

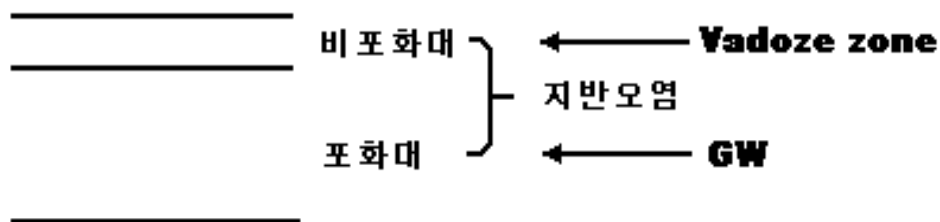
지반환경공학특론 - 1

※ 지반오염영역

What does the Subsurface mean?

Subsurface is the zone below the land surface, being composed of **unsaturated, and saturated zones**.

1. **Saturated zone** is the zone in which the voids in the soil and rocks are filled with water at a pressure greater than atmospheric pressure.
2. **Unsaturated zone** is the zone between the land surface and the water table. It also includes capillary fringe.



※ 지반오염의 정의 (Subsurface contamination)

=> Introduction of hazardous foreign materials into the ground by human activities; such as accidental spills of chemicals or waste materials, leakage of septic tank or buried(underground) storage tank (UST), improper injection of liquid waste, unmanaged dump site, land application of agricultural pesticide, operation of landfills (leachate), and industrial or residual disposals. (FIG. CJN 67)

And those contaminants are categorized as;

- (1) 유기화합물 (organic hazardous compounds; aliphatic, aromatic, and halogenated hydrocarbons, ex. BTEX, PCBs, solvents, PAHs, etc.)
- (2) 무기물 (heavy metal, inorganic compounds; cyanides, sulfates, nitrates, etc.)
- (3) 방사능 물질 (radio active materials; naturally occurring ^{238}U series(radium, and finally lead), Strontium, Cesium, Plutonium, etc.)
- (4) 미생물 (bacteria, virus)

※ **지반오염원으로의 폐기물**

1. 폐기물 - 사람의 생활이나 사업 활동에 필요하지 아니하게 된 물질 「폐기물 관리법」
2. 처리기술 → 재활용(recycle), 소각(incineration), 매립(landfill)
(전체 폐기물 발생량의 80%)

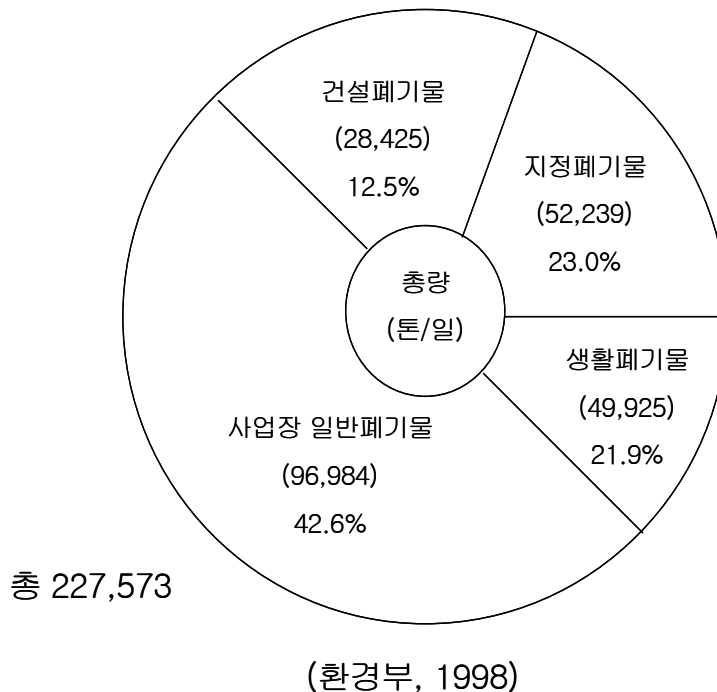
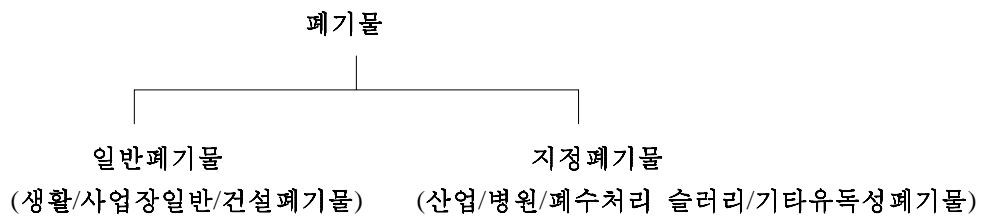
소각 : dioxine 배출문제

↔ biocon 로타리킬른 method(소규모매립장 적용)
(composting)

→ 위생매립시설 필요, 침출수누출 방지시설
(지하수/토양 오염)

3. 폐기물의 성상 : 고체/액체/기체

종류와 발생원 표 4.1장연수



4. 폐기물의 시험 방법

시료채취 → 혼합 or 대표성 갖도록 여러 곳에서 채취

용기 → 무반응성/장기보관 가능한 것 : 무색유리병, 폴리에틸렌병/ 백Tefron 덮개/마개사용
 명기사항 : 명칭, 양, 채취장소, 시간 및 일시, 시료번호, 채취장 이름, 채취방법, 보관상태 등

5. 폐기물 채취방법

고체 : 일정량 채취, 변동계수 20% 이하
 (시료크기의 표준편차 ÷ 시료평균크기 × 100)

액체 : 최종지점 낙하배출구에서 채취
 Tank 저장된 경우 2-3층으로 분리하여 채취

시료의 양은 1회 100g 이상
 대상폐기물 500t 미만인 경우 시료수는 6-30개 정도
 대상폐기물 5000t 미만인 경우 시료수는 50개 정도

보관은 0-4℃ 냉암소 보관, 최소기간 보관 필요

시료 전처리 : 양이 많은 경우 시험전 전처리 필요 → 일반적으로 축소한다.
 (함수비 변하지 않게 유의)
 (폐기물은 일반적으로 5mm이하로)

금속성분 측정시 → 유기물 분해 필요
 질산, 질산-염산 분해법, 질산-황산, 질산-과염산 유기물 분해등
 시험법 → 함유량 시험법 (측정대상 오염물질의 전체량 측정-전량시험법)
 용출시험법 (대립시 지하수/강우에 의하여 폐기물에 함유된 성분이 외부로 유출
 되는지 여부 측정)

발생원에 따른 오염물질의 분류(장연수 표 4.21) + 그림 4.8장연수

가장 빈도높은 물질(유기+무기성 오염물) 표 4.24장연수

6. 오염물에 의한 토질 특성 변화

- 강도특성 Φ , C
 ex. NaCl → 모래+벤토나이트 혼합토 NaCl 농도 ↑ 흙강도 ↑
 유기성(유기물함량)흙 → 강도저하, 압축성 증가
 ※ 대한민국의 토양 화강풍화토 → 지반오염의 측면에선 ?
- 확산이중층에 영향을 끼침 → # 16 참조 박준범

※ Related Journals & Sites

1. ASCE - Geotechnical and Geoenvironmental Engineering
2. Water Resources Research
3. Groundwater
4. Journal of Contaminant Hydrology
5. Environmental Science & Technology
6. Environmental Progress
7. Canadian Journal of Geotechnical Engineering
8. Water, air, and soil pollution
9. Groundwater Remediation and Monitoring
10. Water Environmental Research
11. Environmental Geology
12. Journal of Hazardous Material
13. Waste Management Journal
14. www.clu-in.org
15. www.epa.gov
16. www.groundwater.com

※ BTEX

- B - Benzene
- T - Toluene
- E - Ethylbenzene
- X - Xylene

Plume : 오염분포대, 汚染雲

※ Case Study - Seymour, IN (Needs Slides) + 각국지반오염정화비용

1970-79 : Solvent Recovery, Chemical Plant. Bankrupt in 1979. 98USTs and 50,000 drums of chemicals abandoned.

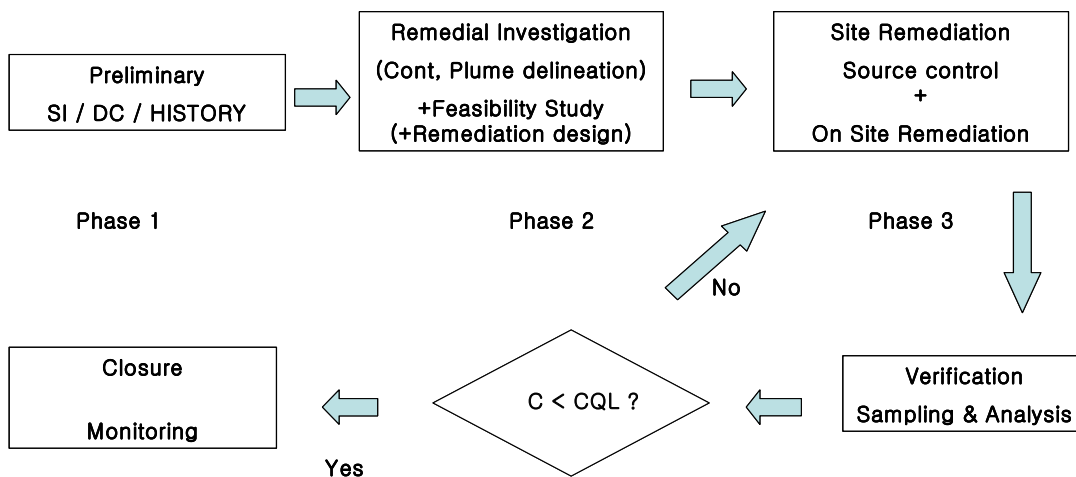
1983 : All Removed. However, unknown amount of chemicals leaked into subsurface.

1983-85 : EPA remedial investigation. (오염물질의 양, 범위, 종류등 조사) Phase I, II

1986 : Feasibility Study for selecting method of remediation

1988-2000 현재 : Remediation Process (P&T, plume stabilization, Bioremediation, Horizontal SVE), \$37M spent so far.

Things we learn from this case :



※ 지하수 오염 제거법

1. Pump and treat
2. Bioremediation → 산소 + 영양분
3. Bioventing → biomass 형성의 문제점
4. Soil washing
5. Thermal desorption
6. SVE : Soil Vapor Extraction

in-situ : 굴착(excavation) 없이 흙을 정화 (↔ ex-situ) : on-site

VOC : Volatile Organic Compound

Key terms relating Contaminated Subsurface

※ porosity (간극률) n :

why important ?

=> for coarse granular soils $n \uparrow$, $k \uparrow$, also $k_{air} \uparrow$ (SVE design consideration)

$$n = \frac{V_v}{V_t} \quad V_v : \text{Void Volume}, \quad V_t : \text{Total Volume}$$

간극비 $e = \frac{V_v}{V_s}$ $n = \frac{e}{1+e}$ $V_s : \text{Solid Volume}$

$$\gamma_t = \frac{G_s + G_s e}{1+e} \gamma_w = \frac{W}{V} \quad G_s \text{ 대입} \rightarrow e \rightarrow n$$

poorly graded soils generally having larger n than well graded soils

Soil type	$n(\%)$
gravel	24 ~ 50
sand	26 ~ 53
silt	34 ~ 50
clay	34 ~ 60

Dispersive effort of the electrostatic charge of the clay particles repelling each other
 → flocculated structure → higher n

n 은 또, in-situ flushing시 적용조건에도 필요하다.

Surfactant → Surface Active Agent

┌ Anionic (-) ← 정화 효과

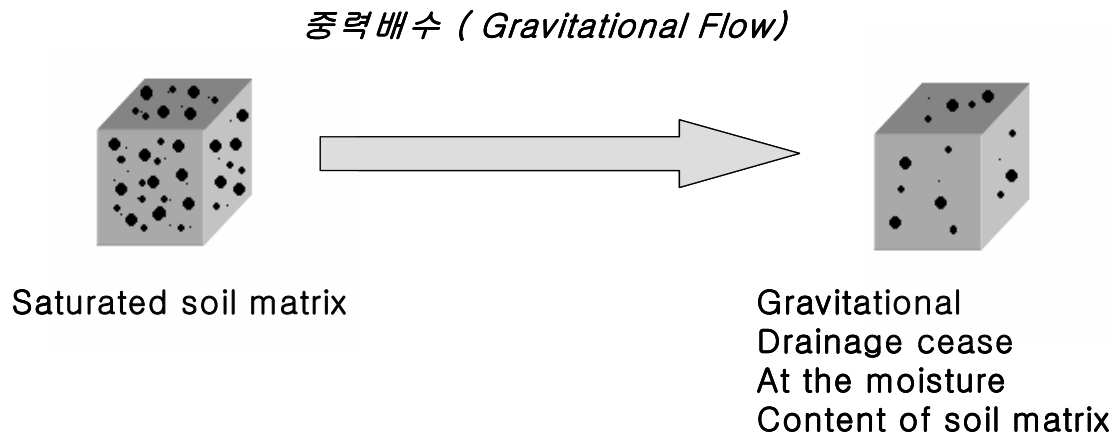
└ Nonionic (0) ←

┌ Cationic (+) ← 오염 확산 방지 (기술자료1 중 '계면활성제를 이용한 오염정화방법 소개' 참조)

effective porosity, n_{eff} : porosity available for fluid flow considering only interconnected pores. Then,

$n \gg n_{eff}$ for general use?? Peyton et al (1986) found that even in clay matrix, water molecules can pass through all the pore throats, so that the $n_{eff} \simeq n$ for fluid flow.

※ Specific yield (S_y)



포화된 지하수층에서, Volume of water that drains due to gravity to the total volume of the porous media, S_y

* Fine Grained soil yields little water and Coarse Grained soil yields significant amount of water. why? FGS has more surface area.

→ more surface clinging water (pendular water) by surface tension.

→ yields less water.

* Specific retention, S_r

$$S_r = \frac{V_r}{V_t}$$

Volume of water a soil matrix can retain against gravity drainage to the total Vol. of soil matrix.

$$n = S_r + S_y = \frac{V_v}{V_t}$$

Generally, gravity drainage will proceed until the forces of surface tension and molecular attraction to the soil particles become equal to the force of gravity.

* Aquifers (대수층)

Fig. (CJN 17, SLIDE)

Geological formation that contains sufficient saturated permeable material to yield significant quantities of water.

1. Unconfined Aquifer(비피압대수층)

=> an aquifer with no confining bed below the zone of saturation and the surface.

Water table(free water surface, where atmospheric pressure applies) exists.

2. Confined Aquifer(피압대수층)

=> an aquifer overlain by a confining bed.(=aquitard, aquiclude). An aquifer that is sandwiched between two impermeable layers.

There will be a potentiometric
|
piezometric |-(surface)

potentiometric(piezometric) surface - represents the level to which water will rise in piezometer(or well). water table = potentiometric surface for unconfined aquifer.

참고 : 건설교통부 자료(1998)에 의하면, 우리나라의 지하수 이용 가능량은 $132.6 \times 10^8 \text{m}^3/\text{yr}$ 이며, 용도별 지하수 이용 비율은 농업용수 6.63%, 공업용수 3.94%, 생활용수 0.40% 순이다. 실제 이용하고 있는 지하수량은 $2.8 \times 10^8 \text{m}^3/\text{yr}$ 로 국내 수자원 부존량의 약 2%에 해당한다.

지층 - 대수층(aquifer)와 난대수층(aquiclude)으로 구분. 대수층은 지하수가 보존될 수 있고, 물이 통과할 수 있는 충분한 트기의 공간이나 틈이 발달되어야 한다. 따라서 이층은 대부분 모래, 자갈, 사암, 석회암등 퇴적암, 균열이 심한 분출암이나 결정질 암층이 된다. 반면, 난대수층은 점토와 같은 세립질로 구성되어 투수성이 낮은 관계로 지하수가 잘 통과할 수 없는 포화지층을 말한다. 대표적 난대수 지층은 점토, 혈암(shale) 및 균열이 발달되지 않은 결정질암이 있다. 화강암은 대부분 암석내에 공극이 적어 난대수층으로 간주되지만 우리나라에 발달된 화강암은 암반내에 절리가 많이 발달되어 있어 상당량의 지하수를 포함하고 있으므로 지하수 개발이 가능하다. -오염물질이 화강풍화암의 절리로 유입되는 경우에 대한 문제.

* 수두(hydraulic head)

총수두(total head, h) = 위치수두(elevation head, z) + 압력수두(pressure head, ψ) + 속도수두(velocity head)

$$h = z + p/Y_w + v^2/2g$$

p/Y_w : 압력수두, ψ

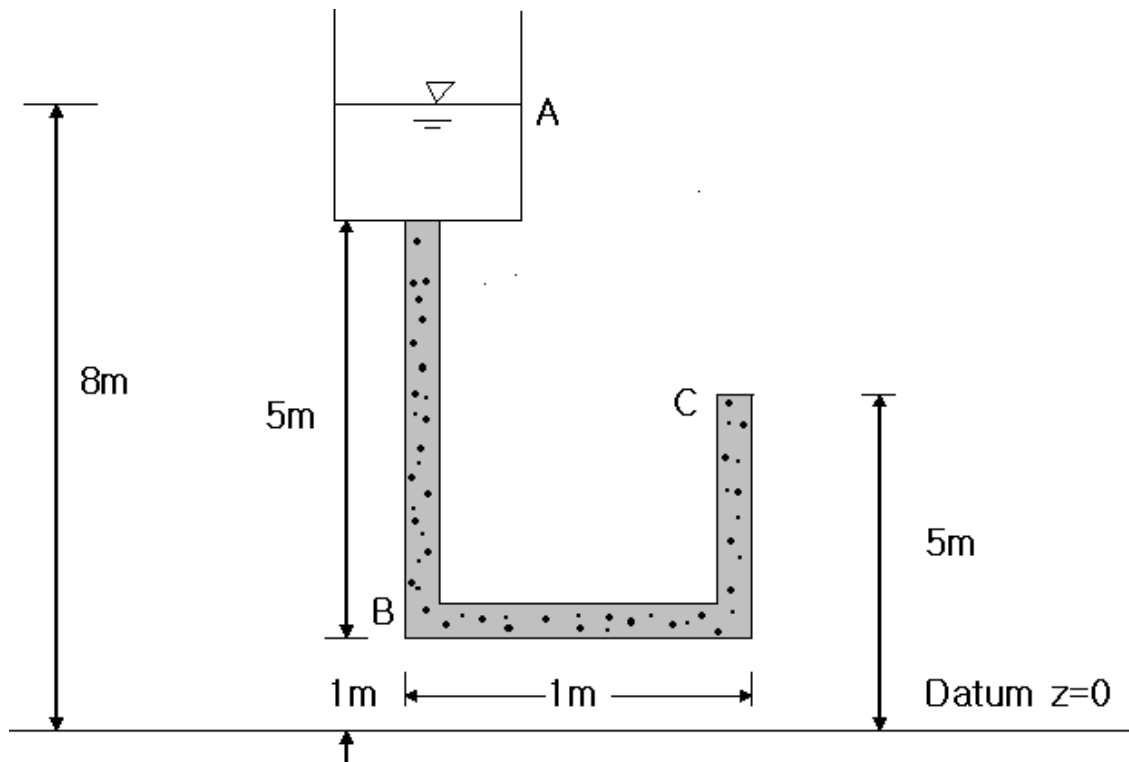
$v^2/2g$: 속도수두 (흙을 통과하는 유속은 대단히 느리므로 negligible)

따라서 흙 속에서의 물의 흐름의 총수두는,

$$h = z + p/Y_w = z + \psi$$

Example : 그림에 보인 바와 같은 chamber내에서 다음을 계산하여라

- 1) A — C 의 수두손실
- 2) B 점의 전수두
- 3) A 점의 압력수두
- 4) A 점의 전수두
- 5) B 점의 압력수두



풀이)

- 1) $\Delta h_{AC} = h_A - h_C = 3 \text{ (m)}$
- 2) $h_B = \psi_B + z_B = (8 - 1) + 1 = 8 \text{ (m)}$
- 3) $\Psi_A = h_A - z_A = 8 - 8 = 0 \text{ (m)}$
- 4) $h_A = \Psi_A + z_A = 0 + 8 = 8 \text{ (m)}$
- 5) $\Psi_B = h_B - z_B = 8 - 1 = 7 \text{ (m)}$

※ Darcy's law (Darcy's law effective for subsurface flow with $R < 10$)

The flow rate through porous media is proportional to the head loss and inversely proportional to the length of flow path.

The flow rate is also proportional to the cross-sectional area of the porous media

$$Q = k \frac{\Delta h}{L} A$$

↙ hydraulic gradient I

$$Q = VA, \quad V = ki$$

V : discharge velocity, V_s : seepage velocity, actual velocity

Fig. (CJN 18, Slide)

Relationship $V_s > V$?

$$\therefore V_s = \frac{VA}{A_v} = \frac{V(A_v + A_s)L}{A_v L} = \frac{V(V_v + V_s)}{V_v} = \frac{V(1 + e)}{e} = \frac{V}{n}$$

$$Q = kiA \quad k : \text{Coefficient of permeability or hydraulic conductivity [L/T]}$$

$k \rightarrow$ indication of how well an aquifer can transmit water.

