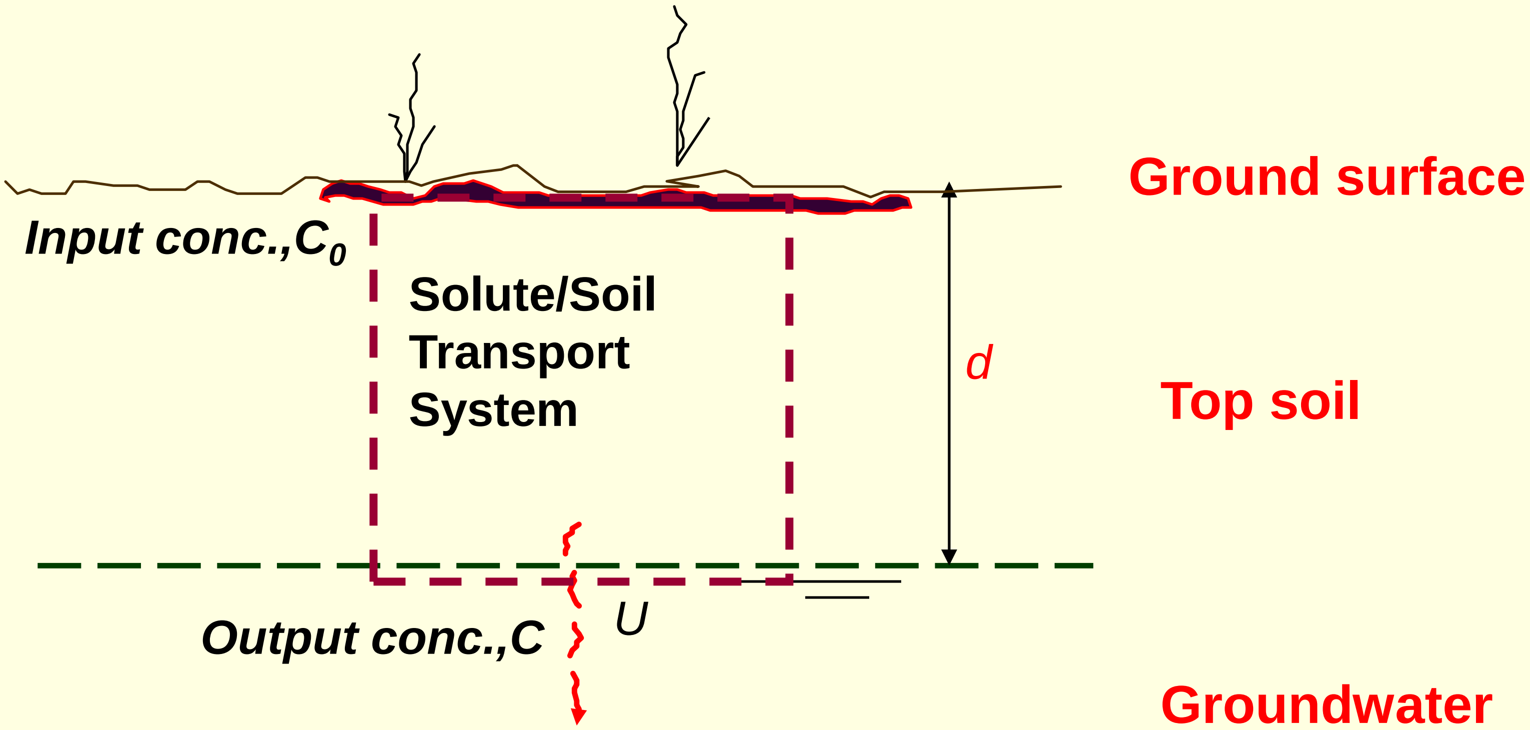
第五單元:土壤與地下水水質模式的建立和應用
Session 5: Formulation and Application of Soil and Groundwater Modeling

1. 污染物在土壤內傳輸的簡易和複雜模式
   Mathematical Modeling of Contaminant Transport in Upper Soils
2. 污染物在地下水內傳輸的簡易和複雜模式
   Mathematical Modeling of Contaminant Transport in Groundwater
3. 地下水污染的風險評估
   Groundwater Contamination and Risk Assessment
4. 實例分析和小組討論
   Tutorial Session and Group Discussion

1.污染物在土壤內傳輸的簡易和複雜模式

Mathematical Modeling of Contaminant Transport in Upper Soils



Darcy's Law and Continuity Equation for unsaturated Groundwater flow

Darcy's Law

$$\mathbf{q} = -\mathbf{K}(\boldsymbol{\theta}) - \mathbf{D}(\boldsymbol{\theta})\frac{\partial \boldsymbol{\theta}}{\partial \mathbf{z}}$$

One-dimensional Continuity Equation

$$\frac{\partial \boldsymbol{\theta}}{\partial \mathbf{t}} = -\frac{\partial \mathbf{q}}{\partial \mathbf{z}}$$

Flow Sub-model (Richard’s Equation)

- Unsaturated Groundwater flow equation is formulated by combining the continuity equation and the Darcy’s law

$$\frac{\partial \theta}{\partial t} = \frac{\partial [D(\theta)\frac{\partial \theta}{\partial z}]}{\partial z} + \frac{\partial K(\theta)}{\partial z}$$

Reference:

Philip,J.R.(1969). “Theory of infiltration” in Advances in Hydroscience (Chow, V.T., ed.), Academic Press.

Transport Sub-model (Advection-Dispersion Equation)

Continuity Equation

$$\frac{\partial \boldsymbol{\theta}}{\partial \mathbf{t}} = -\nabla \mathbf{F} - \mathbf{r}$$

Generally, mass flux in soils (F) is caused by advection and dispersion of solute only. With the Fick's law of diffusion,

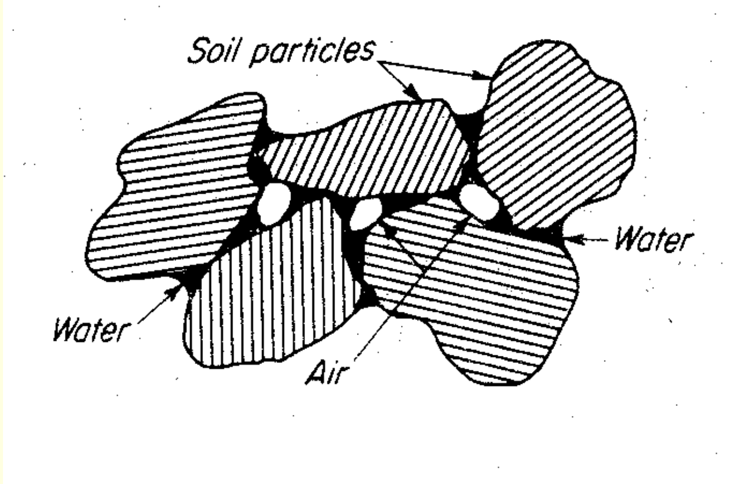
$$\mathbf{F} = -\mathbf{D}\nabla(\boldsymbol{\theta}\,\mathbf{C}) + \mathbf{V}(\boldsymbol{\theta}\,\mathbf{C})$$

Expression of Total Concentration in terms of Solute Concentration

- Assume linear isotherms, we have:
  - $S = K_D C$, K_D is adsorption coefficient
  - $C_G = K_H C$, K_H is Henry's Law constant

$$C_T = (\rho K_D + \theta + a K_H) C$$

C_T = Total resident concentration
C = Resident fluid concentration



Estimation of Adsorption Coefficient and its Estimation

Adsorption Coefficient K_D can be expressed as

$K_D = K_{oc} \cdot \%OC$

K_{oc} is the ratio of the amount of chemical adsorbed per unit weight of organic carbon(OC)in the soil to the the concentration of the chemical in soil solution at the equilibrium

Values of K_{oc} may range from 1 to 10,000,000(Lyman, et al.,1982)

Transport Sub-model

- A general 3-D model of solute transport in unsaturated soils (with a first-order reaction kinetics) is:

$$\frac{\partial}{\partial \mathbf{t}}(\boldsymbol{\rho}\mathbf{K}_{\mathbf{D}} + \boldsymbol{\theta} + \mathbf{aK}_{\mathbf{H}})\mathbf{C} =$$