$k = f_n(\text{fluid, porous media})$

↑ ↑
water soil

water = $f_n(\mu, \gamma_w)$ ↙ 입자의 모양 (형상계수)

soil = $f_n(D, e, Sr, GSD, C)$

↑ ↑
포화도 grain size distribution

$$k = f_n(\mu, \gamma_w, D)$$

$$\mu = \frac{M}{LT} = ML^{-1}T^{-1}$$

$$\gamma_w = F/L^3 = ML^{-2}T^{-2}$$

$$D : L$$

$$k = LT^{-1} \quad \therefore n = 4 \text{ physical variable, 3개의 basic dimension}$$

Buckingham π -theorem

$n - 3 = 1$: dimension group

$$k = C\gamma^{x_1}\mu^{x_2}D^{x_3}$$

↑

무차원상수

$$LT^{-1} = C [ML^{-2}T^{-2}]^{x_1} [ML^{-1}T^{-1}]^{x_2} [L]^{x_3}$$

$$\therefore X_1 = 1, X_2 = -1, X_3 = 2$$

$$\therefore k = C \frac{\gamma_w}{\mu} D^2$$

Kozeny-Carmen equation. (only available for coarse grained round shape particles)

$$k = CD^2 \frac{e^3}{1+e} \frac{\gamma_w}{\mu}$$

Derivation of Kozeny-Carmen Equation (Note#14)

C : 형상계수

Factors affecting k for sandy soils,

$$k = CD_{10}^2 \dots \text{Hazen equation}$$

┌ D ↑ - k ↑

└ e ↑ - k ↑ $k \propto e^2$ by Casagrande

T ↑ ┌ γ_w ↑ ... 무시할만함

└ μ ↓ ... 이 영향을 받아, 투수계수는 증가한다.

$\therefore k \uparrow$ as T ↑

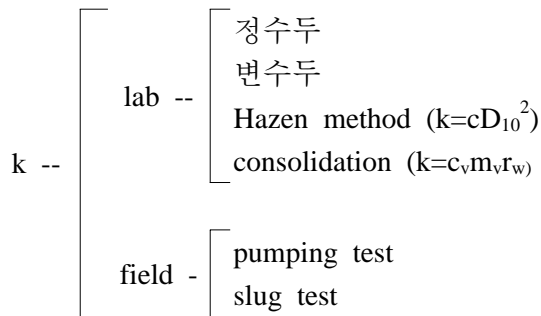
C : 1 ~ 1.5 As particle gets rounder, k ↑

↑ ↙
rough round & smooth

$$k_{20^\circ\text{C}} = \frac{\mu_{T_C}}{\mu_{20^\circ\text{C}}} k_{T_C}$$

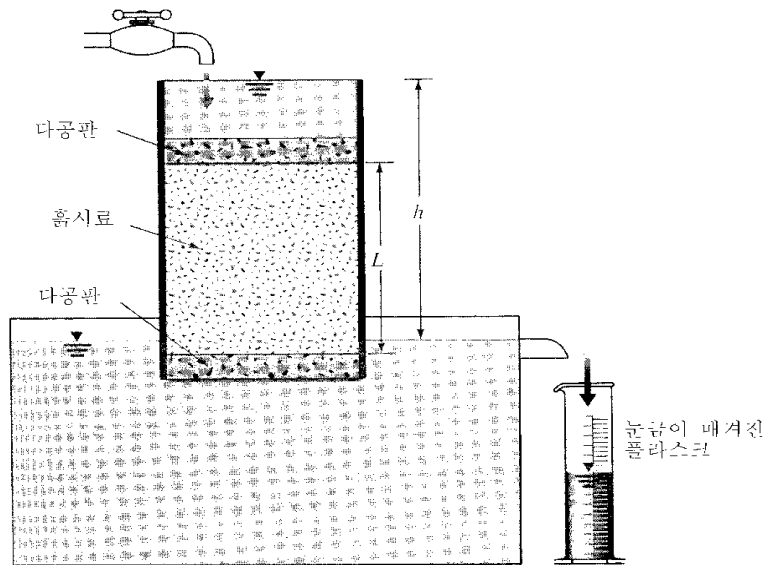
포화도 $S_r \uparrow \rightarrow k \uparrow$ If we have bubbles, air pockets in the pores, those airs can cause surface tension to overcome for flow through porous media.

Grain Size Distribution for k well g. < poorly g.



1) 정수두 투수시험

정수두 투수시험의 대표적인 시험장치는 다음과 같다. 이 실험 장치에서는 물을 공급하는 입구를 조정함으로써 실험하는 시간동안 물의 입구와 출구사이의 수두차를 일정하게 유지하도록 하였다. 물의 흐르는 양이 일정하게 되었을 때, 물을 일정한 시간동안에 실린더에다 집수한다. 집수된 총유량은 다음과 같이 계산된다.



$Q = Avt = A(ki)t$ 여기서 Q : 집수량 A : 흙시료의 단면적 t : 집수시간
그리고, 동수경사 i 는

$$i = \frac{h}{L} \quad \text{여기서, } L : \text{시료의 길이}$$

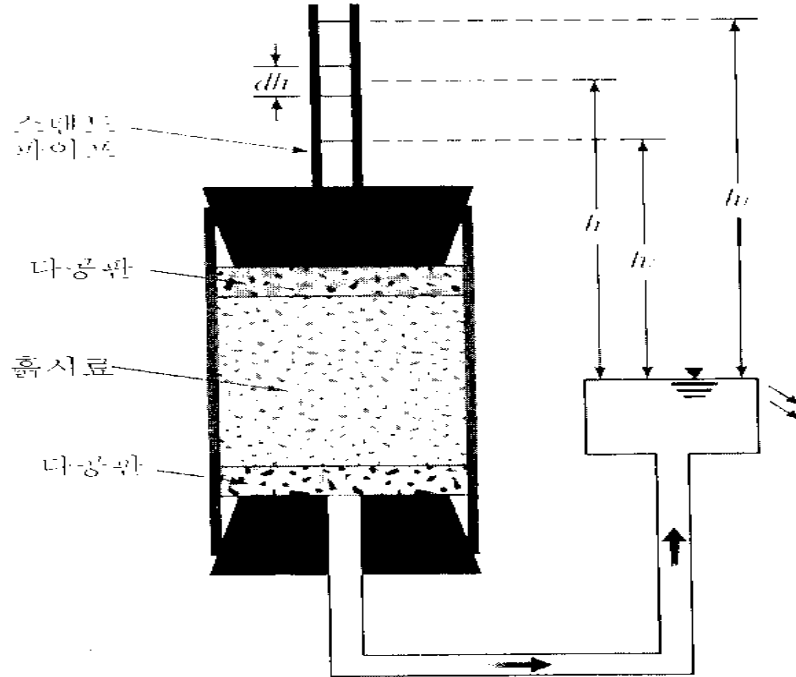
윗 식에 대입하면 최종식은

$$Q = A \left(K \frac{h}{L} \right) t \quad \text{또는} \quad k = \frac{Q L}{A H t}$$

정수두 투수시험은 높은 투수계수를 갖는 조립토에 더 적합하다.

2) 변수위 투수시험

변수위 투수시험의 대표적인 시험장치가 다음그림에 나와있다. 물은 스탠드파이프로부터 흡속으로 흐른다. $t=0$ 일 때 초기수두차 h_1 을 기록하고, 물이 흡 시료를 통해 흐르게 한 후 $t=t_2$ 일때의 최종 수두차 h_2 를 기록한다.



임의의 시간 t 에서 시료를 통해 흐르는 유량은 다음과 같다.

$$q = k \frac{h}{L} A = -a \frac{dh}{dt}$$

여기서, q : 유량 a : 스탠드파이프의 면적 A : 흡시료의 단면적
위 방정식을 정리하면

$$dt = -\frac{aL}{Ak} \left(-\frac{dh}{h} \right) \text{ 또는 } k = 2.303 \frac{aL}{At} \log_{10} \left(\frac{h_1}{h_2} \right)$$

변수위 투수시험은 낮은 투수계수를 갖는 세립토에 더 적합하다.

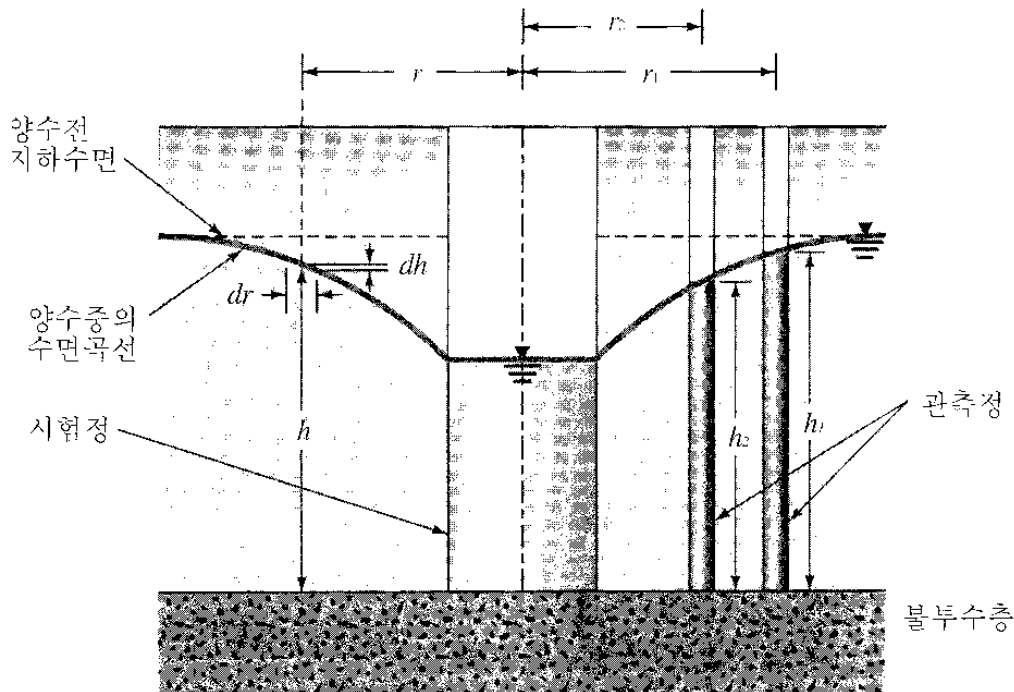
3) Pumping Test

현장에서 물의 흐름방향으로 흙의 평균투수계수는 양수시험에 의하여 측정할 수 있다. 아래 그림은 투수계수를 측정해야 될 상부투수층이 비피압상태에 있고 하부에 불투수층을 형성하고 있는 경우에는 투수시험을 하는 동안에 다공관을 소지한 시험정으로부터 물을 일정하게 퍼낸다. 시험정 주위에 여러 개의 관측정들을 여러 방사선마다 설치한다. 물을 퍼내기 시작하여 정상상태에 도달할 때까지 시험정과 관측정내의 수심을 계속 관측한다.

시험정과 관측정내의 수심이 일정하게 될 때 정상상태에 도달한다. 지하수가 시험정안으로 흘러들어가는 양, q 가 물을 양수하여 퍼올리는 양과 같을 때, 이 상황을 방정식으로 표현하면 다음과 같다.

$$q = k \left(-\frac{dh}{dr} \right) 2\pi r h \quad \text{또는} \quad \int_{r_2}^{r_1} \frac{dr}{r} = \left(-\frac{2\pi k}{q} \right) \int_{h_2}^{h_1} h \, dh$$

현장관측결과 q , r_1 , r_2 , h_1 , 그리고 h_2 를 안다면, 투수계수는 방정식에 주어진 간단한 관계식으로부터 구할 수 있다.

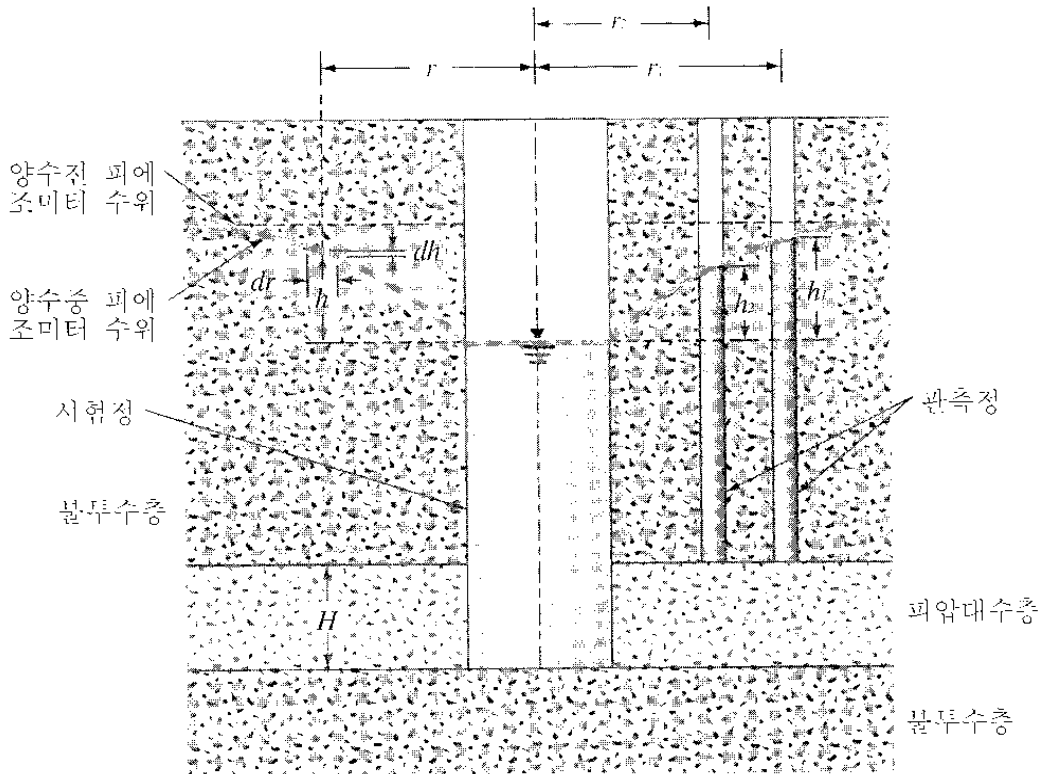


피압대수층(confined aquifer)의 평균투수계수는 대수층까지 완전 관입된 다공관을 통하여 양수시험을 실시하여, 그림에 도시된 것과 같이 여러 방사거리에 위치한 관측정의 지하수위(piezometer level)를 관측함으로써 결정할 수 있다. 일정한 유량 q 를 계속적으로 펴내면 정상상태에 도달한다. 물은 대수층 두께 H 를 통해서 시험정으로 들어가기 때문에 정상상태의 유출량은 다음과 같이 계산할 수 있다.

$$q = k \left(\frac{dh}{dr} \right) 2\pi r H \quad \text{또는} \quad \int_{r_2}^{r_1} \frac{dr}{r} = \int_{h_2}^{h_1} \frac{2\pi k H}{q} dh$$

투수계수는

$$k = \frac{q \log_{10} \left(\frac{r_1}{r_2} \right)}{2.727 H (h_1 - h_2)} \quad \text{이다.}$$



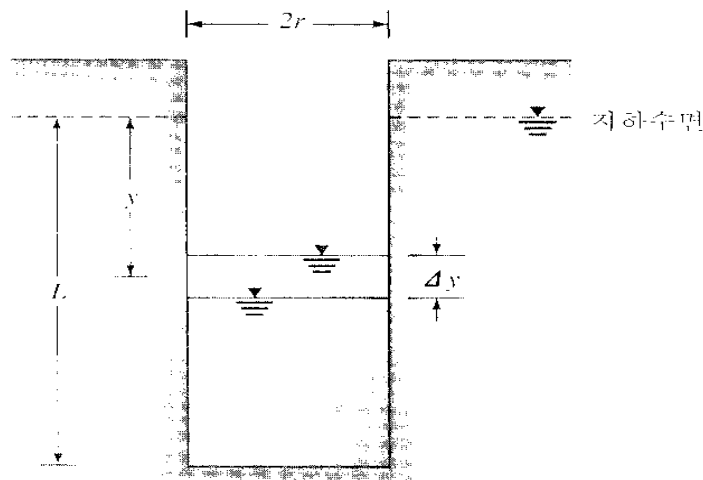
4) Slug Test

현장에서 투수계수는 다음 그림과 같이 하나의 시추공에 의하여 측정할 수 있다. 이런 식의 시험법은 흔히 느린시험 (slug test)이라고 부른다. 현장에서 지하수위아래 심도 L까지 시추를 한다. 먼저 시추공내의 물을 퍼낸다. 이렇게 하면 시추공 주위와 바닥으로부터 시추공으로 물이 흘러들어가게 된다. 경과시간에 따른 시추공내의 수위상승을 기록한다. 이 기록으로부터 다음과 같이 투수계수를 계산한다.(Ernst, 1950; Dunn, Anderson & Kiefer, 1980)

$$k = \frac{40}{\left(20 + \frac{L}{r}\right) \left(2 - \frac{L}{r}\right)} \frac{r}{y} \frac{\Delta y}{\Delta t}$$

여기서, r : 시추공의 반경(m)

y : 경과시간 Δt (m)에 따른 시추공내의 평균상승거리(m)



이 방정식에서 L 과 Δy 의 단위는 m이고, k 의 단위는 경과시간 Δt 의 단위에 따라 m/sec 또는 m/min이다. 시추공을 이용한 투수계수 측정은 정확하지는 못하지만 개략적인 k 값을 제공한다.

※ Diffuse Double Layer and the Structures of Clay Soil

In dry clay, the negative charge is balanced by exchangeable cation like Ca^{2+} , Mg^{2+} , Na^+ , and K^+ surrounded the particle being held by electrostatic attraction when water is added to clay, these cations and small number of anions float around particles. this is referred to as a "Diffuse Double Layer". The cation concentration decrease with the distance from the surface of particle. (박준범 #16)

※ **Transmissivity**

=> 흙 속에서 물이 단위 동수구배 하에서 대수층의 전두께와 단위폭으로 이루어진 면을 통하여 투수되는 물의 양을 투수량계수(transmissivity, T)라고 하며, 투수계수와 다음과 같은 관계를 가진다.

$$T = kb \quad (k : \text{투수계수}, b : \text{대수층의 두께})$$

이 값이 0.015 m²/sec 이상이면 지하수 개발을 할 수 있을 정도의 좋은 대수층임을 의미한다.

※ **Flow through Porous Media**

=> When stress is applied to a unit mass of saturated sand aquifer, compressibility of porous media is expressed by three mechanism by which a volume reduction can be achieved.

- Vol. reduction $\left\{ \begin{array}{l} \textcircled{1} \text{ Rearrangement of soil particles} \\ \quad | \quad (\text{into more closely packed configuration}) \\ \text{┆} \textcircled{2} \text{ Compression of water in pore volume} \\ \text{└} \textcircled{3} \text{ Compression individual soil particles} \leftarrow \text{ignorable} \end{array} \right.$

① Effective Stress Concept (Karl Terzaghi, 1925)

σ_T (Total Stress, Wt of soil, rock, water) is supported by pore water pressure (P) and granular skeleton pressure (or effective stress, σ') in equilibrium.

$$\sigma_T = \sigma' + P$$

For clay layer confined by sandy layers, any change in σ_T will be totally carried by ΔP ($\because k_{\text{clay}}$ is very low, and water incompressible), thus $\Delta \sigma_T = \Delta P$ at entire depth. Water dissipates (squeezes out), $\Delta P \downarrow$. Then, the stress is carried by soil skeletons, thus, the effective stress increases. Rearrangement of soil skeletons will cause volume reduction (Consolidation for the Clay Case).

평형상태에서 물이 빠져나가 평형이 깨짐 \rightarrow 변형 \rightarrow soil skeleton 이 하중을 받게 됨 : consolidation

① \rightarrow change of effective stress에 의해 발생

$$\begin{aligned} d\sigma_T \quad (\approx 0) &= d\sigma' + dP \\ -dP &= d\sigma' \\ \therefore dP &= \rho g dh \end{aligned}$$

Compressibility of porous media

$$\alpha = \frac{-dV_T/V_T}{d\sigma'} \quad \text{체적압축량}$$

$$dV_t = dV_v + dV_s$$

$$\therefore dV_t = dV_v$$

(dV_s is almost negligible) ($dV_v = dV_w$)

$\alpha = f_n$ (applied stress) ← stress history, previous loading history.

「Darcy's law applies to the laminar flow condition in porous media applicable to most groundwater system」

For saturated media,

$$\begin{aligned} dV_w &= dV_v = dV_T \\ &= \alpha V_T d\sigma_1' \end{aligned}$$

For unit volume $V_T = 1$

$$\text{and } d\sigma' = -dP = -\rho g dh$$

For a unit decline of hydraulic head

$$dh = -1$$

$$dV_w = \alpha \rho g$$

② compression of water

$$\beta = \frac{-dV_w/V_w}{dP} = \frac{d\rho/\rho}{dP}$$

ρ : fluid density

$$\beta : 4.4 \times 10^{-10} \text{ (Pa}^{-1} \text{ , m}^2/\text{N)}$$

↑

considered as constant

Soil type	$\alpha(\text{Pa}^{-1})$
clay	$10^{-6} \sim 10^{-8}$
sand	$10^{-7} \sim 10^{-9}$
gravel	$10^{-8} \sim 10^{-10}$
Jointed rock	$10^{-8} \sim 10^{-10}$
sounded rock	$10^{-9} \sim 10^{-11}$
water	β

$$dV_w = -\beta V_w dP, \quad V_w = nV_t$$

For a unit volume $V_T = 1$

$$dP = \rho g dh, \quad dh = -1$$

$$dV_w = \beta n \rho g \text{ -- ②}$$

※ **Specific Storage**

The amount of water released from or taken into storage per unit vol. of porous media per unit change in head

$$\begin{aligned}
 S_s &= \text{the sum of two terms given by ①+②} \\
 &= dV_w + dV_w \\
 &\quad \text{①} \quad \text{②} \\
 &= \rho g (\alpha + n\beta) [1/L]
 \end{aligned}$$

※ **Storage Coefficient, S(Storativity, 저류계수)**

=> Vol. of water that a permeable unit will adsorb or expel from storage per unit surface area per unit change in head.

흐름이 시간에 따라 변동하는 transient flow의 해를 구할 때 사용되는 대수층의 물을 저장할 수 있는 능력을 나타내는 계수이다. 대수층의 단위면적을 가지는 연직 흡기둥에 단위 1의 수두가 저하될 때 이 흡기둥에서 배출되는 수량을 의미한다.

For confined aquifer (head may decline but still saturated),

$$S = b S_s (\text{무차원}) \rightarrow \text{conf. aq } S < 0.005$$

For unconf. aquifer, $S = \alpha S_s + S_y$ ($S \approx S_y$ $S = 0.02 \sim 0.3$)

↓
0

The vol. of water drained from an aquifer as the head is lowered can be expressed as,

$$V_w = S A \Delta h$$

A : surface area overlying the drained aquifer

Δh : average decline in head [L]

Ex. Unconf. aquifer with $S=0.13$ has an area of 123 mi^2 . The water table drops 5.23ft during draught. How much water was lost from storage?

$$\begin{aligned}
 V_w &= S A \Delta h \\
 &= 0.13 \times 123 \times 2.7878 \times 10^7 \times 5.23 = 2.3 \times 10^9 \text{ ft}^3 \text{ for unconfined aquifer.}
 \end{aligned}$$

If the same aquifer had been confined with $S = 0.0005$

$$V_w = 0.0005 \times 123 \times 2.7878 \times 10^7 \times 5.23 = 9.0 \times 10^6 \text{ ft}^3 \text{ for confined aquifer.}$$

(장연수 161, 예제 5.4)

- a) 어떤 수평대수층의 상부에 15m의 포화점토층이 놓여있다. 포화점토층의 단위중량 $r_{sat} = 1.8 \text{ t/m}^3$ 이라면 대수층의 상부에 작용하는 전응력을 계산하여라
- b) 피압상태의 대수층에 걸린 간극수두는 20m이었다. 대수층내의 유효응력은 얼마인가?
- c) 대수층에 양수정을 뚫어 간극수두가 10m 저하되었다고 할 때 대수층내의 전응력, 유효응력, 압력수두의 크기를 계산하여라.
- d) 대수층의 체적압축량이 $\alpha = 1.4 \times 10^{-5} \text{ m}^2/\text{kN}$ 이고 대수층의 두께가 8m이며 간극률 $n = 0.3$, 투수계수 $K = 5 \times 10^{-4} \text{ cm/sec}$ 이라고 할 때 투수량계수와 저류계수를 계산하여라 (이 때 물의 압축계수는 $4.4 \times 10^{-7} \text{ m}^2/\text{kN}$ 으로 가정)
- e) 대수층내 지하수 포텐셜 저하로 인한 유효응력 증가가 10 t/m^2 이라 할 때 발생하는 대수층의 다짐에 의한 침하량을 계산하여라.

풀이)

- a) 전응력은 포화단위중량과 점토층 두께의 곱이므로

$$\begin{aligned} \sigma &= r_{sat}H \\ &= (1.8)(15) = 27 \text{ t/m}^2 \end{aligned}$$

- b) 유효응력과 전응력, 간극수압의 관계식에서

$$\begin{aligned} \sigma' &= \sigma - u_0 \\ &= 27 - 20 = 7 \text{ t/m}^2 \end{aligned}$$

- c) 간극수두 10m 저하식

$$\begin{aligned} u &= u_0 - \Delta u = 20 - 10 = 10 \text{ t/m}^2 \\ \sigma' &= 27 - (20 - 10) = 17 \text{ t/m}^2 \\ \sigma &= \sigma' + u = 17 + 10 = 27 \text{ t/m}^2 \end{aligned}$$

따라서 전응력의 크기는 변화가 없다.

- d) 투수량계수 계산

$$T = Kb = 5 \times 10^{-4} \left(\frac{1}{100} \right) (8) = 4 \times 10^{-5} \text{ m}^2/\text{sec}$$

저류계수의 계산

$$\begin{aligned} \text{물의 밀도 } \rho &= 1 \text{ t/m}^3, g = 9.8 \text{ m/sec}^2 \\ S &= \rho gb (\alpha + n\beta) \\ &= (1)(9.8)(8) \{ 1.4 \times 10^{-5} + (0.3)(4.4 \times 10^{-7}) \} \\ &= 78.4 \{ 1.4 \times 10^{-5} + 1.32 \times 10^{-7} \} \\ &= 1.1 \times 10^{-3} \end{aligned}$$

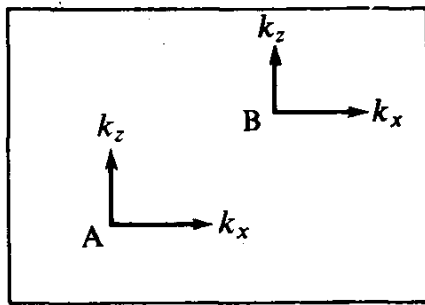
- e) 대수층의 다짐에 의한 침하량을 s 라 하면

$$\begin{aligned} s &= \alpha \cdot b \cdot \Delta \sigma' \\ &= 1.4 (10^{-5}) \cdot (8) \cdot (9.8 \times 10) \\ &= 0.011 \text{ m} = 1.1 \text{ cm} \text{ 이다.} \end{aligned}$$

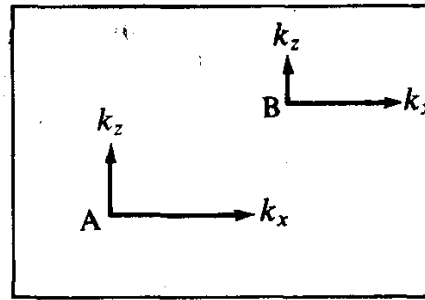
*Isotropic / Homogeneous → value (x,y,z) = const
 ↓ ↓
 Property independent of direction of measurement at a point independent of position

(Drawing Needed) 투수계수의 비등방성과 비균질성

흙이 퇴적되어 자연지반을 이루었다면 흙입자의 형상때문에 대략 평행한 층을 이루면서 퇴적되므로 연직방향과 수평방향의 투수계수가 다르다. 다시 말하면 수평방향의 투수계수는 연직방향의 투수계수보다 일반적으로 더 큰 값을 보이며 그 비는 10:1 이상되는 경우도 있다. 이와 같이 한 위치에서 방향에 따라 투수계수가 다르다면 이것을 비등방(anisotropy)이라고 한다.



(a) 등방, 균질
 $k_x = k_z, k_x(A) = k_x(B)$
 $k_z(A) = k_z(B)$



(b) 비등방, 비균질
 $k_x \neq k_z, k_x(A) \neq k_x(B)$
 $k_z(A) \neq k_z(B)$

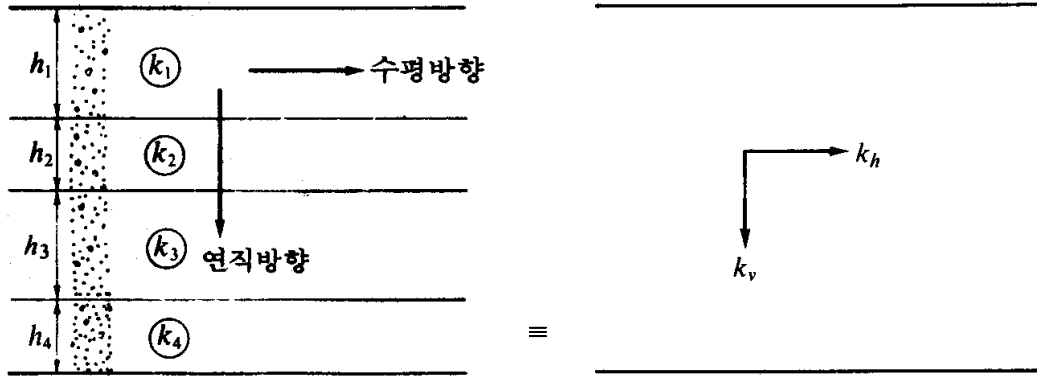
투수계수의 등방성과 비등방성 및 균질성과 비균질성

또한 흙이 두 위치에서의 투수계수가 다를 때, 이것을 비균질(nonhomogeneity)하다고 말한다. 흙이 퇴적되는 과정에서 퇴적환경이 달라졌다면 각 토층의 투수계수는 비균질이다. 엄격히 말하면, 자연지반의 투수계수는 비등방성이고 비균질성이다.

다층지반의 토층에 대한 등가투수계수

투수계수가 각각 다른 이질의 토층에 대하여 수평 및 연직방향의 등가 투수계수를 구해두면 여러가지 계산이 대단히 간소화될 수 있다. 아래그림에서 각 토층의 투수계수는 등방성이나 토층마다 각각 다른 투수계수를 가지고 있다고 가정한다. 이러한 경우에 대한 투수계수를 결정하기 위해서는 각 층으로부터 불교란시료를 채취하여 각 투수계수를 결정한 후 다음과 같은 방법으로 등가투수계수를 구하여 침투유량을 산정하여야 한다.

그림은 이층으로 된 자연지반을 보인다. $h_1, h_2 \dots h_n$ 을 각 토층의 두께라 하고, 각 층에 대응하는 투수계수를 각각 $k_1, k_2 \dots k_n$ 이라 하자. 지금 물이 토층에 평행한 방향으로 흐른다고 하면 동수경사는 각 층마다 동일하므로 Darcy의 법칙에 의해 유출속도 v 는 다음과 같이 기술할 수 있다.



$$v = k_h i = \frac{1}{h} (v_1 h_1 + v_2 h_2 + \dots + v_n h_n)$$

$$= \frac{1}{h} (k_1 i h_1 + k_2 i h_2 + \dots + k_n i h_n)$$

여기서, $h = h_1 + h_2 \dots + h_n$

이것을 정리하면,

$$k_h = \frac{1}{h} (k_1 h_1 + k_2 h_2 + \dots + k_n h_n) = \frac{1}{h} \sum_{j=1}^n (k_j h_j)$$

여기서 k_h 는 수평방향으로의 등가투수계수이다.

만일 토층에 직각 방향으로 물이 흐른다고 하면 각 층을 통해 흐른 침투유량은 동일하나 동수경사는 각 층마다 다르다는 것을 알 수 있다. 지금 각 층의 동수경사를 각각 $i_1, i_2 \dots i_n$ 이라 하고, 전 토층의 두께를 h , 전수두손실을 Δh 라 하면

$$v = k_v \frac{\Delta h}{h} = k_1 i_1 = k_2 i_2 = \dots = k_n i_n$$

즉

$$v = k_1 \frac{\Delta h_1}{h_1} = k_2 \frac{\Delta h_2}{h_2} = k_n \frac{\Delta h_n}{h_n}$$

따라서,

$$\Delta h_1 = v \frac{h_1}{k_1}$$

마찬가지로,

$$\Delta h_2 = v \frac{h_2}{k_2}$$

.....

$$\Delta h_n = v \frac{h_n}{k_n}$$

전수두손실은

$$\Delta h = \Delta h_1 + \Delta h_2 + \dots + \Delta h_n = \frac{vh_1}{k_1} + \frac{vh_2}{k_2} + \dots + \frac{vh_n}{k_n}$$

$k_v = \frac{h}{\Delta h} v$ 이므로 이 식의 Δh 대신 위식을 대입하고 정리하면

$$k_v = \frac{h}{\frac{h_1}{k_1} + \frac{h_2}{k_2} + \dots + \frac{h_n}{k_n}} = \frac{h}{\sum_{j=1}^n \left(\frac{h_j}{k_j} \right)}$$

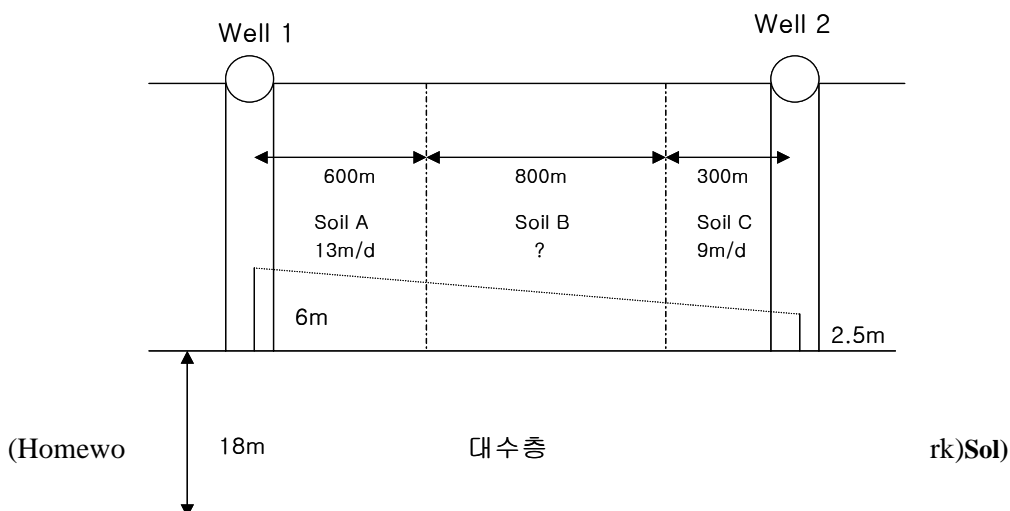
여기서 k_v 는 연직방향으로의 등가 투수계수이다.

* For Vertical and Horizontal Flow, the k values are determined as;

① Vertical flow (Q = const)	② Horizontal flow (i = const)
$b = \sum b_i$	$Q = Q_1 + Q_2 + Q_3$
$\Delta h = \sum \Delta h_i$	
$k_v = \frac{b}{\sum \frac{b_i}{k_i}}$	$k_h = \frac{\sum k_i b_i}{b}$

(Homework)

Example : Two observation wells 1700m apart have been constructed in a confined aquifer with variable hydraulic conductivity in the x-direction. The flow rate is 0.008 m³/h per unit width of the confined aquifer. Well 1 is drilled in Soil A with hydraulic conductivity 13 m/d, and Well 2 is drilled in Soil C with hydraulic conductivity 9 m/d. The soil zone B is between the wells, 600 m from Well 1 and 300 m from Well 2. The Potentiometric surface is 6 m above the upper confining unit in Well 1 and 2.5 m above the upper confining unit in Well 2. Evaluate the hydraulic conductivity of Soil B. The thickness of the aquifer is 18m.



$$Q = k_v i A = k_v \frac{\Delta h}{h} A$$

$$k_v = \frac{Q \cdot h}{\Delta h \cdot A} = \frac{0.008 \times 1700}{(6 - 2.5) \times 1.8 \times 1} = 0.216 \text{ m/h}$$

$$k_v = \frac{h}{\frac{h_A}{k_A} + \frac{h_B}{k_B} + \frac{h_C}{k_C}}$$

$$0.216 = \frac{1700}{\frac{600}{0.542} + \frac{800}{k_B} + \frac{300}{0.375}}$$

$$\therefore k_B = 0.134 \text{ m/h} = 3.20 \text{ m/d}$$

*Direction / Gradient of GW Flow (Slides Needed)

✱ Steady State flow and Transient flow

Steady state occurs when at any point in a flow field the magnitude and direction of the flow velocity are constant with time. Otherwise → transient flow

$$\left(-\frac{\partial v}{\partial t} \neq 0 \right)$$

If Δh constant, flow net will not change with time.

$$v = -\frac{\partial h}{\partial l} k \text{ remains constant with time.}$$

In Steady state condition, velocity may vary from point to point, but it won't vary with time at any given point. (Derivation Needed)

Flow net instantly changes with time

v is not constant with time

Important for well hydraulics, ground water recharge, and many Geotechnical applications.

※ SS saturated Flow

Homogeneous / Isotropic unit vol.

(Drawing Needed)

Conservation of mass

$M_{in} - M_{out} = \text{changes in storage/time}$

$$= 0$$

+ Darcy's law, $k_w = k_y = k_z$

$$- \frac{\partial}{\partial x}(\rho v_x) - \frac{\partial}{\partial y}(\rho v_y) - \frac{\partial}{\partial z}(\rho v_z) = 0$$



$$\frac{\partial^2 h}{\partial x^2} + \frac{\partial^2 h}{\partial y^2} + \frac{\partial^2 h}{\partial z^2}$$

For ss conf. / unconf. condition (Drawing Needed)

$h=h(x,y,z)$

The solution is the hydraulic head at any point in the flow domain.

In 2-D, → equivalent to the graphical flow net

*** Determination of Pressure Head / Effective Stress/ Flow Rater Unit Width.**

※ Transient condition

① Confined Aquifer

For unit volume of soil element, $M_{in} - M_{out} \neq 0$

$$- \frac{\partial}{\partial x}(\rho v_x) - \frac{\partial}{\partial y}(\rho v_y) - \frac{\partial}{\partial z}(\rho v_z) = \frac{\partial}{\partial t}(\rho n)$$

$$\begin{aligned}
 &= - \left(\frac{\partial v_x}{\partial x} - \frac{\partial v_y}{\partial y} - \frac{\partial v_z}{\partial z} \right) = \frac{1}{\rho} \frac{\partial}{\partial t} (\rho n) \\
 &= \frac{1}{\rho} \left(\rho \frac{\partial n}{\partial t} + n \frac{\partial \rho}{\partial t} \right) \\
 &= \frac{\partial n}{\partial t} \\
 &= S_s \frac{\partial h}{\partial t} \\
 \frac{\partial}{\partial x} \left(k_x \frac{\partial h}{\partial x} \right) + \frac{\partial}{\partial y} \left(k_y \frac{\partial h}{\partial y} \right) + \frac{\partial}{\partial z} \left(k_z \frac{\partial h}{\partial z} \right) &= S_s \frac{\partial h}{\partial t} \\
 k_x = k_y = k_z &
 \end{aligned}$$

$$\frac{\partial^2 h}{\partial x^2} + \frac{\partial^2 h}{\partial y^2} + \frac{\partial^2 h}{\partial z^2} = \frac{S_s}{k} \frac{\partial h}{\partial t} \qquad \begin{aligned} S &= S_s b \\ T &= kb \end{aligned}$$

$$\nabla^2 h = \frac{S}{T} \frac{\partial h}{\partial t}$$

This is the governing equation for transient flow for confined aquifer. Solution gives $h = h(x,y,z)$, hydraulic head at any point at any time in flow domain.

② Unconfined aquifer

Saturated thickness can change with time.

The general flow eq. for 2-D unconfined eq. is known as the "Boussinesq eq."

$$\frac{\partial}{\partial x} \left(h \frac{\partial h}{\partial x} \right) + \frac{\partial}{\partial y} \left(h \frac{\partial h}{\partial y} \right) = \frac{S_y}{k} \frac{\partial h}{\partial t}$$

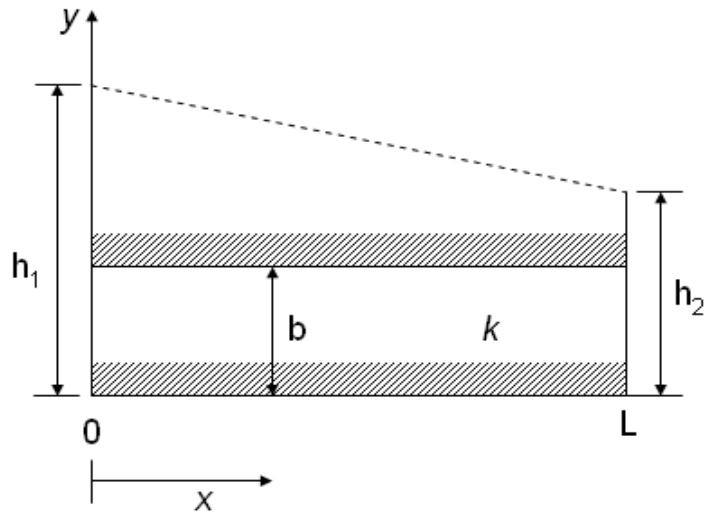
If drawdown $\leq 10\%$ of the original thickness

$$S \approx S_y, \quad \frac{\partial^2 h}{\partial x^2} + \frac{\partial^2 h}{\partial y^2} = \frac{S_y}{kb} \frac{\partial h}{\partial t}$$

basically, the same form as confined transient flow

※ Head and Flow rate

① Confined aquifer (SS condition)



Head will decrease linearly as,

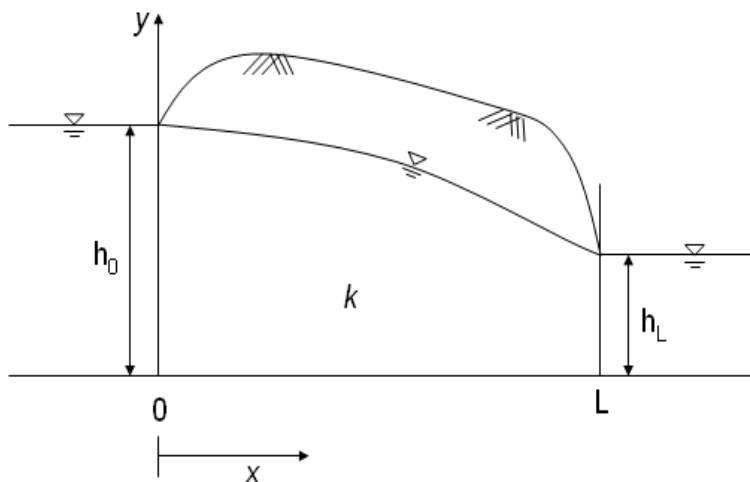
$$L : h_1 - h_2 = x : h_1 - h_x$$

$$h(x, y) = h_1 - (h_1 - h_2) \frac{x}{L}$$

$$Q = ki (bw)$$

$$i = \frac{dh}{dl}$$

② Unconfined aquifer (SS condition)



✱ **Dupuit's Assumption**

- ① Flow line is assumed horizontal,
Equipotential line is vertical (Water table is slightly inclined)
- ② Slope of Water table = Hydraulic gradient

✱ **Flow rate (b ≠ constant)**

$$\text{Darcy's law } q = -kh \frac{dh}{dx} \qquad \begin{array}{ll} x = 0, & h = h_o \\ x = L, & h = h_L \end{array}$$

$$\int_0^L q \, dx = \int_{h_o}^{h_L} -kh \, dh$$

$$qL = \frac{-k}{2}(h_L^2 - h_o^2) = \frac{k}{2}(h_o^2 - h_L^2)$$

$$\therefore q = \frac{k}{2L}(h_o^2 - h_L^2)$$

Called as 'Dupuit's equation'

Head at point X (from Dupuit's parabola)

$$q = -kh \frac{dh}{dx}$$

$$\int_0^x \frac{q}{-k} \, dx = \int_{h_o}^{h_x} h \, dh$$

$$-\frac{qx}{k} = \frac{h_x^2 - h_o^2}{2} \quad \therefore h_x^2 = h_o^2 - \frac{2qx}{k} \text{-----(1)}$$

From Dupuit's equation,

$$q = \frac{k}{2L}(h_o^2 - h_L^2)$$

$$h_x^2 = h_o^2 - \frac{x}{L}(h_o^2 - h_L^2)$$

(head at X)

Keep work on Dupuit's equation with Recharge ([Example 2.3 on CJN pp 32.](#))

※ Well in a Uniform Flow Field

A typical problem in well mechanics involves the case of a well pumping from a uniform flow field (See Below, CJN pp.45). A vertical section and plan view indicate the sloping piezometric surface and the resulting flow net.