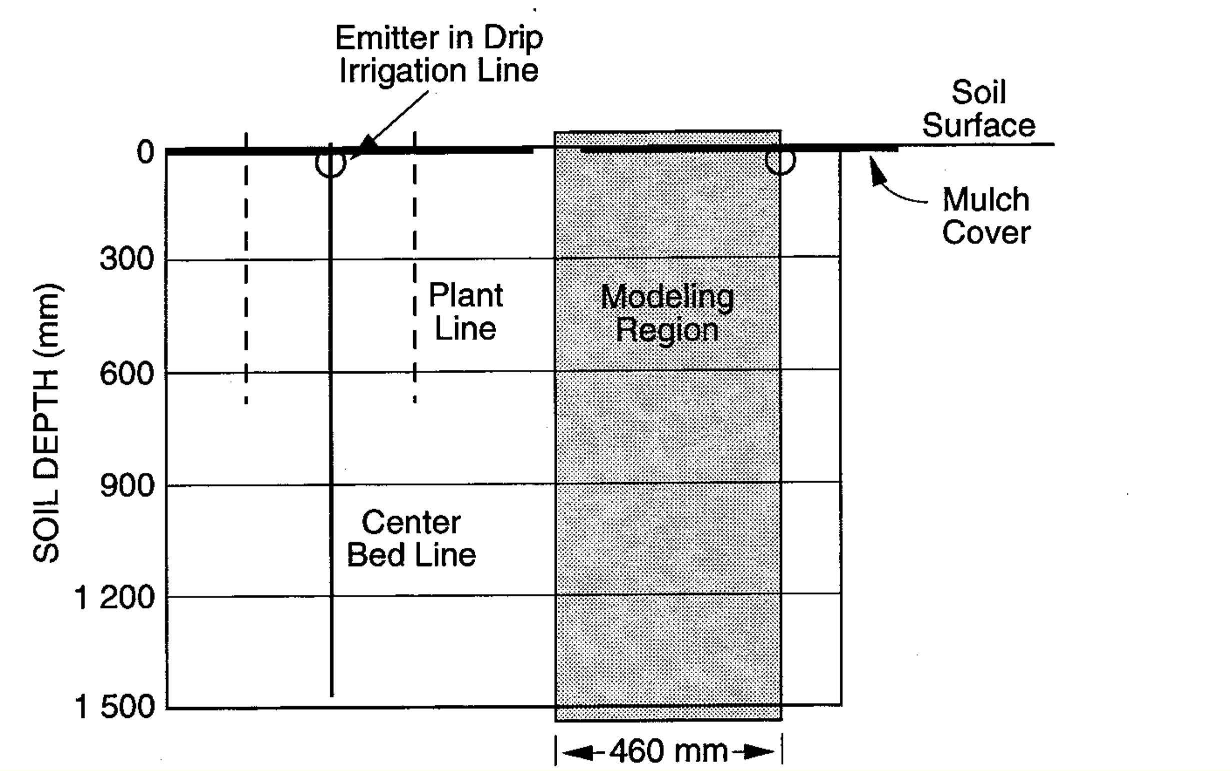
$$\nabla(\mathbf{D}\nabla\boldsymbol{\theta}\mathbf{C}) - \nabla\mathbf{V}(\boldsymbol{\theta}\mathbf{C}) - \mathbf{k}(\boldsymbol{\rho}\mathbf{K}_{\mathbf{D}} + \boldsymbol{\theta} + \mathbf{aK}_{\mathbf{H}})\mathbf{C}$$

Complex Models

(1) Three-Dimensional Flow and Transport Modeling

- To solve coupled 3-D flow and transport equations.
- Numerical schemes must be used.
- Example:
  - *Liu, C. C.K., Loague K., and Feng J. (1991).“Fluid flow and solute transport processes in unsaturated heterogeneous soils: Preliminary numerical experiments”, J. Contaminant Hydrology, 7:261-283.*

(2) Two-dimensional Transport Modeling

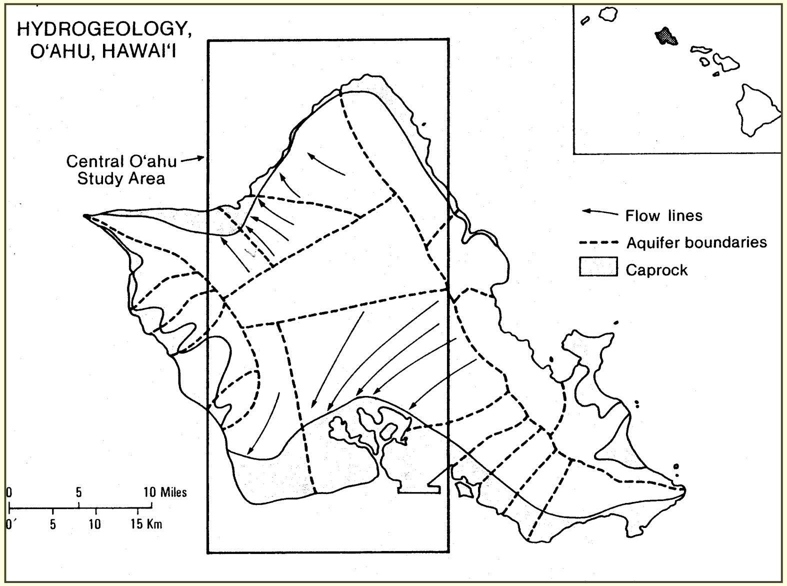


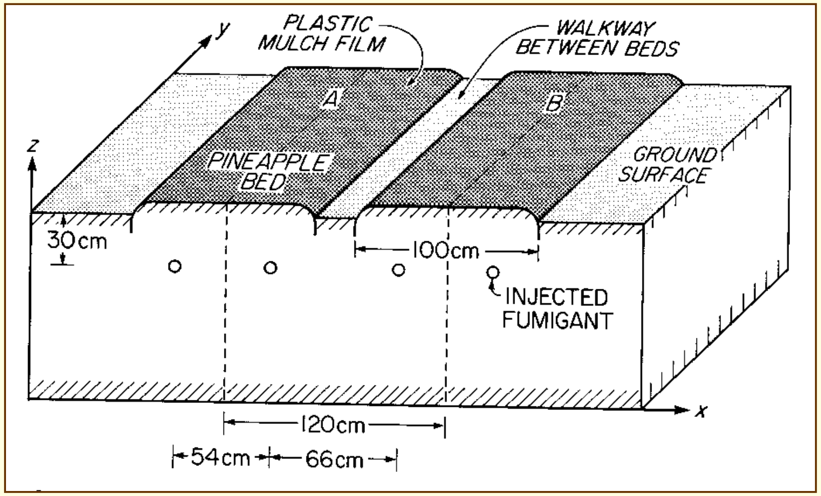
Reference:

Lin, P. Liu, C.C.K. and Green, R.E. (1995). "Simulation of 1,3-dichloropropene in topsoil with pseudo first-order kinetics", J. Contaminant Hydrology,18:307-317.

Agricultural Use of Volatile Organic Chemicals in Hawaii and Groundwater Contamination

The use of Soil Fumigants DBCP and EDB in Hawaii



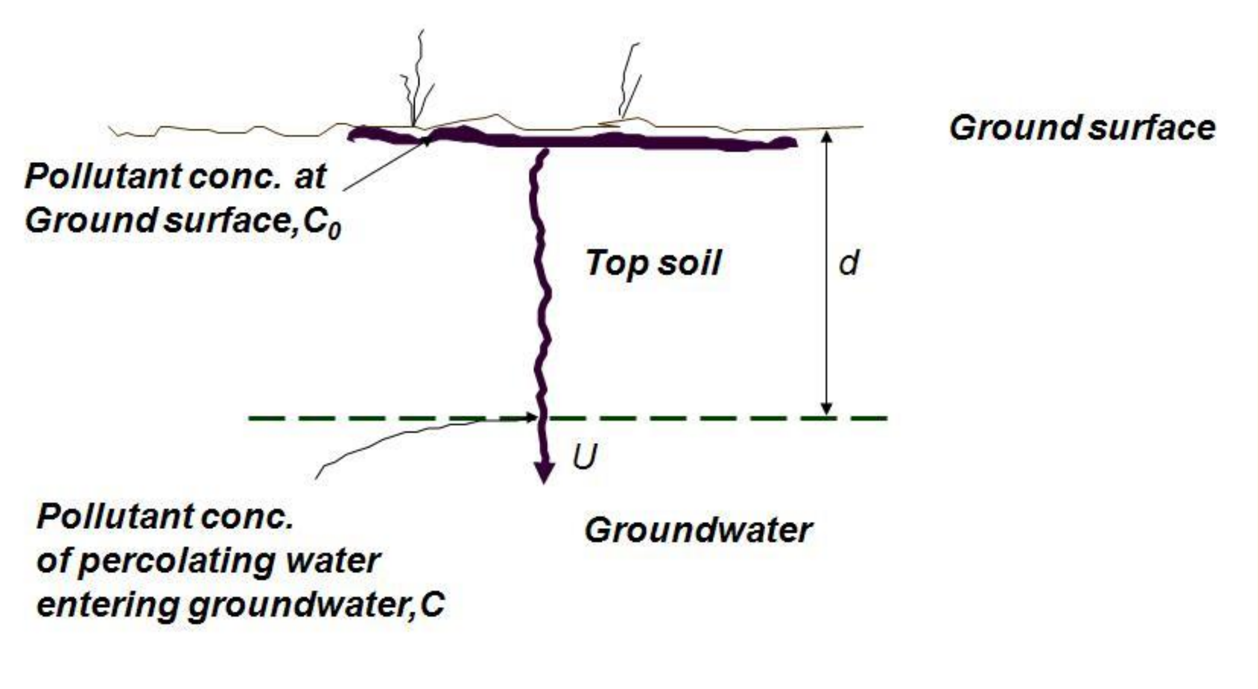


(3) One-Dimensional Flow and Transport Modeling
US EPA PRZM Model

- PRZM is a dynamic compartment model for use in simulating one-dimensional chemical movement in unsaturated soil systems with and below the plant root zone.
- PRZM allows the user to perform dynamic simulations of potentially toxic chemicals, particularly pesticides, that are applied to the soil or plant foliage.
- Reference:
  - *Loague, at el, (1989). "Simulation of organic chemical movement in Hawaii soils with PRZM",J. Pacific Science, 43:67-95.*