The GW divide between the region that flows to the well and region flowing by the well can be found from

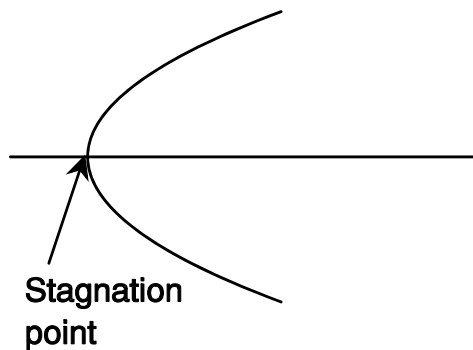
$$-\frac{y}{x} = \tan \left(\frac{2 \pi k b i}{Q} y \right)$$

----- ①

Eq ① comes from the superposition of radial and 1-D flow field solution, where i is the original piezometric slope gradient. It can be shown that

as $x \rightarrow \infty$, $y_L = \pm \frac{Q}{2 k b i}$

----- ②



and stagnation point (no flow) occurs at

$$x_s = - \frac{Q}{2 \pi k b i} \quad \text{at } y = 0 \quad \text{----- ③}$$

Equations (2) and (3) may be applied to unconfined aquifers for cases of small drawdowns (less than 10% of original thickness), when b is replaced by h_0 (average original saturated aquifer thickness). An important application of the well in a uniform flow field involves the evaluation of pollution sources and impacts on downgradient well fields and the potential for pumping and capturing a plume as it migrates downgradient.

✱ **Transient well hydraulics**

Generally, it takes a long time to reach steady state in the field. Transient state well hydraulics are more frequently applied in the field.

① Theis Method (CJN pp. 49-54)

For confined aquifer pumped at a constant rate

Governing eq.

$$\frac{\partial^2 h}{\partial x^2} + \frac{\partial^2 h}{\partial y^2} = \frac{S_s}{k} \frac{\partial h}{\partial t} = \frac{S}{T} \frac{\partial h}{\partial t}$$

In polar coordinates,

$$\frac{\partial^2 h}{\partial r^2} + \frac{1}{r} \frac{\partial h}{\partial r} = \frac{S}{T} \frac{\partial h}{\partial t}$$

Boundary Condition

$h = h_0$, for $t = 0$

$h \rightarrow h_0$, as $r \rightarrow \infty$ for $t \geq 0$

Assuming that the well is a mathematical sink of constant strength with the B.C.,

$$S' = \frac{Q}{4\pi T} \int_u^\infty \frac{e^{-u}}{u} du = \frac{Q}{4\pi T} w(u)$$

S' : drawdown

Q : discharge at the well

$w(u)$: well function

$$u = \frac{r^2 S}{4 T t}$$

$$w(u) = -0.5772 - \ln u + u - \frac{u^2}{2 \cdot 2!} + \frac{u^3}{3 \cdot 3!} - \dots$$

We obtain T, S by only one observation well and a relatively short pumping period.

Assumptions for This Solution

- (1) Aquifer is homogeneous and isotropic, having uniform thickness and infinite extent.
- (2) Prior to pumping, the piezometric surface is horizontal.
- (3) Pumping rate is constant.
- (4) Flow is horizontal within the aquifer.
- (5) Storage within the well can be neglected.
- (6) Water removed from storage responds instantaneously with a declining head.

In field, seldom completely satisfied, but still most useful and accurate method.

$$S' = \frac{Q}{4\pi T} w(u)$$

$$\frac{r^2}{t} = \frac{4T}{S} u$$

----> graphically solution

$$w(u) : u$$

---> type curve

overlapped over

$$r^2 / t : S'$$

Find position of well-matching by Trial and error.

② Cooper-Jacob Method

(Need Writing)

※ Organic Compounds (OC)

= Compounds containing Carbon.

exception : CO_2 , CO_3^{2-} , CN^-

C forms four covalent bonds capable of bonding to other atoms, =, ≡ bonds.

Diverse physical/chemical properties C - H, O, P, S, N, Cl, etc.

Transport Behavior Affected.

※ Physico-chemical properties of OC

① Name, MW. (molecular weight), Structure (formula)

② melting point, boiling point (1 atm 기준)

→ 지층에서 gas, liquid, solid state 결정 → Remediation Method Selection

* 같은 basic structure를 가진 OC는 MW이 증가할수록 Boiling Point가 커진다.

Alkane, C _n H _{2n+2}	# of C	Boiling Point (°C at 1atm)
Butane (C ₄ H ₁₀)	4	0
Pentane (C ₅ H ₁₂)	5	36
Hexane (C ₆ H ₁₄)	6	69
Heptane(C ₇ H ₁₆)	7	98
Octane(C ₈ H ₁₈)	8	126
Nonane(C ₉ H ₂₀)	9	151
Decane(C ₁₀ H ₂₂)	10	174

③ Specific gravity

$G_s = (\text{Wt. of a given volume of substance at typically } 20^\circ\text{C}) / (\text{Wt. of same volume of water at } 4^\circ\text{C})$

If $G_s \leq 1$: Floater, LNAPLs (BTEX, etc.) NAPL : Non Aqueous Phase Liquid

$G_s > 1$: Sinkers, DNAPLs (TCE, PCE, etc.)

Remediation Method Selection

④ Water Soluble

Completely	soluble	-	insoluble
	miscible	-	지층에서 생화학적으로 분해가 용이 (degraded decompose)

More soluble materials have a greater potential of mobility in the environment, moving along GW, easily decomposed. (Natural Attenuation applicable)

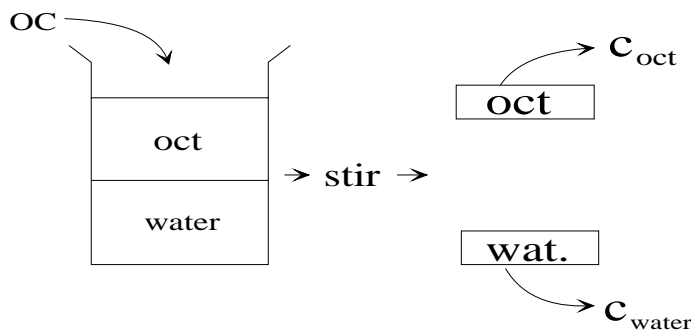
unit : mg dissolved / L of distilled water

example : benzene 1780mg/L, Ethylbenzene 150mg/L, Anthracene 0.073mg/L,
generally as the number of benzene ring increases, water solubility decreases.

⑤ K_{ow} (Octanol-Water partition coefficient)

↳ hydrophobicity

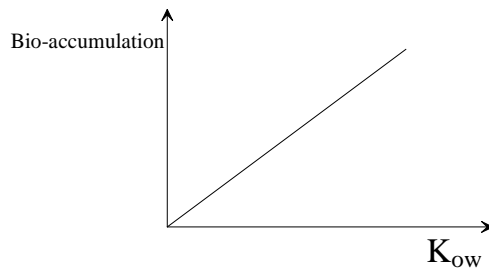
Measure of the degree to which an organic substance will preferentially dissolve in water or an organic solvent.



$$K_{ow} = \frac{C_{oct}}{C_{water}}$$

benzene : $K_{ow} = 139$ $\log K_{ow} = 2.13$

DDT : $K_{ow} = 10^{6.19}$ $\log K_{ow} = 6.19$



As K_{ow} increases, Natural Organic material 에 더 흡착된다.

→ 이동성 저하

→ 처리에 어려움

CRC handbook

Merck Index

⑥ Henry's (law) constant

$$H_L = \frac{P_x}{C_x}$$

P_x : Partial pressure of gas in equilibrium (atm)

C_x : Equilibrium concentration of the gas in solution (mol/m³ water)

As H_L increases, the greater the rate of volatilization from soil or water. Soil Vapor Extraction, Steam Injection, Air Sparging, etc. applicable.

⑦ Vapor Pressure

Measure of the tendency of a substance to pass from a solid or a liquid to a vapor state. Pressure of the gas in equilibrium with liquid or the solid at a given temperature.

As vapor pressure increases, more volatile of the substance.

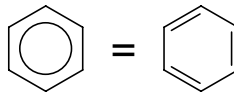
※ Classification of Organic Compounds

C 공유결합 with H, O, N, P, S, Cl, Br etc.

유기물의 특징은 가연성이 있으며 수용성이 낮고(hydrophobic) 비등 및 용해점이 낮으며 유기물질의 근원은 석유처럼 자연적으로 생성된 것이 있는가 하면 합성 및 발효에 의하여 만들어 진다.

C와 H로 기본구조를 이루는 것을 탄화수소(hydrocarbon)

HC	{	Aliphatic HC (지방족) : no benzene ring (straight chain, branched chain, ring chain)
		Aromatic HC (방향족) : contains benzene ring (aromatic chain)



Aliphatic HC

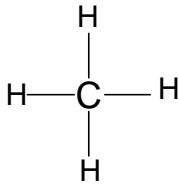
- Alkane : Single bond, C - C ; saturated HC
- Alkene : double bond, C = C ; unsaturated HC
- Alkyne : triple bond, C ≡ C ; unsaturated HC

Alkanes

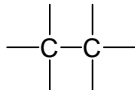
C_nH_{2n+2} : straight chain and branched chain structures (**Environmentally, straight chains are more easily broken and degraded than branched chains**)

포화탄화수소를 일명 alkanes 또는 파라핀(paraffins) 및 메탄계열 탄화수소라 한다. 대체적으로 불활성(inert)이며 원천은 휘발유, 경유를 위시한 원유들로서 아래의 물질이 대표적인 물질이다. (한정상 pp651)

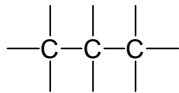
Methane 가장 간단한 탄화수소. 하수 슬러지나 유기폐기물을 혐기성처리할 때, 최종 생성물로 얻어짐(매립장 가스 LFG의 주성분). 공기중에 5-15%의 메탄이 포함되면 폭발 가능함. 메탄은 주요 온실가스(greenhouse gas)의 하나. 성층권의 메탄농도는 지구의 열수지(heat balance)와 온난화에 영향을 미친다.



Ethane

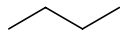


Propane

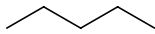


Butane C_4H_{10}

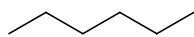
두 개의 이성질체가 존재. (n-butane, isobutane)



Pentane



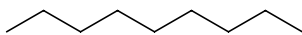
Hexane C_6H_{14}



Heptane C_7H_{16}

Octane C_8H_{18}

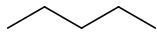
Nonane C_9H_{20}



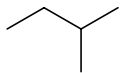
Decane $C_{10}H_{22}$

75개의 이성질체 존재. 탄소수가 증가함에 따라 이성질체의 수도 증가

Structure isomers(이성질체) : same formula, different structure →물성이 달라짐
example C₅H₁₂ (3 isomers are possible)



pentane



2- methylbutane



2,2-Dimethylpropane

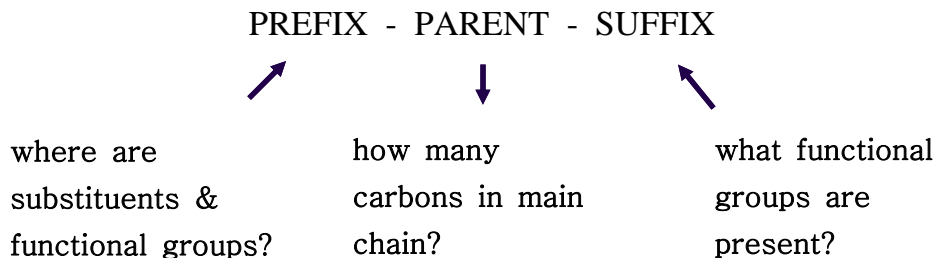
만일 탄소와 결합하고 있는 수소이온이 할로젠물질로 치환되면 이를 halogenated alkanes라 한다. (한정상 pp652, 표 12-24)

포화탄화수소는 색과 냄새가 없고 물에 잘 녹지 않으며, 특히 탄소수 5개 이상의 것은 물에 거의 녹지 않는다. 그러나 유기용매에는 대부분이 잘 녹으며, 실온에서 C₃까지의 탄소수를 가진 탄화수소는 기체, C₆-C₁₇은 액체, C₁₇이상은 고체이다.

※ Alkane 명명법 (Nomenclature) (박준범 slides)

IUPAC(International Union of Pure and Applied Chemistry)

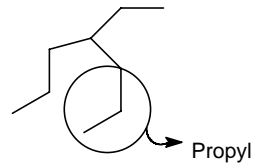
A chemical name has three parts on the IUPAC system



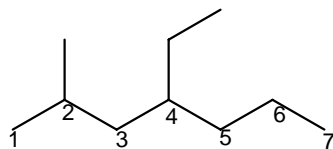
As we cover different functional groups in later chapters, IUPAC rules will be given.
For now, let's see how to name branched-chain alkanes.

- ① base name - longest chain alkane
- ② Any branch from straight chain is named as alkyl group

ex. Methyl CH_3 -
 Ethyl CH_3CH_2 -
 Propyl $CH_3CH_2CH_2$ -



- ③ Location of functional group is indicated by numbering the carbon atoms in the longest chain, with end carbon closest to the position of the first functional group being carbon #1

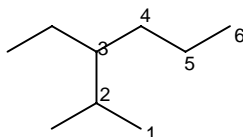


2-methyl-4-ethyl-heptane

- ④ , , ... C_nH_{2m}
 cyclopropane cyclobutane

※ 5 Steps to naming branched alkanes :

Step1 - Find the parent hydrocarbon - the longest carbon chain. If 2 different chains of equal length are present, select the one with the most branch points.

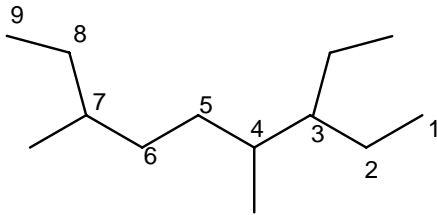


3-ethyl-2-methyl hexane

chain의 길이가 같을 때 **branch point**가 더 많은 것을 택함

Step2 - Number the atoms in the main chain beginning at the end nearer the first branch point. If 2 branch points are the same distance from each end, begin numbering

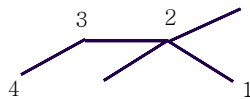
at the end nearer the 2nd branch point.



3-ethyl-4,7-dimethyl nonane

두 번째 branch가 먼저 나오는 쪽으로
순번을 정한다.

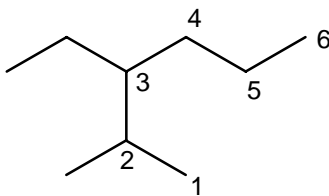
Step3 - Identify and number the substituents. If there are 2 substituents on the same carbon, assign them both the same number.



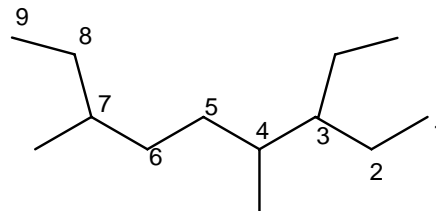
2,2-dimethyl butane

같은 번호 반복

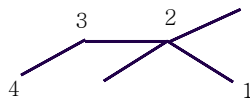
Step4 - Write out the name as a single word using hyphens to separate the different prefixes and using commas to separate numbers. If 2 or more different substituents are present, cite them in alphabetical order. If 2 or more identical substituents are present, use one of the prefixes di-, tri-, tetra-, etc. Don't use these prefixes for alphabetizing purposes, however.



3-ethyl-2-methyl hexane

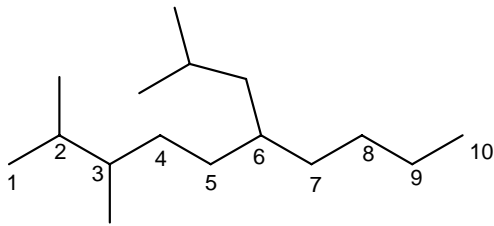


3-ethyl-4,7-dimethyl nonane

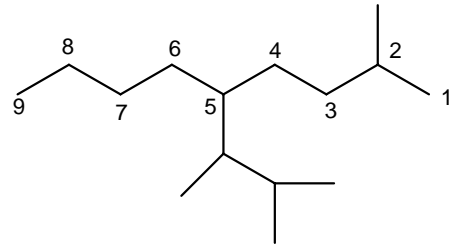


2,2-dimethyl butane

Step5 - needed when a substituent has a sub-branch - name the complex substituents - begin numbering at the point of attachment to the main chain.



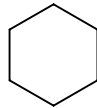
2,3-dimethyl-6(2-methyl propyl) decane
cycloalkane



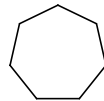
2-methyl-5(1,2-dimethyl propyl) nonane



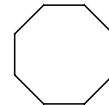
cyclopentane



cyclohexane



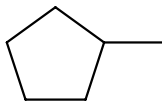
cycloheptane



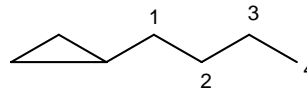
cyclooctane

✳ cycloalkane

1.



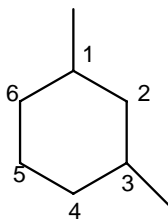
methylcyclopentane



1-cyclopropyl butane

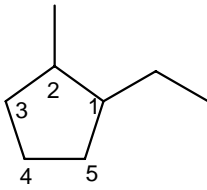
2.

a)

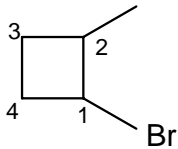


1,3-dimethyl cyclohexane

b)

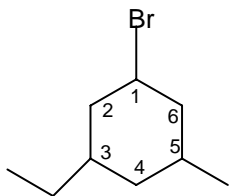


1-ethyl-2-methyl cyclopentane

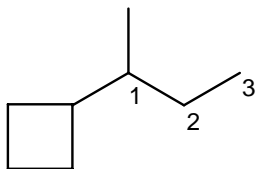


Halogens are treated exactly like alkyl groups

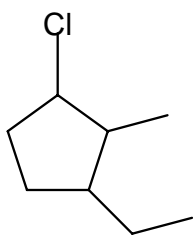
1-bromo-2-methylcyclobutane



1-bromo-3-ethyl-5-methyl cyclohexane



(1-methylpropyl) cyclobutane



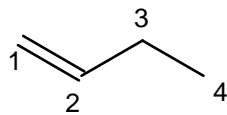
1-chloro-3-ethyl-2-methyl-cyclopentane

※ Alkene

C_nH_{2n} , double, unsaturated, olefin
(-ene, ylene)

alkenes는 주로 석유생성공정에서 제조되며 적은 분자가 폴리머(polymer)라 불리우는 거대한 분자를 이루는 중합반응(polymerization)을 통해 고분자를 형성한다. ethylene 혹은 ethene의 수소가 할로젠 원소인 Cl로 치환되면 chlorinated alkene으로 바뀌는데 이들은 내성이 강하고 독성이 매우 큰 물질로서 생분해에 의해 분해되는 경우 독성이 증폭될 수 있는 물질이다. PCE(Perchloroethylene, or Tetrachloroethylene)가 미생물에 의하여 지중에서 분해되면 TCE-DCE를 거쳐 VC(Vinylchloride, C_2H_3Cl)로 바뀌면서 염소이온이 유리되어 나온다. VC는 PCE보다 독성이 훨씬 크다. (한정상 표 12-26) VC는 PVC의 제조에 사용되며, 오염된 지하수와 위생매립지로부터 발생하는 기체 속에서 흔히 검출된다. 휘발성이 강하여 대기오염문제도 일으킨다. MCL은 2 ug/L이다.

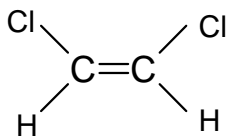
The carbon atoms in the straight chain are numbered straight at the end nearest the double bond.



1-butene

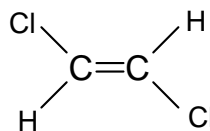


2-butene



(one side)

cis-1,2dichloroethane



trans-1,2dichloroethane

※ Alkynes (아세틸렌계열)

불포화탄화수소. 이웃한 두 탄소 원자사이에 삼중결합을 가진다.

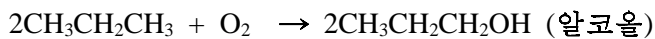
H-C≡C-H (ethyne, 에틸렌)

환경공학적인 문제를 거의 일으키지 않는다.

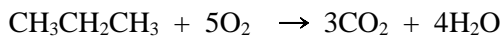
일반적으로 포화화합물(saturated HC)에 비하여 불포화화합물(unsaturated HC, 이중, 혹은 삼중결합화합물)은 산화되기 쉬우므로 미생물에 의하여 지중에서 더 쉽게 산화된다.

Aliphatic HC - Aromatic에 비해 지중 박테리아에 의해 유산소상태에서 분해가 잘 된다. 따라서 방향족 화합물에 비하여 환경에 미치는 영향이 작다.

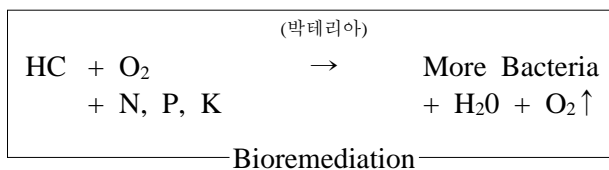
탄화수소는 호기성 조건(aerobic condition)에서 박테리아에 의하여 산화된다. 이 산화 반응의 제 1단계는 느린 생물학적 반응으로 말단의 탄소원자를 공격하여 알코올로 전환시킨다. 이를 오메가 산화(omega oxidation)라고 한다.



이후 여러 단계의 산화반응을 거쳐 탄화수소를 이산화탄소와 물로 전화시키며, 이 과정에서 에너지를 얻는다.

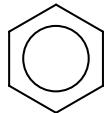


이를 지반환경정화에 응용한 방법이 생분해법(bioremediation)이다.



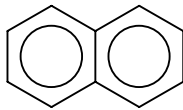
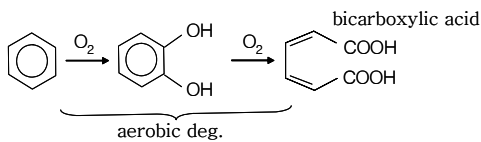
※ Aromatic Compounds

→ containing benzene ring (Generally, aliphatic compounds are more easily degraded than aromatic compounds, which means aliphatics are less toxic to environment.) 지중에서 지방족보다 난 분해성. 분해속도는 구성물질에 따라 다르지만 대체적으로 수용성이 좋고 단순한 구조일수록 생분해가 잘된다.



carcinogenic!

벤젠의 지중분해과정



벤젠링이 2개 이상 연결된 것

Naphtalene

Polycyclic nuclear Aromatic Hydrocarbon (PAH)

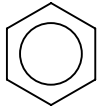
4개 이상 extremely- carcinogenic (ex. benzopyrene 벤젠링 5개 MCL 0.2 ug/L)

PAH는 아스팔트, 콜타르, 및 크레오소트(creosote)와 같은 물질의 정제 시 생산되며 주로 염색가공, 물편이나 알카로이드 제조공정에서 사용한다. 이들 물질은 소수성 (hydrophobicity)이 크기 때문에 지하수 내에서 거동은 활발하지 않으나 지속성이 있고 독성/발암성 물질이다. 이와 같이 벤젠링이 증가할수록 발암성이 커지고, 박테리아에 의한 분해가 어려워진다.

벤젠링이 3개인 것은 anthracene과 phenanthrene (이성질체)

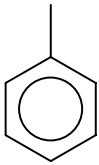
(BTEX) 석유류 지반오염물질, 폐수와 침출수에서 10-1,000mg/L까지 검출됨. 주로 UST의 누출에 의하여 발생됨.

Benzene (석유 내에 평균 2% 함유, MCL 5ug/L)

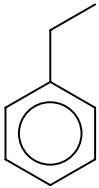


주로 코올타르나 원유에 함유되어 있으며 석유정제, 유기화합물의 합성플랜트, 고무산업과 관련된 폐수에 포함되어 있다. 장기 복용 시 백혈병의 원인이 될 수 있다. 페놀은 벤젠에 수산기(OH)가 결합된 물질로서 석탄이나 석유공정의 산업 폐수에서 생산되며 살균제로 이용된다. 저농도의 페놀은 미생물에 의해 생분해가 되나 고농도에서는 오히려 독성을 띠므로 살균제로 이용한다.

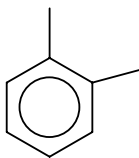
Toluene (석유 내에 평균 15% 함유, MCL 1mg/L)



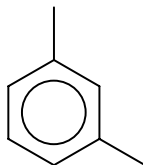
Ethylbenzene (석유 내에 평균 2% 함유, MCL 700ug/L)



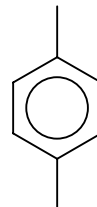
Xylene (dimethylbenzene) (석유내에 평균 10% 함유, MCL 이성질체 총합 10mg/L)



o-Xylene
(ortho-)



m-Xylene
(meta-)



p-Xylene
(para-)

BTEX 물성

출처 E.Wertheim and H.Jeskey, 'Introductory Organic Chemistry' 3rd ed. McGraw-Hill, New York, 1956.

방향족 탄화수소의 염소화합물(chlorinated aromatic compound)은 환경에 비교적 오래 잔류하므로 지방족 염소화합물(chlorinated aliphatic compound)과 마찬가지로 생태계에 대한 피해가 크다. 벤젠 염소화물(chlorinated benzenes)과 다염화 바이페닐(polychlorinated biphenyl, PBCs)의 두 가지가 가장 중요한 유형이다.

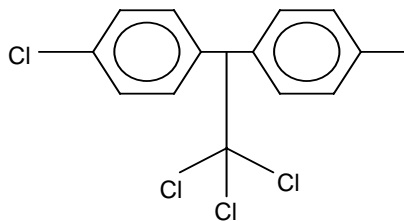
이름	화학식	M.P.(°C)	B.P.(°C)	비중 (20°C/4°C물)
benzene	C ₆ H ₆	5.5	80.1	0.879
toluene	C ₆ H ₅ CH ₃	-95.0	110.8	0.866
ethylbenzene	C ₆ H ₅ C ₂ H ₅	-93.9	136.2	0.867
<i>o</i> -xylene	C ₆ H ₄ (CH ₃) ₂	-29.0	144.0	0.875
<i>m</i> -xylene	C ₆ H ₄ (CH ₃) ₂	-53.6	138.8	0.864
<i>p</i> -xylene	C ₆ H ₄ (CH ₃) ₂	13.2	138.5	0.861

※ 벤젠 염소화물

벤젠에서 한 개 이상의 수소가 염소로 치환된 화합물이다. 이들은 solvent와 살충제로 광범위하게 사용되는 공업약품이다. 지방족 염소화합물과 마찬가지로 매립지와 여러 폐수와 침출수에서 발견된다. 휘발성이 크고 물에 잘 녹지 않는 소수성이다. chlorobenzene은 먹는물 MCL이 100 ug/L로 정하여져 있으며 세 개의 이성질체(*o*-, *m*-, *p*-)가 있다. 또, hexachlorobenzene은 여러 가지 클로로벤젠의 합성에 사용되며 지하수 오염물질 중에서 검출되고 있으며, MCL은 1 ug/L이다.

※ PCBs

벤젠고리가 다른 그룹과 결합하는 경우에 phenyl 이라는 용어를 사용한다. 다음 그림과 같이 두 개의 벤젠고리가 결합하고 Cl이온에 의해 치환된 물질을 PCB : Polychlorinated Biphenyl 이라고 한다. 이는 방향족 탄화수소의 염소화합물(chlorinated aromatic hydrocarbon)의 일종이고, 자연계에서 난분해성(recalcitrant)이다.



Dichloro-diphenyl-trichloroethyne
= DDT

209종의 PCB가 존재하며(이를 congener, 동속체라 한다.), 비슷한 숫자의 염소원자를 가진 동속체군은 'arochlor'라 불린다. 증기압이 낮고, 유전상수가 큰 안정한 화합물로, 변압기와 축전기의 절연유, 가소제(plasticizer), 용매, 열매체, 농약 등의 용도로 사용한다. K_{ow}값이 크고(hydrophobic), 이에 따라 생체축적(bioaccumulation)이 잘되어, EPA기준은 총 PCB에 대하여 0.5µg/L 이다. 염소원자가 많은 것들은 혐기성 미생물에 의하여 분해되며, 적은 것들은 호기성 미생물에 의하여 분해된다. 그러나 변환속도가 매우 느리기 때문에 일반적으로 난분해성으로 간주된다.

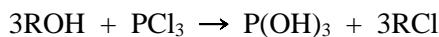
※ Halogenated Hydrocarbons (HH)

Aliphatic HHs and Aromatic HHs are characterized by the presence of one or more halogen atoms (F, Cl, Br, etc.). (CJN pp.86)

HHs are very hard to treat, recalcitrant to decompose. Typically, they are denser than water ; if spilled on the ground in quantities great enough to overcome the residual saturation, the pure phase may migrate vertically downward through an aquifer. 버려진 쓰레기 매립지와 산업 및 도시하수에서 검출되는 화합물이다. 대표적인 지하수 오염물질인 TCE, PCE의 MCL은 공히 0.5µg/L 이다.

화학식 CHCl=CHCl을 가진 할로젠화 에텐은 기하이성질체(geometric isomer)라고 하는 특별한 형태의 이성질현상을 나타내는 화합물의 예이다. cis-1,2-dichloroethene에서는 염소원자들이 같은 쪽에 있으며, 반면 trans-1,2-dichloroethene에서는 염소원자들이 서로 반대쪽에 있다.

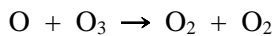
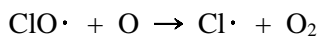
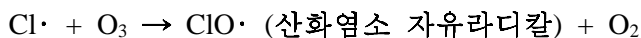
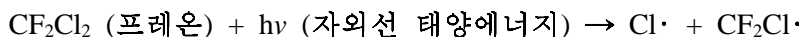
간단한 할로젠화 알킬(R-X)은 알코올과 PCl₃의 반응으로 제조할 수 있다.



예) 3CH₃CH₂CH₂OH + PCl₃ → P(OH)₃ + 3C₃H₇Cl (n-염화프로필, n-propyl chloride)

※ CFC(chlorofluorocarbons)

일명 프레온(Freon)으로 불리며 안정하고 불연성이며 무독성이어서 오랫동안 냉동제, 용매 및 연무제로 널리 사용되어 왔다. 자외선에 의하여 다음과 같이 반응하여 성층권의 오존층을 파괴하는 현상에 관여하는 것으로 밝혀졌다.



CFC는 온실가스로도 알려져 있으며, 오존층 파괴와 온실효과 때문에 전 세계적으로 그 제조와 사용을 규제하고 있다.

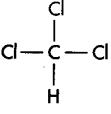
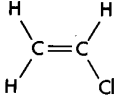
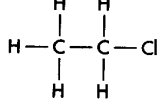
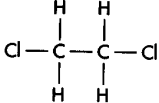
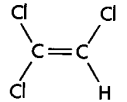
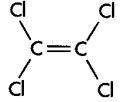
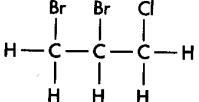
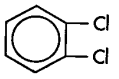
Name	Structure	Uses and Other Sources
Trichloromethane (chloroform)		Liquid used in manufacture of anesthetics, pharmaceuticals, fluorocarbon refrigerants and plastics. Used as solvent and insecticide. Formed from methane when chlorinating drinking water.
Vinyl chloride (chloroethene)		Gas used in the manufacture of polyvinyl chloride. End product of microbial degradation of chlorinated ethenes.
Chloroethane		Liquid used to manufacture tetraethyl lead. Degradation product of chlorinated ethanes.
1,2-Dichloroethane		Liquid used to manufacture vinyl chloride. Degradation product of trichloroethane.
Trichloroethene (Trichloroethylene)		Solvent used in dry cleaning and metal degreasing. Organic synthesis. Degradation product of tetrachloroethene.
Tetrachloroethene (perchloroethene) (perchloroethylene)		Solvent used in dry cleaning and metal degreasing. Used to remove soot from industrial boilers. Used in manufacture of paint removers and printing inks.
1,2-Dibromo-3-chloropropane (DBCP)		Soil fumigant to kill nematodes. Intermediate in organic synthesis.
o-Dichlorobenzene (1,2-dichlorobenzene)		Chemical intermediate. Solvent. Fumigant and insecticide. Used for industrial odor control. Found in sewage from odor control chemicals used in toilets.

FIGURE 7.4 Organic halides found in hazardous waste.

※ Alcohols

알코올은 탄화수소의 일차 산화생성물



- An alcohol has one or more hydroxyl group, -OH, substituted for hydrogen atoms on an aliphatic HC (R-OH, R : aliphatic backbone) CH₃-OH (Methanol).
- Alcohols are named by finding the longest HC chain that includes the carbon atom to which -OH is attached. That becomes the base name, to which suffix, -ol is added. The position of the C to which -OH is attached is indicated by a numerical prefix. If there are two -OH groups, then suffix -diol is used.

Alcohols are miscible with water and hence have a potential for significant mobility in groundwater. Many are also readily biodegraded. 미생물은 호기성 조건에서 일차와 이차 알코올을 쉽게 분해한다. 최종 생성물은 물과 이산화탄소이지만 중간 생성물로 알데하이드와 케톤이 존재하는 것으로 알려져 있다. 삼차 알코올은 미생물에 의한 분해가 매우 어려우며, 탄화수소에서와 마찬가지로 먼저 말단의 메틸기가 산화되는 것으로 알려져 있다.

Name	Structure	Uses and Sources
Methanol (wood alcohol)	$\begin{array}{c} \text{H} \\ \\ \text{H}-\text{C}-\text{H} \\ \\ \text{OH} \end{array}$	Solvent. May be added to gasoline. Manufacture of formaldehyde and methyl halides.
Ethanol (grain alcohol) (ethylalcohol)	$\begin{array}{c} \text{H} \quad \text{H} \\ \quad \\ \text{H}-\text{C}-\text{C}-\text{H} \\ \quad \\ \text{H} \quad \text{OH} \end{array}$	Preparation of distilled spirits. Solvent. Manufacture of acetaldehyde, acetic acid, ethyl ether, etc. Preparation of lacquers, perfumes, cosmetics, over-the-counter medicines. Degradation of ethyl acetate in excess of water.
Ethylene glycol (1,2-ethanediol)	$\begin{array}{c} \text{H} \quad \text{H} \\ \quad \\ \text{H}-\text{C}-\text{C}-\text{H} \\ \quad \\ \text{OH} \quad \text{OH} \end{array}$	Antifreeze (engine coolant) compound. Manufacture of polyester fiber and film. Deicing compound for airplanes at gate. Solvent base.
Propanol	$\begin{array}{c} \text{H} \quad \text{H} \quad \text{H} \\ \quad \quad \\ \text{H}-\text{C}-\text{C}-\text{C}-\text{H} \\ \quad \quad \\ \text{H} \quad \text{H} \quad \text{OH} \end{array}$	Released from fermentation of whisky and during sewage treatment and decomposition of organic matter. Solvent in printing, used in nail polish, brake fluid, lacquers, cleaners, polishes.
1,2-Propanediol (propylene glycol)	$\begin{array}{c} \text{H} \quad \text{H} \quad \text{H} \\ \quad \quad \\ \text{H}-\text{C}-\text{C}-\text{C}-\text{H} \\ \quad \quad \\ \text{H} \quad \text{OH} \quad \text{OH} \end{array}$	Solvent used in paints, inks, and coatings. Antifreeze formulations.
2-Methy-2-butanol	$\begin{array}{c} \text{H} \quad \text{CH}_3 \quad \text{H} \quad \text{H} \\ \quad \quad \quad \\ \text{H}-\text{C}-\text{C}-\text{C}-\text{C}-\text{H} \\ \quad \quad \quad \\ \text{H} \quad \text{OH} \quad \text{H} \quad \text{H} \end{array}$	Solvent.
t-Butanol (2-methyl-2-propanol)	$\begin{array}{c} \text{H} \quad \text{CH}_3 \quad \text{H} \\ \quad \quad \\ \text{H}-\text{C}-\text{C}-\text{C}-\text{H} \\ \quad \quad \\ \text{H} \quad \text{OH} \quad \text{H} \end{array}$	Manufacture of flotation agents, flavors, and perfumes. Solvent. Paint removers. Octane booster in gasoline. Lacquer. Solvent for pharmaceuticals.
4-Methyl-2-pentanol	$\begin{array}{c} \text{H} \quad \text{H} \quad \text{H} \quad \text{H} \quad \text{H} \\ \quad \quad \quad \quad \\ \text{H}-\text{C}-\text{C}-\text{C}-\text{C}-\text{C}-\text{H} \\ \quad \quad \quad \quad \\ \text{H} \quad \text{OH} \quad \text{H} \quad \text{CH}_3 \quad \text{H} \end{array}$	Solvent.

FIGURE 7.5 Alcohols found in hazardous waste.

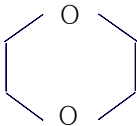
※ Ethers

· Ethers have an oxygen atom bonded between two Cs. (C-O-C, CH₃-O-CH₂CH₃ → ethyl-methyl ether)

naming two HCs followed by the word ether.

알코올을 탈수하여 제조. 에테르는 생물학적 산화를 거의 받지 않으나, 물에 잘 녹지 않으므로 부상분리(floatation)나 기울여 따름(decantation)으로 산업폐수에서 분리할 수 있다.

· Two cyclical ethers ; persistent contaminant in GW.



ex.

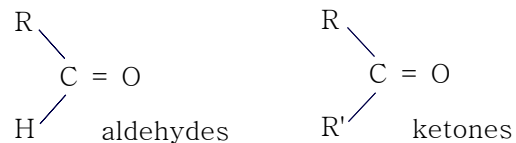
1,4-Dioxane ; miscible w/water, great mobility, extremely resistant to biodegradation. EPA designated toxic waste.

· Hazards (1) high degree of flammability, (2) formation of unstable peroxides(-O-O-) which can explode.

※ Aldehydes and Ketones

알데하이드는 일차알코올(R-OH)의 산화생성물이며, 케톤은 이차알코올(R-CHOH-R')의 산화 생성물이다.

· Both contain the carbonyl group,

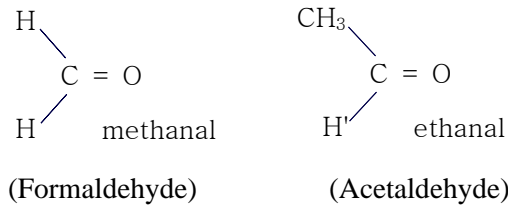


· Aldehyde has at least one H bonded to C ; naming the HC and adding the suffix -al.

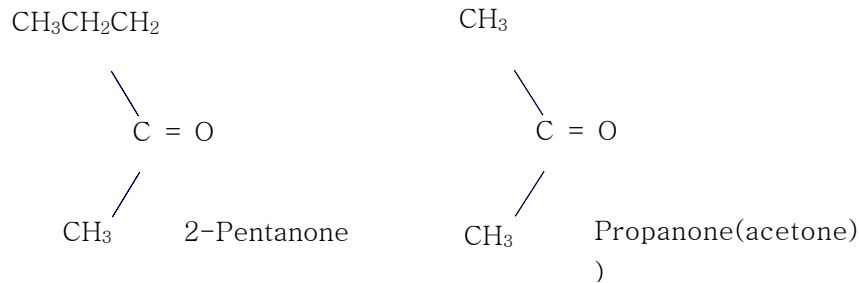
메틸알코올을 산화하면 포름알데하이드가 생성된다.

포름알데하이드는 독성이 있어, 미생물에 의한 분해가 어려우나, 1,500 mg/L이하로 하면 미생물에 의한 분해가 가능하며, 최종 생성물로 이산화탄소와 물을 생성한다.

에틸알코올을 산화하면 아세트알데하이드가 된다.



· 케톤은 이차알코올의 산화생성물
ketones have carbonyl group bonded to two HCs ; naming the HC and ending w/ the suffix -one. 아세톤은 가장 간단한 케톤이며, 아이소프로필 알코올의 산화에 의해 생성된다.