Simple Models

(1) 1-D Transport Model of Contaminants in Soil with Constant Percolating Velocity



Reference: *Liu, C.C.K. et al. (1983). Modeling analysis of pesticide (DBCP) transport in soils of Kunia area in Central Oahu, Phase 1 Completion Report to US EPA, Pacific Biomedical Research Center, University of Hawaii.*

Example: Application of 1-D Transport Model

A farmer took his spraying rig to a nearby pond to wash it out. When finished he dumps 10 cubic feet of rinse water back into the pond with an approximate concentration of 100 mg/L. This non-toxic spray has a very strong taste and can be detected at concentration above 0.001 mg/L. The following day his kids refused to drink their well water because of its unbearable taste. The local health officials are notified and brought in to identify the problem. After a thorough check they discover that the well was located a short distance from the contaminated ponds . The well is encased down to 40 feet and then screened in the underlying groundwater table. The health officials assured them that there was no worry because the inflow to the pond would eventually dilute the initial spray concentration. The pond is rectangular in shape (50 feet long, 10 feet wide, and 2 feet deep) and its inflow (equal to its outflow) is 5,000 ft^3/day.

What the famer wanted to know, however, was how long it take before the taste returned to normal. The health official could not say and a groundwater hydrologist consultant was called in. The consultant conducted a few tests and concluded that the contaminated water percolated vertically into the groundwater table with a constant seepage velocity, u = 15 ft/day and with a dispersion coefficient D = 2 ft^2/day/. Thus, the spray waste travels vertically towards the well and decreases in concentration by biodegradation in the soil. At the same time, the waste concentration in the pond decreases continuously with time by the fresh water inflow.

You , as an expert modeler, have been hired by the consultant to conduct a modeling analysis and to tell him how long the water will taste bad (i.e. C > 0.001 mg/L) under conditions of (1) adsorption coefficient is 0, and (2) adsorption coefficient is 0.5 cm^3/water/g soil.

(2) Index Model and Simplifying Assumptions

A simple index model of solute transport in soils can be formulated with the following assumptions:

1. Hydraulic behavior represented by an Ideal Plug Flow Reactor (PFR).
2. Attenuation effect represented by a first order decay.
3. Retardation effect of sorption kinetics represented by a linear isotherm.

Derivation of the Index Model of Contaminant Movement through Soils

$$\frac{\partial C}{\partial t} = D_R \frac{\partial^2}{\partial z^2} - V_R \frac{\partial C}{\partial z} - kC$$

Assume a steady – state plug flow

$$V_R \frac{dC}{dz} = -kC$$

$$C = C_0 \exp(-k \frac{z}{V_R})$$

And, $\frac{z}{V_R} = t_R =$ time of travel

Index Model of Contaminant Movement through Soils

Attenuation Factor,AF

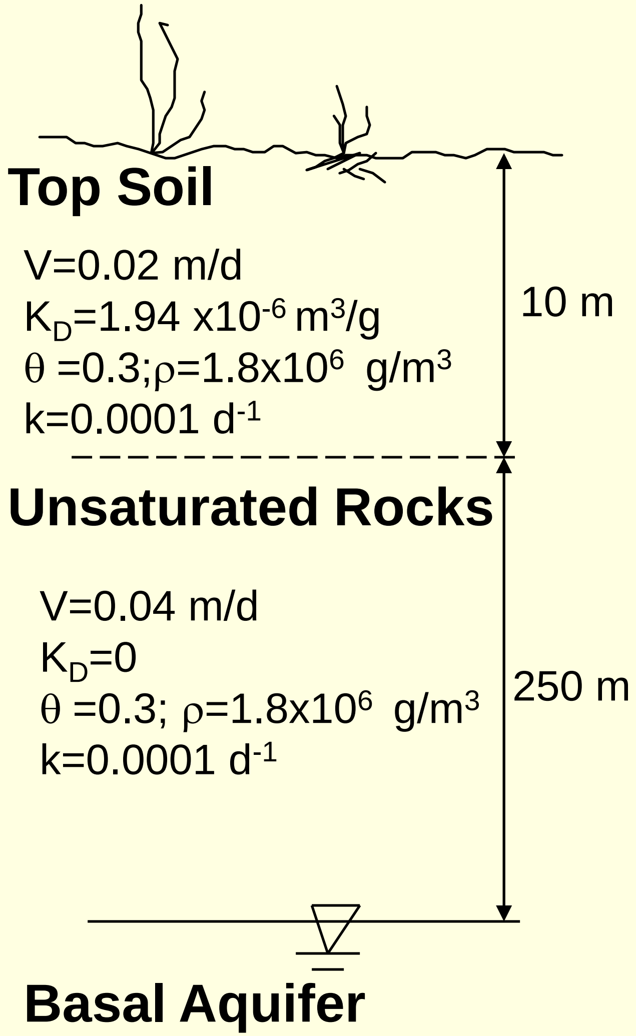
$$\mathbf{AF = \exp(-kt_r) = \exp[-k(d/V_R)]}$$