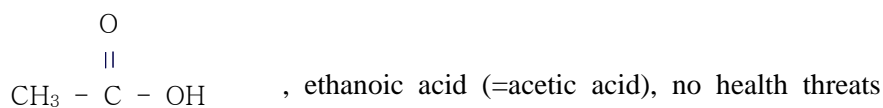


알데하이드와 케톤은 여러 미생물에 의하여 유기산(organic acid)으로 쉽게 산화. 유기산은 다시 미생물에 의하여 분해되어 최종으로 이산화탄소와 물로 분해된다. 산(acid)는 유기화합물이 가질수 있는 가장 높은 산화상태이다. 계속 산화되면, 무기화합물인 물과 이산화탄소로 된다.

※ Carboxylic Acids

유기산은 모두 R-COOH를 가지고 있으며, 이것을 $\begin{array}{c} \text{O} \\ \parallel \\ \text{R} - \text{C} - \text{OH} \end{array}$ carboxyl기라고 부른다.

- Carboxylic acids have the carboxyl group,
- 폐기물 매립장의 악취의 주 원인 물질
- named by taking the stem name and adding -oic acid.

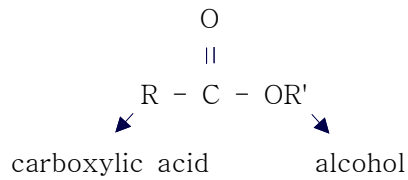


- Carboxylic acids are weak acids and do not strongly dissociate in water.

※ Esters

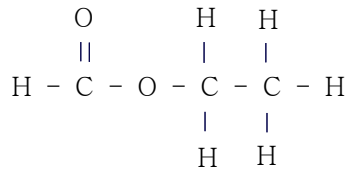
· Result of the combination of a carboxylic acid w/ an alcohol.
 무기화학에서는 산과 염기의 반응으로 생성되는 염에 해당한다.

· The functional group is :



· Named by the alcohol group by the name of the carboxylic acid w/ -ate.

· Ethanol + Formic acid = ethyl formate



· Applications and uses for solvents for polymers, flavoring agents.

· Toxicity increases w/ an increase in alkyl chain length.

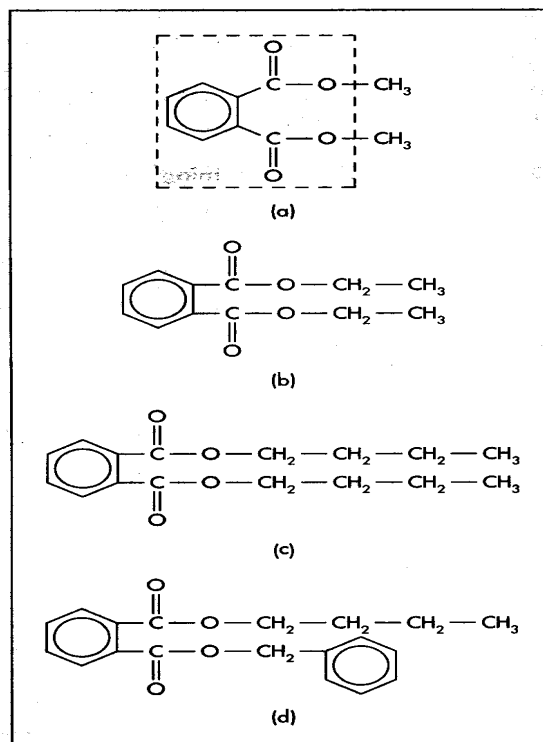

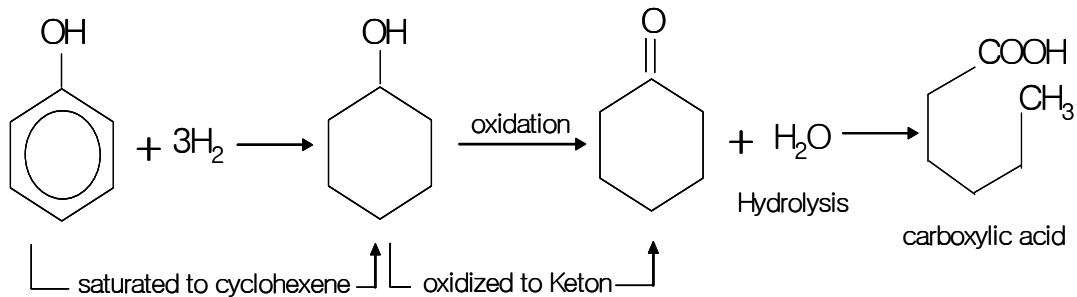


FIGURE 7.6 Structure of some phthalates. (a) Dimethyl phthalate; (b) diethyl phthalate; (c) *di-n*-butyl phthalate; (d) butyl benzyl phthalate.

※ Phenols

· Phenols are based on a hydroxyl radical bonded to 

벤젠의 모노하이드록시 유도체. 강한 독성물질. 최근의 연구결과 최고 500 mg/L까지는 호기성 박테리아에 의하여 심각한 독성 영향 없이 분해할 수 있는 것으로 밝혀짐. 혐기성상태의 분해도 가능하며 아래와 같은 분해과정을 거치게 된다.



· common GW contaminant(most of US superfund sites), due to its use in many industrial process

· Cresol ; a methyl group attached to benzene ring of phenol (hydroxytoluene, methyl phenol) 살균력이 페놀보다 강하나 사람에게 대한 독성은 약하다. 크레졸은 목재의 방부제로 사용되는 creosote의 주성분이다. 크레졸류가 섞여있는 산업폐수는 생물학적 처리가 거의 불가능하다.

· Phenols are weakly acidic(pH 6.0)

3 major classes of phenolic compounds of commercial apply(?)

- ① alkyl phenols (cresol)
- ② chlorophenols (pentachlorophenol)
- ③ nitrophenolw (2,4-Dinitrophenol)

· highly toxic (EPA priority pollutants) but most of phenols are biodegraded in nature

· Some phenols found in hazardous waste

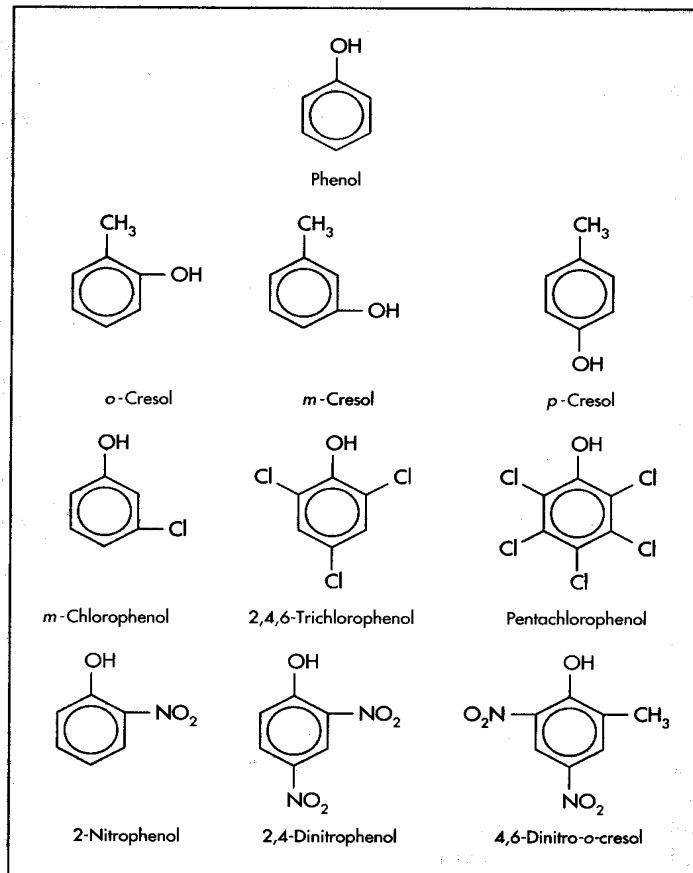


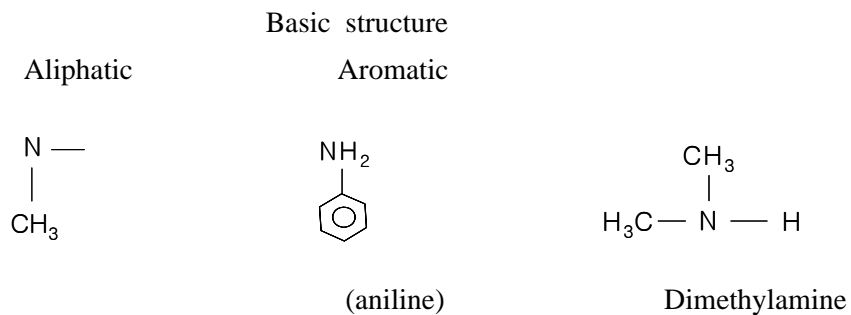
FIGURE 7.7 Structure of phenols.

※ Organic Compounds Containing Nitrogen

ex) TNT (2,4,6-trinitrotoluene)

Explosive, soil contaminant in the areas of waste disposal from manufacture of munition and explosive. 생분해에 대한 내성이 비교적 큰 화합물이다.

① Amines ; base molecule is ammonia and one or more hydrogen atom is replaced by a HC group.



② Amides

Acrylamide

③ Nitriles ; have a cynde group ($C\equiv N$)

ex) Atrazine

widely used herbicide quickly degraded in nature

위의 세 가지 화합물이 대표적인 질소화합물이나, 이밖에 환경적으로 중요한 화합물에는 isocyanate가 있다. 일반식은 $R-N=C=O$ 로 표시된다. 공업용약품으로 널리 이용된다. methylisocyanate, $CH_3-N=C=O$ 는 인도 보팔의 유니온 카아바이드 화학공장폭발로 1,000명 이상이 죽고, 수천 명이 부상당한 사고를 낸 물질이다. 휘발성이 커서 대기오염문제도 일으킬 수 있다.

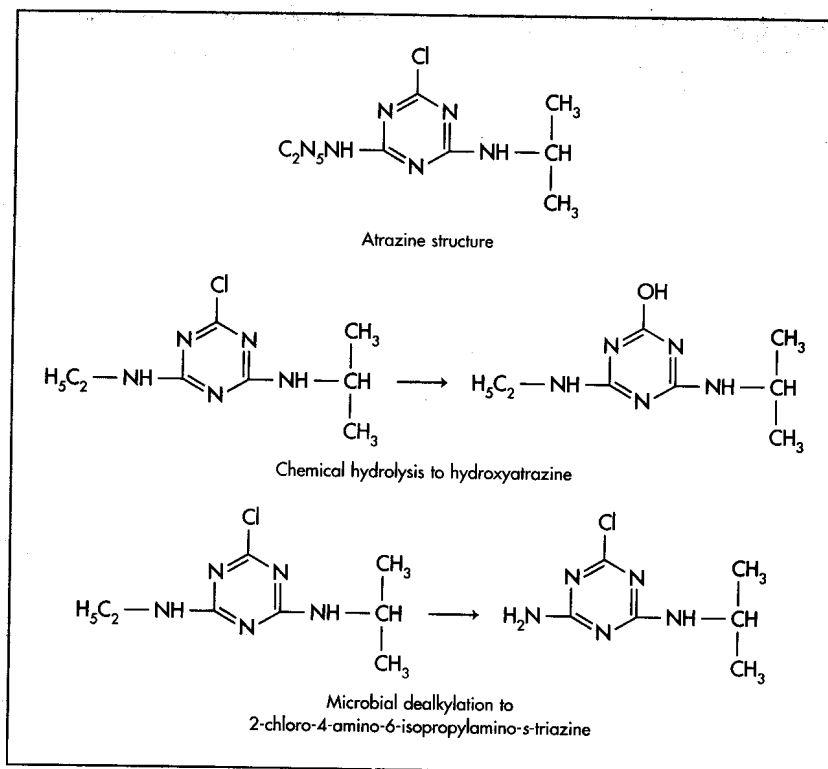
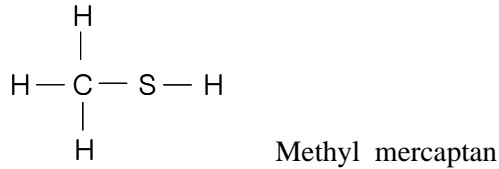


FIGURE 7.8 Structure of atrazine and metabolic pathways leading to degradation.

※ Organic Compounds Containing Sulfur and Phosphorus

- organosulfur . . . offensive odor



- Many pesticides includes sulfur, phosphorus or both in their composition.
- GW contamination source materials. 미국 26개주의 지하수에서 46종의 농약이 검출되었다. 유기염소계 농약은 독성 잔류성으로 사용이 제한됨.

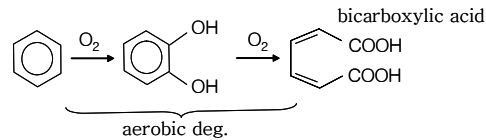
Name	Structure	Use
Captan		Fungicide used on foliage
Disulfone		Systemic insecticide used on plants
Aldicarb		Systemic insecticide and nematocide
Endosulfan		Insecticide
Malathion		Insecticide
Parathion		Insecticide and acaricide
Asulam		Herbicide

FIGURE 7.9 Structure and uses of organosulfur and organophosphorus pesticides.

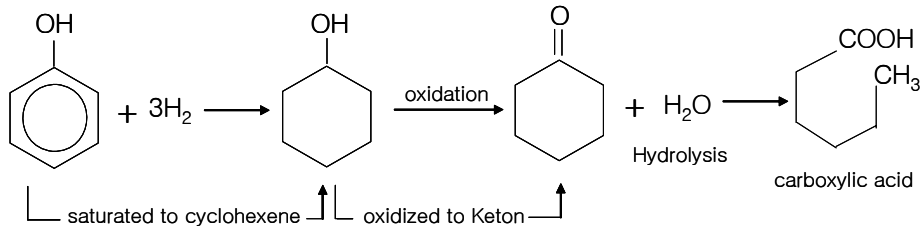
※ Degradation of Organic Compounds

↳ "the process of an organic molecule becoming smaller by chemical or biological means"

- The ultimate product of degradation of a HC is methane or CO₂ and water
- Branched-chain HCs are more resistant to microbial degradation than normal alkanes.



- Aromatic HC ;
- Phenol can undergo anaerobic degradation



During the process, the Nitrate(M(NO₃)_x, M : metal) is reduced to nitrogen.

· DDT

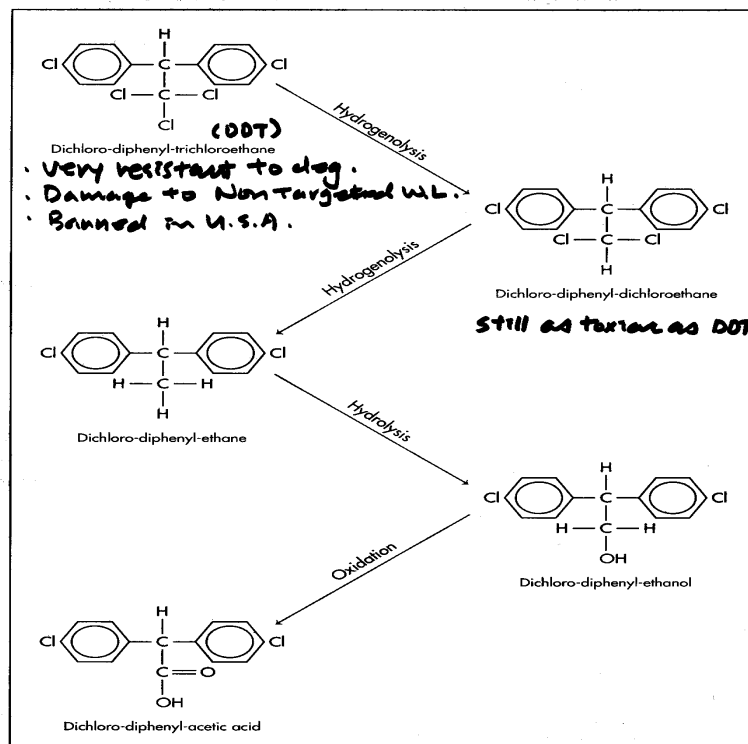
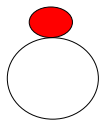


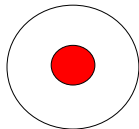
FIGURE 7.14 Metabolic pathway for the degradation of dichloro-diphenyl-trichloroethane (DDT).

※ Sorption and Chemical reaction

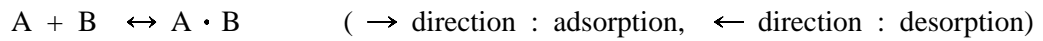


표면 Adsorption

⇒ sorption



흡수 Absorption



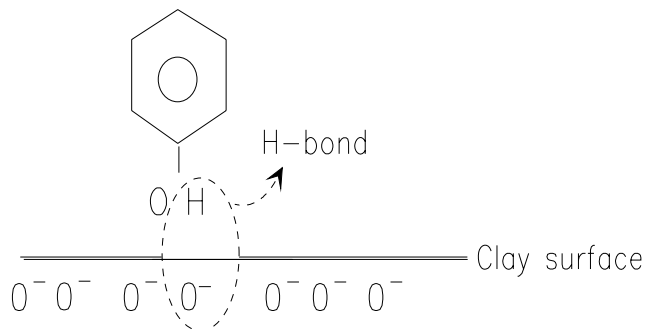
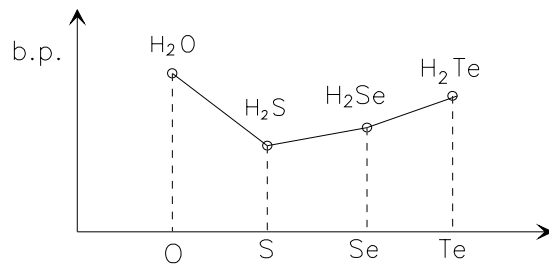
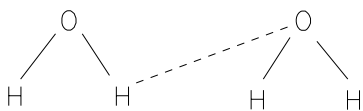
A : sorbate(chemical compound), B : sorbent(soil)

partitioning ----- Contaminant distribution between solution and solid phase

※ Sorption Mechanism

① Hydrogen bonding

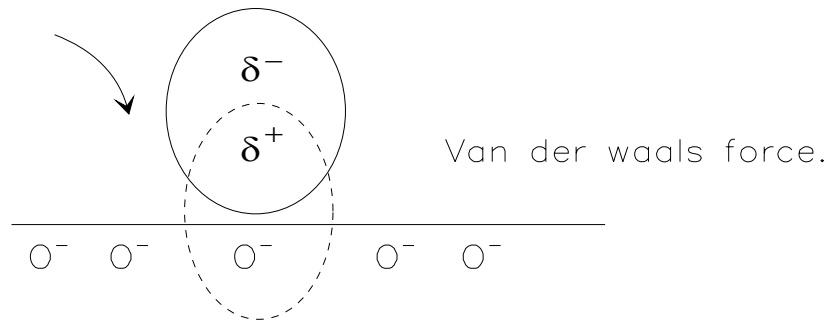
Intermolecular bond between molecules in which hydrogen is bonded to a strongly electro-negative elements(O, F, N). Example : Boiling point of water(H₂O) has higher than those of H₂S, H₂Se, H₂Te.



② Van der Waals force.

Weak electrostatic force b/w atoms, ions, and molecules that are caused by electron fluctuations that produce instantaneous dipoles.

비극성 유기오염물



③ Hydrophobic Sorption(소수성 흡착)

Natural Organic Matter(NOM) adsorbs hydrophobic organic compounds correlated with K_{ow} , f_{oc} , S (solubility of the compound)
 $S < 10^{-3}M$, $f_{oc} > 1\%$ (Karickhoff(1985))

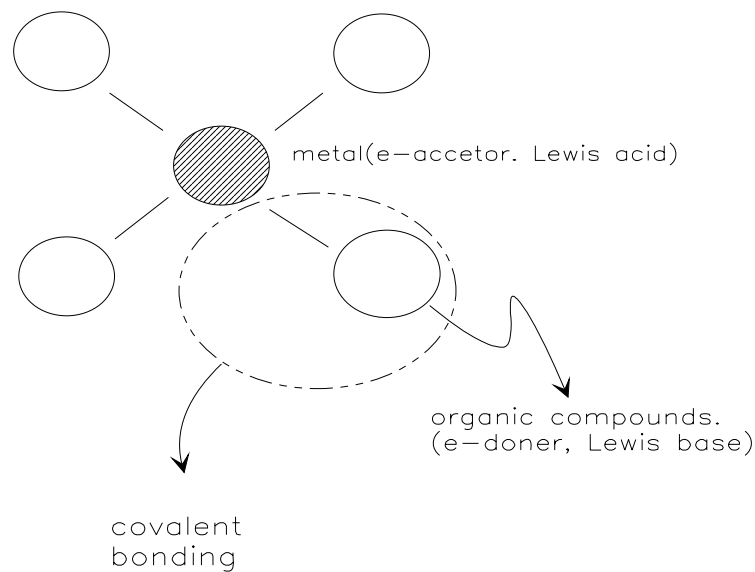
④ Ion Exchange

Alcohols(OH-), Amines(-N=), and Carbonyls(-CO).
 → positively charged in the soil matrix
 → adsorbed on clay minerals.

⑤ Coordination(or Chelation)

Ions or group of nonionic polar organic compounds that are coordinated or attached to a central metallic atom (Mg^{2+} , Al^{3+} , Si^{4+}) of a clay matrix.

Preferentially coordinate with molecules containing oxygen as a electron donor such as carbonate(CO_3^{2-}), hydroxide(OH⁻)



Generally, for charged compounds, opposites attract, for uncharged compounds, likes interact with likes.