Retardation Factor,RF

$$\mathbf{RF = 1 + \frac{\rho K_D}{\theta}}$$

The reduction of pollutant concentration, $C/C_0 = AF$

Application of Index Model: (a) Transport of DBCP in soils in Central Oahu



How long dose it take for DBCP residue to pass through the top soil?

$RF = 1 + (\rho K_D)/\theta = 1+(1.8\text{x}10^6)(1.94\text{ x}10^{-6})=12.64$

$t_R = 10/(0.02/12.64)=6329$ d

How long dose it take for DBCP residue to reach the groundwater?

$t = t_R + 250/0.04 = 6329 + 250/0.04 = 12579$ d

Determine the attenuation factor.

$AF = C/C_0 = \exp(-k\ t) = \exp(-\ 0.0001\text{x}12579) = 0.284$

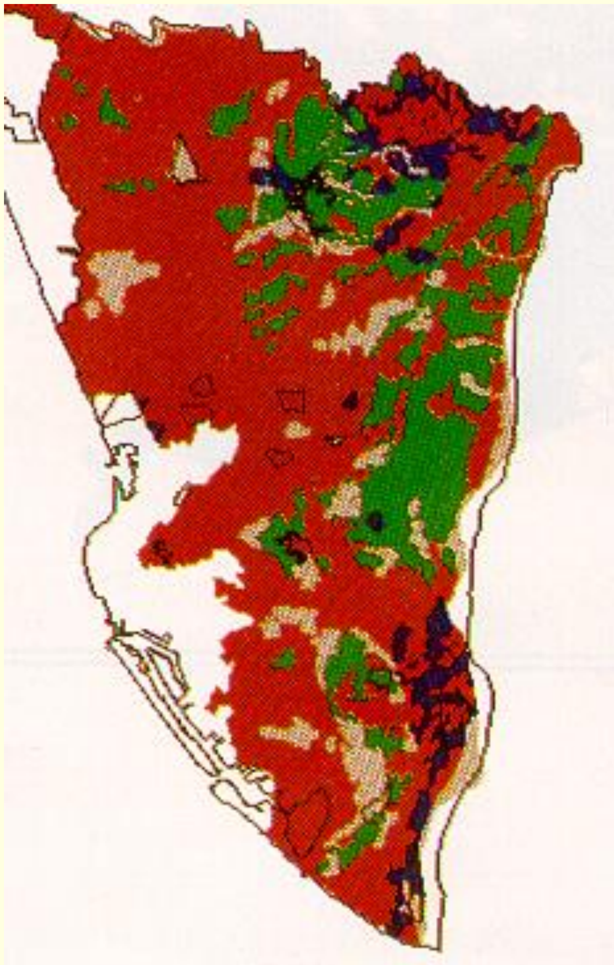
Application of Index Model: (b) Risk Assessment of Groundwater Contamination

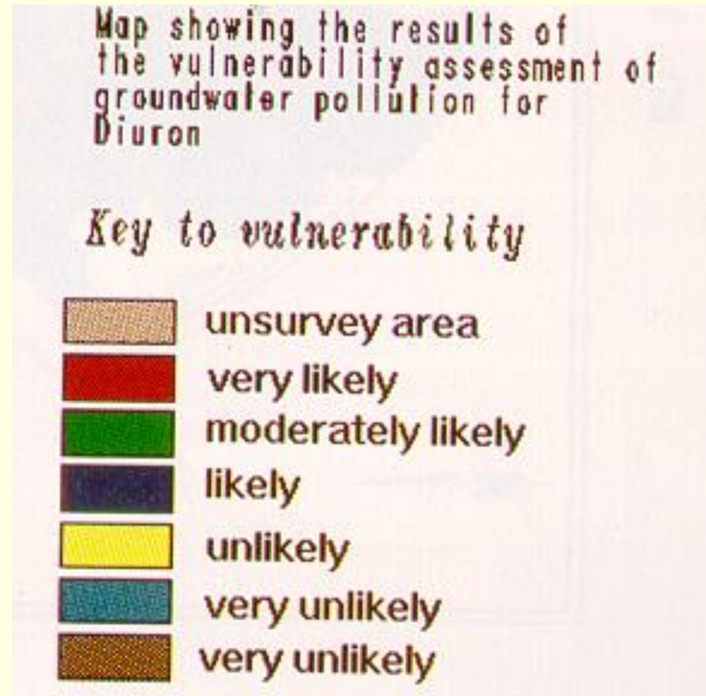
Index Model was used in a conjunctive application with geographic information system (GIS) to study the potential risk of chemicals in soils in the Kaohsiung Area, Southern Taiwan.