※ Factors Affecting Sorption

(1) Contaminant Characteristics

- Water Solubility (High S, Low Adsorption)
- Charged character
- Octanol-water partition coefficient (The more hydrophobic the contaminant is, the more likely it is to partition onto soils and to have low S.)

(2) Soil Characteristics

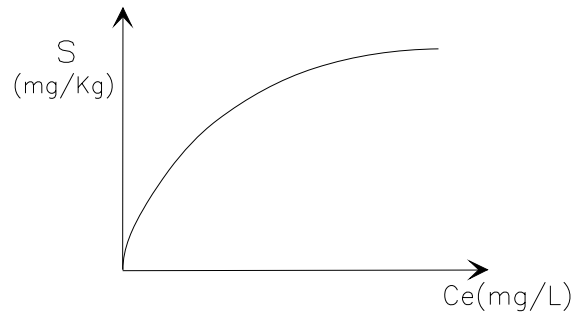
- Mineralogy (silt, clay, and sand)
- Permeability
- Organic carbon content
- Surface charge
- Surface area

(3) Fluid Media Characteristics

- pH (ex. pentachlorophenol $\text{pH} < 4.7$ uncharged, $\text{pH} \geq 4.7$ anion)
- Salt content

※ Adsorption Isotherm

The constant-temperature equilibrium relationship b/w the quantity of sorbate(contaminant) per unit of sorbent(soil), S , and the equilibrium concentration of sorbate in solution, C_e , is called "adsorption isotherm." Sorption isotherm can be linear, concave, convex, or complex combination of all the shapes.

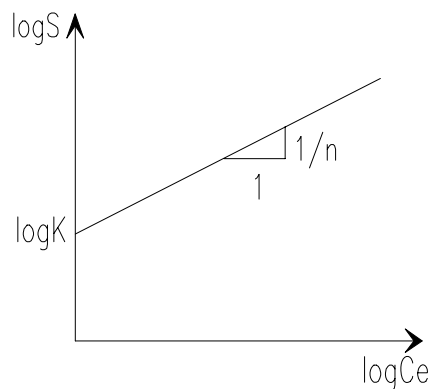


The most common relationship is the \Rightarrow Freundlich Isotherm equation

$$S = K C_e^{1/n}$$

and can be linearized as,

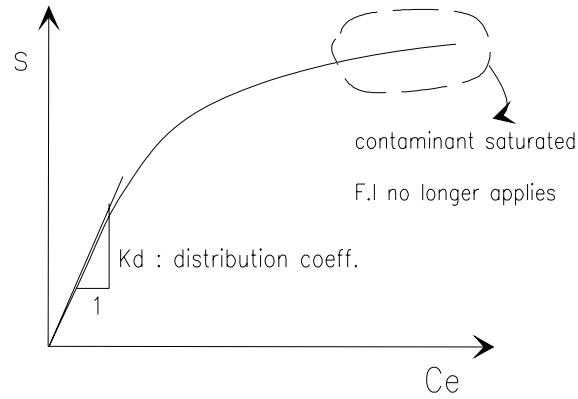
$$\log S = \log K + \frac{1}{n} \log C_e$$



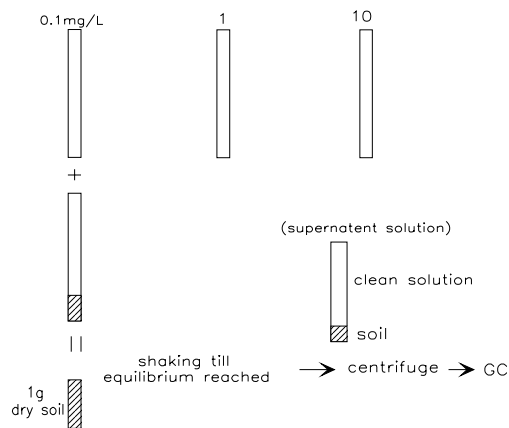
$K, 1/n$: Freundlich constants.

K relates to the capacity of sorbent for sorbate, and $1/n$ is a function of the strength of adsorption (The smaller the $1/n$, the stronger the adsorption bond is.)

When $1/n=1$, the equation can be $S=K_d C_e$, where K_d is the distribution coefficient.



* For obtaining F.I., a number of solutions containing various contaminants of the contaminant are well mixed with the solid, and the amount of contaminant removed is determined.



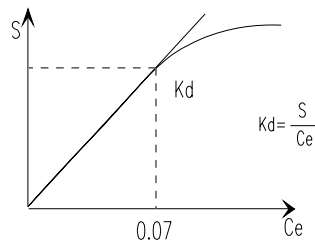
	C_0 :	0.1	1	10
	C_e :	0.07	0.67	

0.03mg/L

↓

0.0003 mg

$$\therefore S = \frac{0.0003 \text{ mg}}{1 \text{ g}} = 3 \times 10^{-7} \text{ mg/Kg}$$

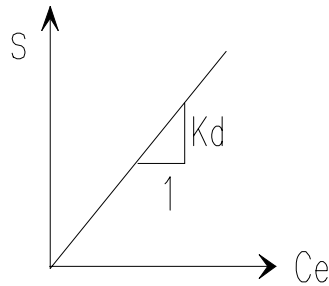


Retardation Factor

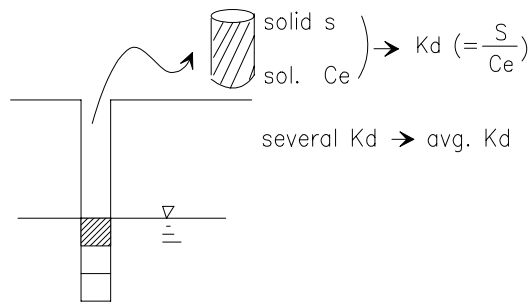
$$R = \frac{V_{GW}}{V_{cont.}} \quad R = 1 + \frac{\rho_b}{n} K_d$$

ρ_b, n : from Lab (각각, 흙의 단위중량, 공극률)

K_d : F. I.



① Field sampling



② Kow 값 이용

K_{ow} : octanol-water partition coefficient (C_{oct} / C_{water}) (환경화학 pp.310)

$$K_d = f_{oc} K_{oc}$$

f_{oc} : organic carbon content in soil(Lab) (mass organics / mass dry soil)

$f_{oc} < 0.0005$ 인 경우, 본 방법 적절치 않음

soil type	f_{oc}
fine sand	0.0002
lake sediment	0.001
silty sand	0.01
clay	보통 0.01 이상
* 김포매립지	0.02 ~ 0.04

K_{oc} : organic carbon partition coefficient

(mg cont./Kg organic carbon) / (mg cont./L solution)

K_{oc} has directly relationship with K_{ow} (CJN Table 7.2 P.174)

$K_{oc} = f_n(K_{ow})$

$$\log K_{oc} = 0.544 \log K_{ow} + 1.377$$

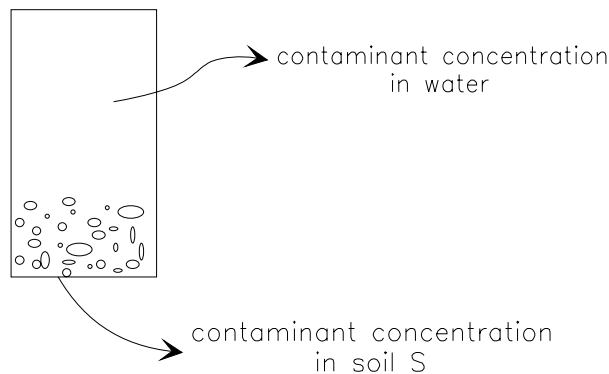
(Kenaga & Goring (1978))

본 방법은 (f_{oc} 가 0.0005 이상인 경우에 사용할 수 있다)

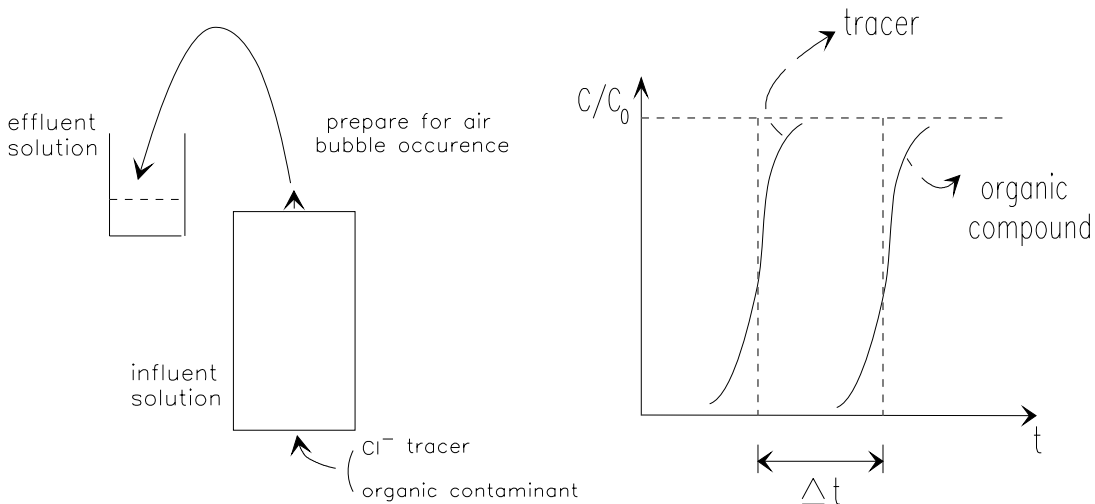
K_{ow} from lab \rightarrow K_{oc} from regression \rightarrow f_{oc} from lab \rightarrow $K_d = f_{oc} \cdot K_{oc} \Rightarrow R$

③ Lab test

i) Batch test (회분식 시험)



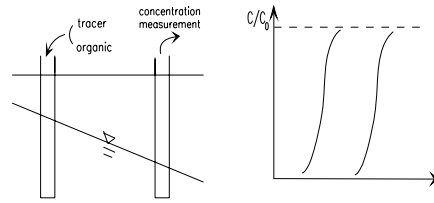
ii) column test (주상시험)



$$R = V_{gw} / V_{cont.} = V_{cl} / V_{cont.} = 1 + \rho_b/n K_d$$

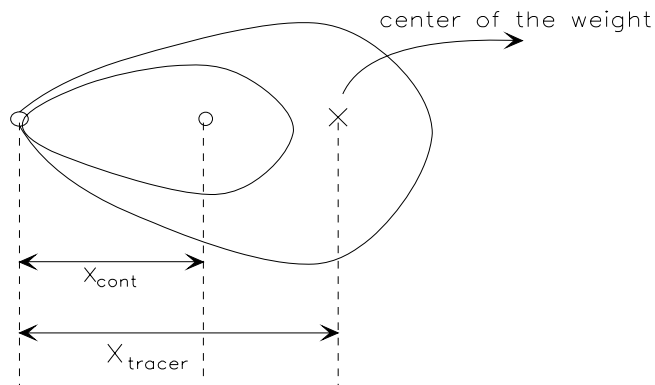
④ Field experiment

Same concept with lab column test (break through test)



⑤ Plume Movement

$$R = X_{cl} / X_{cont.}$$



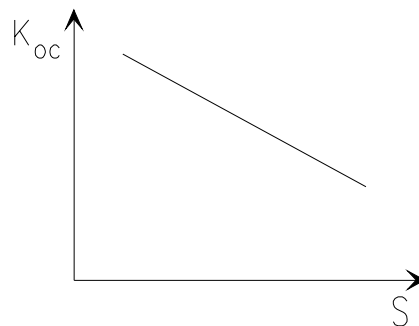
⑥ Solubility S

S has direct relationship with K_{oc} (CJN Table. 7. 2)

$$K_{oc} = f_n(S)$$

S → literature.

$$S \rightarrow K_{oc} \rightarrow K_d = f_{oc} \cdot K_{oc} \Rightarrow R$$



(예제)

다음과 같은 조건을 가진 토양에 대한 클로로폼, 클로로벤젠과 DDT의 지하수의 자연 상태의 흐름에 대한 지체계수(R)을 비교하여라.

조건 : 단위중량 $\rho_b = 2 \text{ Kg/L}$, $f_{oc} = 0.01$, $n = 0.2$

풀이

$K_d = f_{oc} \cdot K_{oc} \Rightarrow R = 1 + \rho_b/n K_d$ 을 활용

$K_{oc} = 0.63(K_{ow})$ (일련의 방향족화합물과 염화탄화수소에 대한 Karickhoff 등(1979)의 식 이용)

문헌으로부터,

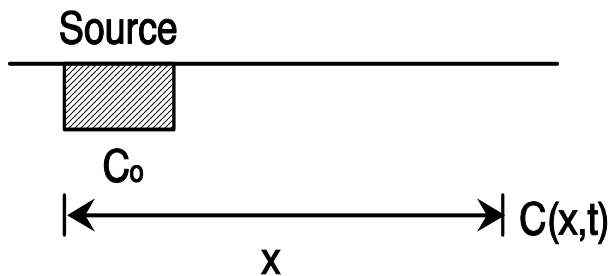
화합물	log Kow	Kow	Koc	Kd	R
chloroform	1.97	93.3	58.8	0.588	6.88
chlorobenzene	2.84	692	436	4.36	44.6
DDT	6.91	8.13×10^6	5.12×10^6	5.12×10^4	5.12×10^5

이 계산으로부터 클로로폼은 계수 약 7만큼, 클로로벤젠은 45만큼, DDT는 계수 약 50,000만큼 지하수 보다 느리게 이동할 것이라는 사실을 알 수 있다. 이 세 화합물들 중에서 클로로폼은 지하수 흐름을 따라 훨씬 빠르게 이동하며, 반면 DDT는 그 오염원으로부터 멀리 이동하지 않을 것으로 예상된다.

※ Contaminant Transport Mechanism (포화대 내의 이송)

지반내의 오염물질 이송에 영향을 주는 요소

- 지반의 수리지질학적 조건 (hydrogeological condition)
- 오염물질 자체의 특성 (유기화합물) (Characteristic of organic compounds)

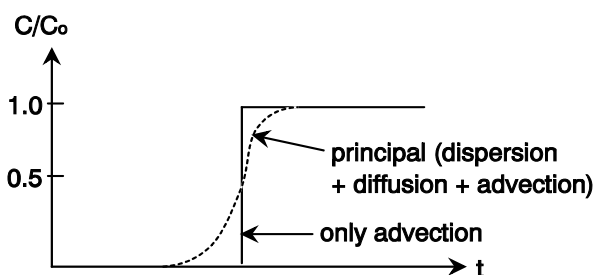


Main Process

- ① Advection 수송
- ② Diffusion 확산
- ③ Dispersion 소산
- ④ Adsorption 흡착
- ⑤ Biodegradation 생분해
- ⑥ Chemical reaction 화학반응

① Advection :

Movement of contaminants along with flowing GW at the Seepage velocity. (average linear velocity). in porous media



Advection에 의한 오염물질의 이동량

Mass flux (F)

단위시간당 단위면적을 통과한 오염물질의 양

$$F = v_s \cdot n C \quad [M/L^2/T] \quad \text{----- (1)}$$

advection transport Eq.

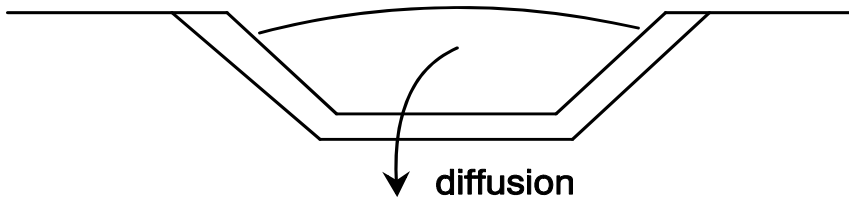
$$\frac{\partial C}{\partial t} = -v_s \frac{\partial C}{\partial x} \quad \text{----- (2)}$$

② Diffusion (확산)

- Contaminant spreading due to concentration gradients.

higher C -----> lower C

$$i = 0$$



- Governing Process for low velocity flow like in clay media
- Diffusion에 의한 오염물질의 이동량 (Fick;s first law)

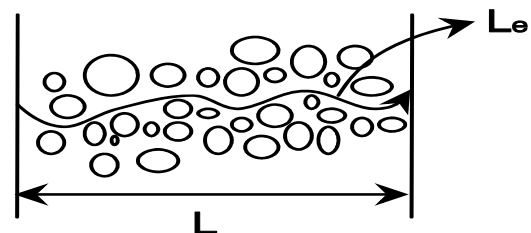
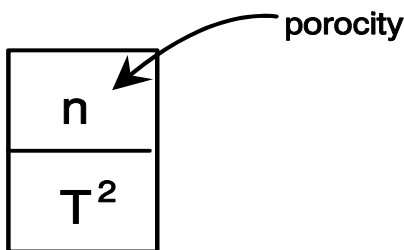
$$F = -D_d \frac{\partial C}{\partial x} \quad \text{----- (3)}$$

D_d : Diffusion coeff. (L^2/T)

effective diffusion coeff. $D^* = wD_d$ ----- (5)

D^* : 지반내의 조건 (입자 존재) 고려

w : tortuosity coeff. = $\frac{n}{T^2}$, $T = \frac{L_e}{L}$: tortuosity



$$0.01 < w < 0.5$$

↑ ↑
well graded uniform

D_d : $1 \times 10^{-9} \sim 2 \times 10^{-9} \text{ m}^2/\text{s}$ at 25°C

5°C 이하이면 50% 값 정도 사용

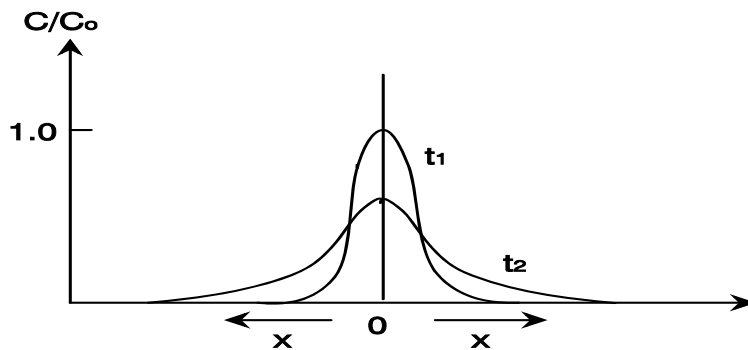
- For System where concentration are change with times, Fick's Second law applies

$$\frac{\partial C}{\partial t} = D_d \frac{\partial^2 C}{\partial x^2} \quad [M/L^3/T] \quad \text{----- (4)}$$

$$C(x, t) = C_o \operatorname{erfc} \left(\frac{X}{2\sqrt{D^*t}} \right) \quad \text{----- (6) : 식 (4)의}$$

해

(Only diffusion)



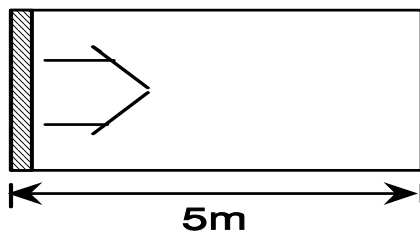
C : the concentration at distance X form the source at times t since diffusion begins.

C_o : initial concentration

ex) $D_d = 1 \times 10^{-9} \text{ m}^2/\text{s}$, $w = 0.5$

$\therefore D^* = 5 \times 10^{-10} \text{ m}^2/\text{s}$

Source



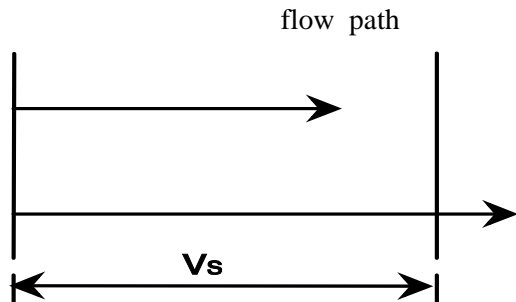
Find C / C_o at 5m after 100yrs of diffusion

sol)

$$\begin{aligned} C / C_o &= \operatorname{erfc} \left(\frac{5}{2\sqrt{5 \times 10^{-10} \times 3.15 \times 10^9}} \right) \\ &= \operatorname{erfc}(1.99) \\ &= 0.005 \end{aligned}$$

③ Dispersion 소산

1. Cause by heterogeneous in medium
creates variations in flow velocity



why?

- ① pore size
- ② path length
- ③ Friction in pores



Cause mixing of contaminants with GW → dilution
Called "Mechanical dispersion"

$\alpha_L v_s$ ← flow path와 같은 방향 (longitudinal dispersion 횡방향)

$\alpha_T v_s$ ← (transverse dispersion)

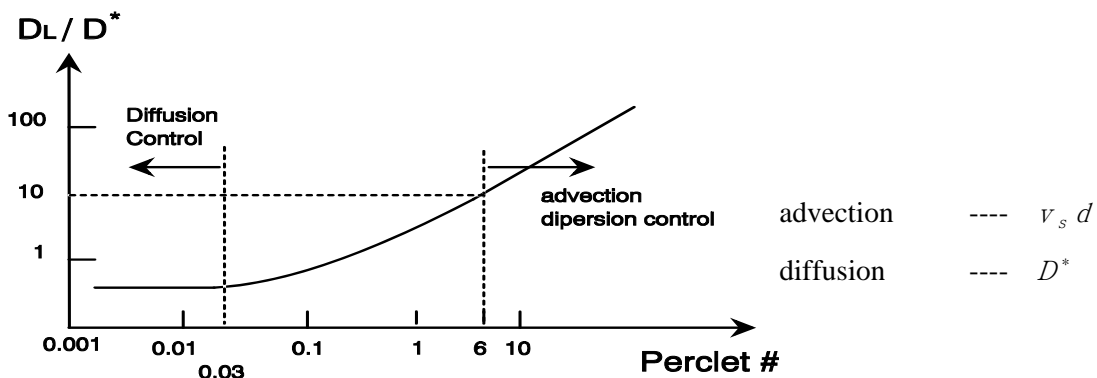
(α : dispersivity [L])

Hydrodynamic Dispersion

$$D_L = \alpha_L v_s + D^* \quad \text{----- (7)}$$

$$D_T = \alpha_T v_s + D^*$$

$$D_L \gg D_T$$



Peclet # : defines the ratio if transport by advection to rate of transport by diffusion

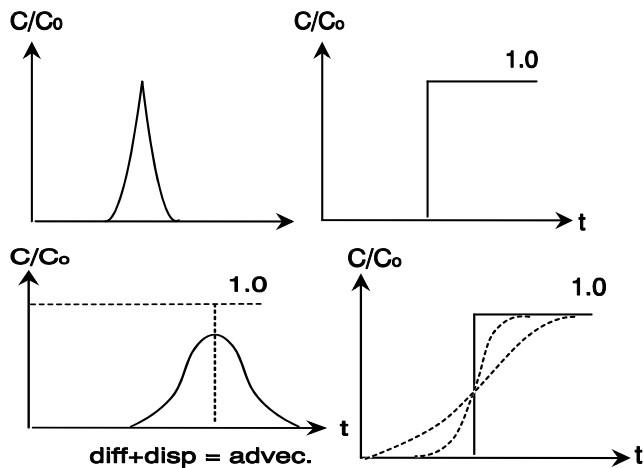
Flux by diagram

$$F + n D_L \frac{\partial C}{\partial x} \quad [M/L^2/T] \quad \text{----- (8)}$$

※ Types of Source

Instantaneous / Slug Source : Short period of time, 시간에 따른 mass의 변화는 없다

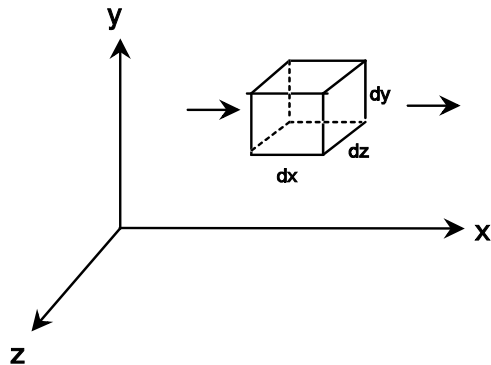
Continuous Source : Long period of time, mass change with time



Advection - Dispersion Eq. 오염물질의 지하수내에서의 이동 방정식
(Diffusion 첨가된 것)

Assumptions

- ① Homogeneous / isotropic
- ② Steady-state flow
- ③ Darcy's law applicable
- ④ Saturated
- ⑤ Contaminant uniformly dissolved
- ⑥ Contaminant conservative (nonreaction)
- ⑦ Water incompressible



Law of Mass conservation

In -Out = net chang

(accumulation)

F_x (Transport by Advection)

$$n C v_{sx} dA \quad [M/T]$$

F_x (Transport by Dispersion)

$$n D_x \frac{\partial C}{\partial X} dA \quad [M/T] \quad (D_x = \alpha_x v_{sx} + D^*)$$

$$\therefore F_x = n C v_{sx} - n D_x \frac{\partial C}{\partial X}$$

$$F_y = n C v_{sy} - n D_y \frac{\partial C}{\partial Y}$$

$$F_z = n C v_{sz} - n D_z \frac{\partial C}{\partial Z}$$

Total amount of contaminant entering the element

$$F_x dydz + F_y dzdx + F_z dxdy$$

Total amount of contaminant leaving the element

$$(F_x + \frac{\partial F_x}{\partial X}) dydz + (F_y + \frac{\partial F_y}{\partial Y}) dxdz + (F_z + \frac{\partial F_z}{\partial Z}) dxdy$$

In- Out

$$= - \left(\frac{\partial F_x}{\partial X} + \frac{\partial F_y}{\partial Y} + \frac{\partial F_z}{\partial Z} \right) dzdydz = \text{the rate of mass change in element}$$

$$= n \frac{\partial e}{\partial t} dxdydz$$

$$\therefore \frac{\partial F_x}{\partial X} + \frac{\partial F_y}{\partial Y} + \frac{\partial F_z}{\partial Z} = - n \frac{\partial C}{\partial t}$$

$$D_x \frac{\partial^2 C}{\partial X^2} + D_y \frac{\partial^2 C}{\partial Y^2} + D_z \frac{\partial^2 C}{\partial Z^2}$$

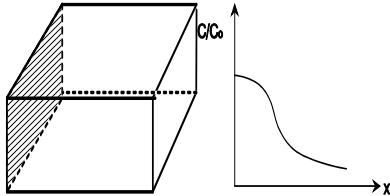
$$- \left[v_{sx} \frac{\partial C}{\partial x} + v_{sy} \frac{\partial C}{\partial y} + v_{sz} \frac{\partial C}{\partial z} \right] = \frac{dC}{dt}$$

(3D Ad-Disp Eq.)

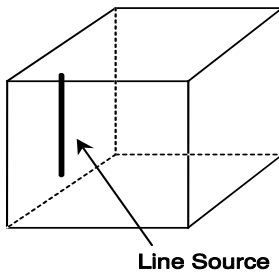
$$2D : D_x \frac{\partial^2 C}{\partial x^2} + D_y \frac{\partial^2 C}{\partial y^2} - \left[v_{sx} \frac{\partial C}{\partial x} + v_{sy} \frac{\partial C}{\partial y} \right] = \frac{dC}{dt}$$

$$\text{For 1-D : } D_x \frac{\partial^2 C}{\partial x^2} - v_{sx} \frac{\partial C}{\partial x} = \frac{dC}{dt}$$

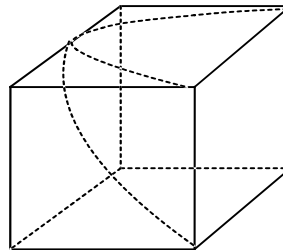
1-D (Plane source)



2-D



3-D (Point source)

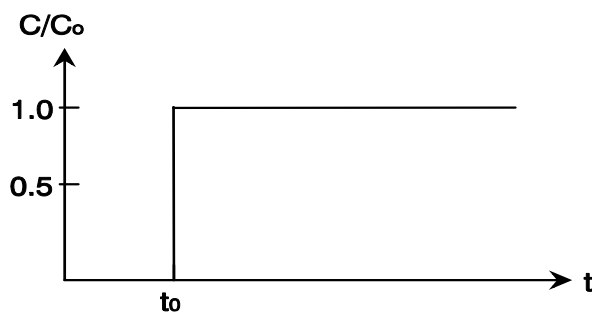


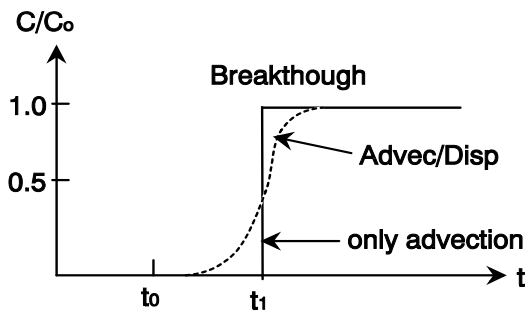
$$D_x \frac{\partial^2 C}{\partial x^2} - v_x \frac{\partial C}{\partial x} = \frac{dC}{dt} \quad \text{--> Laplace formation}$$

i) continuous source

ii) slug source

1) continuous source





$$\frac{C(x, t)}{C_o} = \frac{1}{2} \left[\operatorname{erfc} \left(\frac{x - v_{sx}t}{2\sqrt{D_x t}} \right) + \exp \left(\frac{v_{sx}}{P_x} \right) \operatorname{erfc} \left(\frac{x + v_{sx}t}{2\sqrt{D_x t}} \right) \right]$$

1-D Continuous Source

adv. Disp. eq.

sol.

$$\frac{C(x, t)}{C_o} = \frac{1}{2} \left[\operatorname{erfc} \left(\frac{x - v_{sx}t}{2\sqrt{D_x t}} \right) \right]$$

ex) $x = 30\text{ cm}$ $C_o = 1\text{ mg/L}$ $v_{sx} = 10^{-2}\text{ cm/s}$
 $D_x = 0.018\text{ cm}^2/\text{s}$ $t = 45\text{ min (27000 sec)}$ $C = ?$

ex2)

FIG

$C_o=1000\text{mg/L}$ 1-D condition

$\alpha_L=7.5\text{m}$ ($\alpha_L=10\alpha_D$)

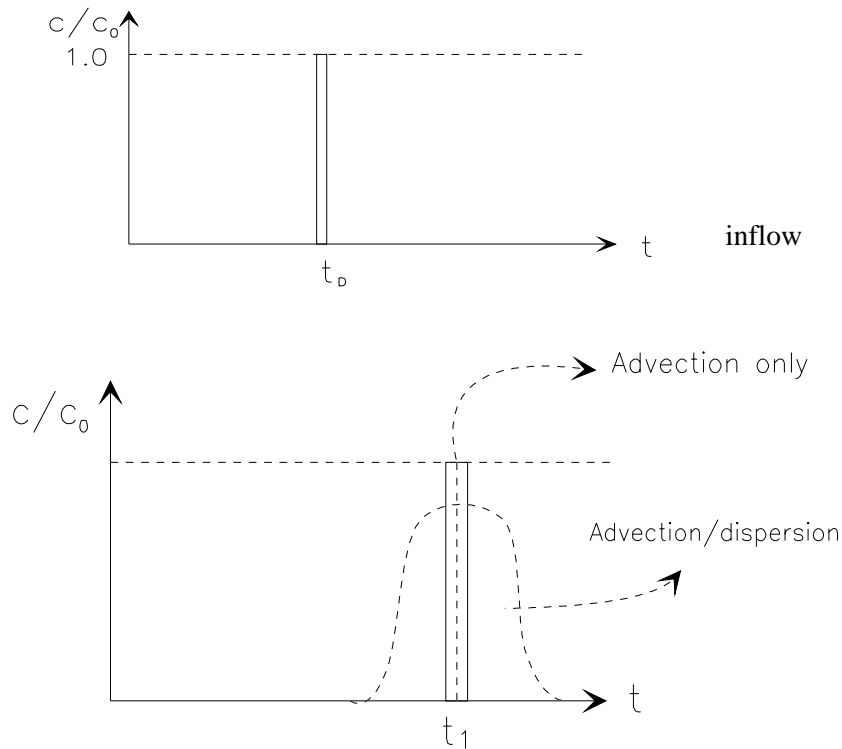
$n=0.1$

$i=0.04\text{m/m}$

$k=2.15\text{m/day}$

$c=100\text{mg/L}$ 일 때 $t=?$

2) Instantaneous Source(slug)



1-D slug source

adv-Dsp.

eq. soil

$$C = \frac{M}{(4\pi D_x t)^{1/2}} \exp\left(-\frac{(x - V_{sx}t)^2}{4D_x t}\right)$$

ex3) $M=10 \text{ mg/cm}^2$
 $x=1\text{m}$

$D_x=10^{-5} \text{ cm}^2/\text{s}$
 $c=8.92 \text{ mg/cm}^3$

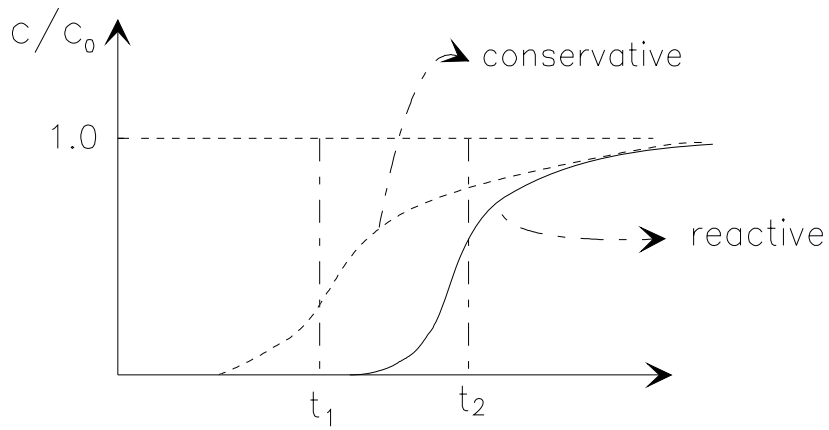
$V_{sx}=10^{-4} \text{ cm/s}$

$t=10,000 \text{ sec}$

iii) adsorption effects

causes " Retardation" 지체

(Accumulation of dissolved substances on solid particles)



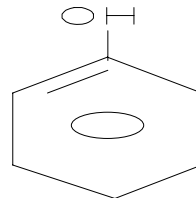
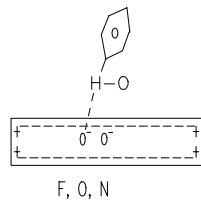
retardation

$$R = \frac{V_s}{V_{cont}}$$

ex) R=1 conservative

R=2~1000

보통 (2~10)



Hydrogen-bonding
Natural organic matter

흡착

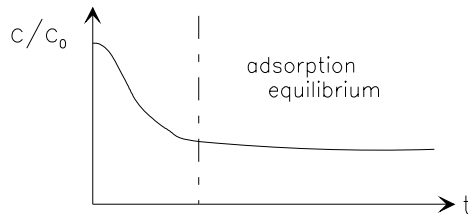
(NOM) 0.5~4%

Van-der Waals force
Chemical bonding
Chelation

K_{ow}

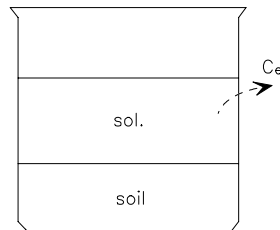
Frendlich Isothem Eq.

$$S = K_d C_e^n$$



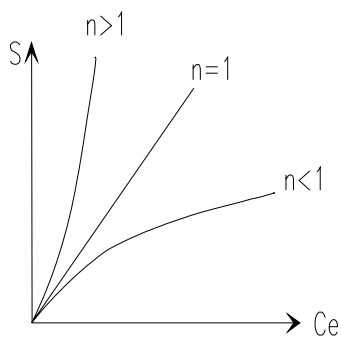
$$S = \frac{\text{mass of cont. absorbed}}{\text{dry mass of soil particles}} \quad \left(\frac{\text{mg}}{\text{Kg}} \right)$$

$$C_e = \text{equilibrium concentration in solution} \quad \left(\frac{\text{mg}}{\text{L}} \right)$$



K_d : distribution coeff. (depends on hydrophobicity of cont. of organic compounds and NOM in soil)

n : experimently drived coeff.



F.I.C.



Adsorption

$$S = K_d C_e^n \quad \text{Freundlich Isocherm eq.}$$

1-D Ad-Disp. eq.

$$D_x \frac{\partial^2 C}{\partial X^2} - V_{sx} \frac{\partial C}{\partial X} - \frac{\rho_b}{n} \frac{\partial S}{\partial t} = \frac{\partial C}{\partial t}$$

↑
흡착 term

where) ρ_b : bulk density
n : porosity

$$- \frac{\rho_b}{n} \frac{\partial S}{\partial t} = - \rho_b \frac{dS}{dC} \frac{\partial C}{\partial t}$$

Freundlich isotherm coeff n=1, linear isotherm

$$\frac{dS}{dC} = K_d$$

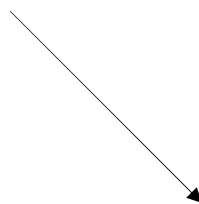
$$\therefore - \frac{\rho_b}{n} K_d \frac{\partial C}{\partial t}$$

$$\therefore D_x \frac{\partial^2 C}{\partial X^2} - V_{sx} \frac{\partial C}{\partial X} = \left(\frac{1 + \rho_b}{n} K_d \right) \frac{\partial C}{\partial t} = R \frac{\partial C}{\partial t}$$

$$R = 1 + \frac{\rho_b}{n} K_d = \frac{V_{GW}}{V_{cont.}}$$

$$\frac{D_x}{R} \frac{\partial^2 C}{\partial X^2} - \frac{V_{sx}}{R} \frac{\partial C}{\partial X} = \frac{\partial C}{\partial t}$$

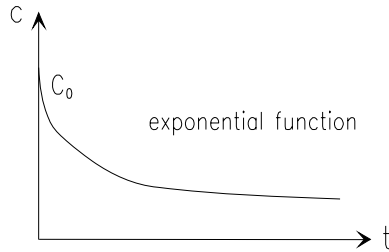
$$C(x, t) = \frac{C_o}{2} [\operatorname{erfc}(Rx - V_{sx}t)] \quad \text{continuous source}$$



adsorption을 고려한 advection-disp. eq

iv) Biological decay (Radioactive Material)

First-order decay



$$\frac{dC}{dt} = -\lambda C \quad \text{where) } \lambda : \text{ first order decay const.}$$

$$C_0 \sim C$$

$$0 \sim t$$

$$\frac{C}{C_0} = e^{-\lambda t}$$

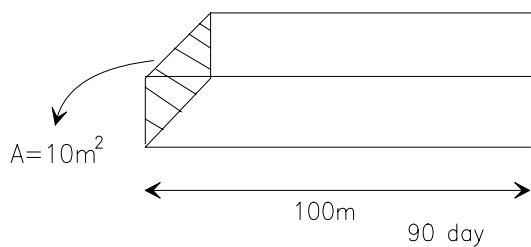
$$t_{\frac{1}{2}} = \frac{\ln 2}{\lambda} \quad \longrightarrow \quad \text{반감기}$$

$$D_x \frac{\partial^2 C}{\partial X^2} - V_{sx} \frac{\partial C}{\partial X} - \lambda C = \frac{\partial C}{\partial t}$$

$$\longrightarrow C(x, t) = \left[\frac{M}{\sqrt{4\pi D_x t}} \exp\left(-\frac{(X - V_{st}t)^2}{4D_x t}\right) \right] \times \exp(-\lambda t) :$$

slug source

ex) 1kg ¹³⁷Cs (half life 33yr) (P.132 6-1, (b))



$$D_x = 6.45 \text{ m}^2/\text{day}$$

$$\lambda = \frac{\ln 2}{t \cdot \frac{1}{2}} = \frac{\ln 2}{33 \times 365} = 5.755 \times 10^{-5} \text{ day}^{-1}$$

$$\therefore C(100, 90) = 10^6 \frac{mg/10m^2}{\sqrt{4\pi \times 6.45}}$$

2 - D

(1) For slug source

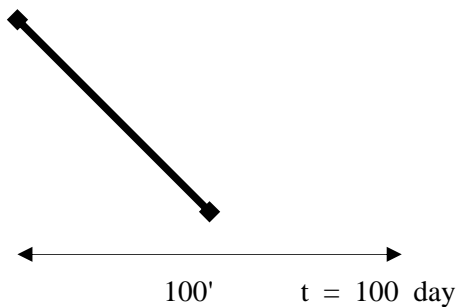
1) $-\lambda c$ 가 없는 경우

$$C(x, y, t) = C_o \frac{A}{4\pi t (D_x D_y)^{1/2}} \exp \left[-\frac{(X - V_{xs} t)^2}{4D_x t} - \frac{y^2}{4D_y t} \right] \quad V_h \gg V_v$$

2) $-\lambda c$ 가 있는 경우

$$C(x, y, t) = C_o \frac{A}{4\pi t (D_x D_y)^{1/2}} \exp \left[-\lambda t + \frac{y^2}{4D_y t} \right]$$

ex) Source



$$V_{sx} = 1 \text{ ft/day} \quad , \quad \lambda = 0.05 \text{ day}^{-1} \quad , \quad D_x = D_y = 10^{-4} \text{ ft}^2/\text{day} \quad ,$$

$$C_o A = 100 \text{ g/ft} \quad ,$$

i) 경우: $C = 795.8 \text{ g/ft}^3$

ii) 경우: $C = 5.4 \text{ g/ft}^3$

※ The dimensions of the plume are reflect to

x 방향의 크기 : $3 \sigma_x$

$$\sigma_x = (2D_x t)^{1/2} \quad : \quad \begin{array}{l} \text{Gaussian Distribution} \\ \text{Standard deviation} \end{array}$$

y 방향의 크기 : $3 \sigma_y$

$$\sigma_y = (2D_y t)^{1/2}$$

* $3\sigma_x$, $3\sigma_y$ represent two standard deviation away from the mean within which 99.7% of the contaminant mass is contained

(2) Continuous source (2-D)

$$C(x,y,t \rightarrow \infty) = \frac{C_o Q}{2\pi(\rho_x D_y)^{1/2}} \exp\left(-\frac{V_{sx} X}{2D_x}\right) K_0\left[\frac{V_{sx}^2}{4D_x} \left(\frac{X^2}{D_x} + \frac{y^2}{D_y}\right)^{1/2}\right]$$

Q : L^3/T : rate at which C_o is being injected.

K_0 : modified bessel function ($\approx \left(\frac{2r}{\pi B}\right)^{-1/2} \exp\left(-\frac{r}{B}\right)$)

$$B = \frac{2D_x}{V_{sx}} \quad , \quad r = \sqrt{\left(X^2 + \frac{D_y}{D_x} y^2\right)}$$

$$r = 1 + \frac{2B\lambda}{V_{sx}}$$

Chapter 7.