Reference

Liu, C.C.K.,Tsai,,J. and Chiang,L (1993) "Assessing groundwater contamination potential in the Kaohsiung area, southern Taiwan" Proceedings of CAAPCON, pp.7.65-7.68

Risk Assessment of Groundwater Contamination in Southern Taiwan by the Index Model and GIS System

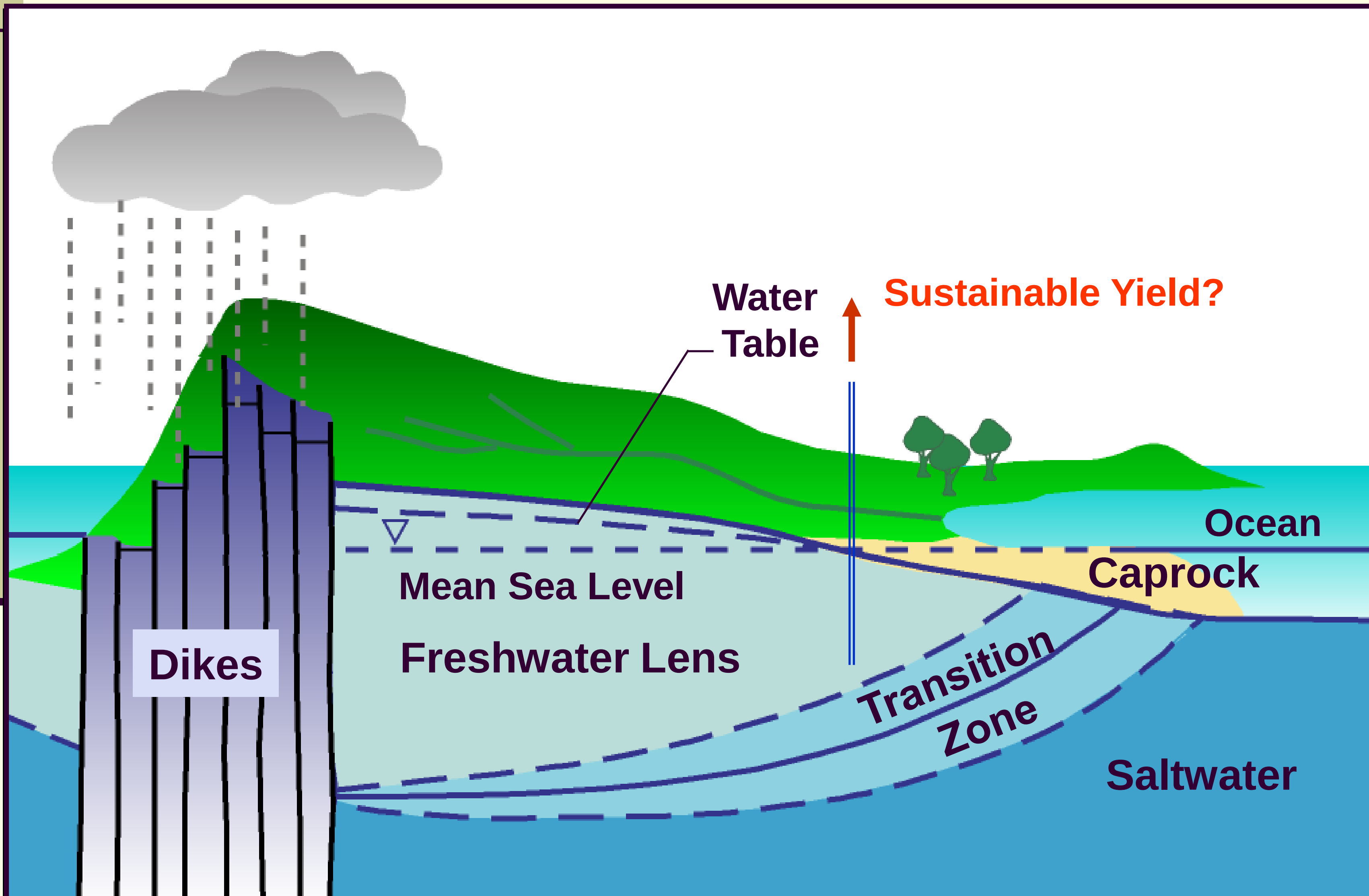




Note page 1

2.污染物在地下水內傳輸的簡易和複雜模式

Mathematical Modeling of Contaminant Transport in Groundwater



Complex 3-D Flow and Transport Modeling of Basal Aquifers

US Geological Survey's SUTRA Model

Flow Sub-model

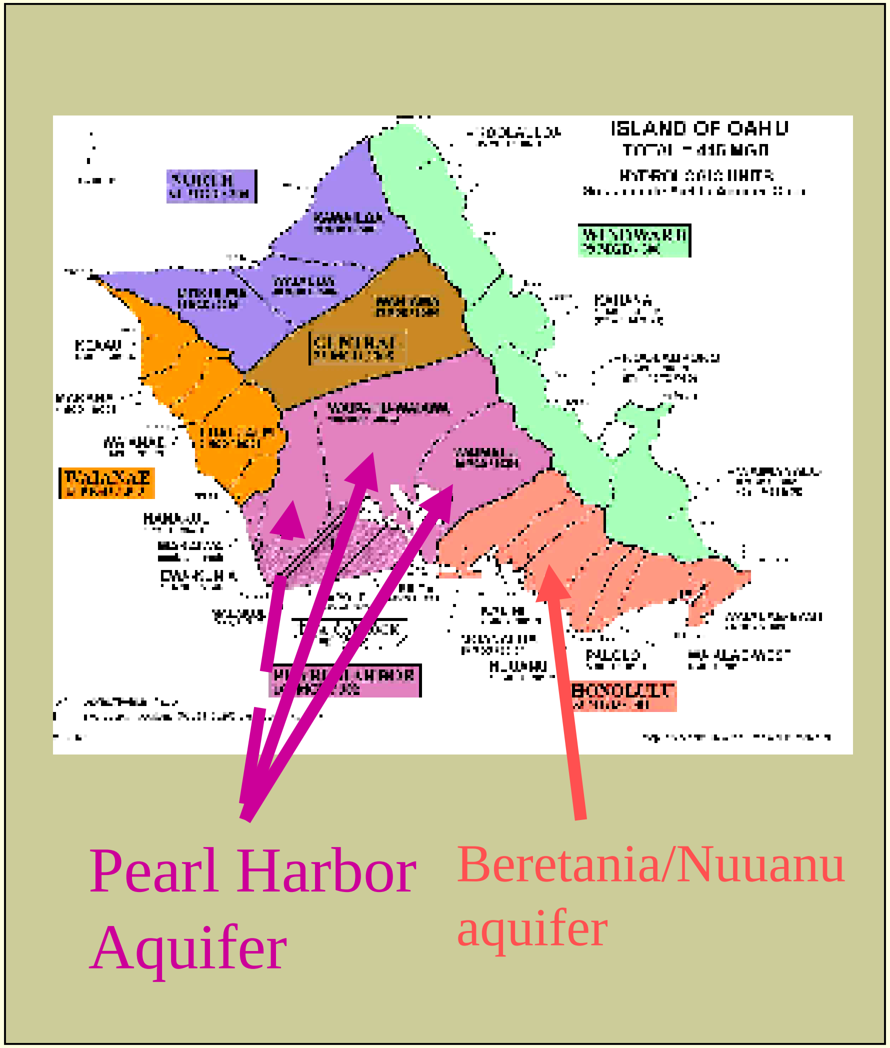
$$\left(S_w \rho S_{op} + \varepsilon \rho \frac{\partial S_w}{\partial p}\right)\frac{\partial p}{\partial t} + \left(\varepsilon S_w \frac{\partial \rho}{\partial C}\right)\frac{\partial C}{\partial t} - \vec{\nabla} \cdot \left[\left(\frac{\vec{\vec{k}}_{sm} k_r \rho}{\mu}\right) \cdot \left(\vec{\nabla} p - \vec{g}\right)\right] = Q_p(x, y, z, t)$$

Transport Sub-model

$$\frac{\partial\left(\varepsilon S_w \rho C\right)}{\partial t} = -\vec{\nabla} \cdot (\varepsilon S_w \rho \vec{v} C) + \vec{\nabla} \cdot \left[\varepsilon S_w \rho \left(D_m \vec{I} - \vec{\vec{D}}\right) \cdot \vec{\nabla} C\right] + Q_p(x, y, z, t) C^*(x, y, z)$$

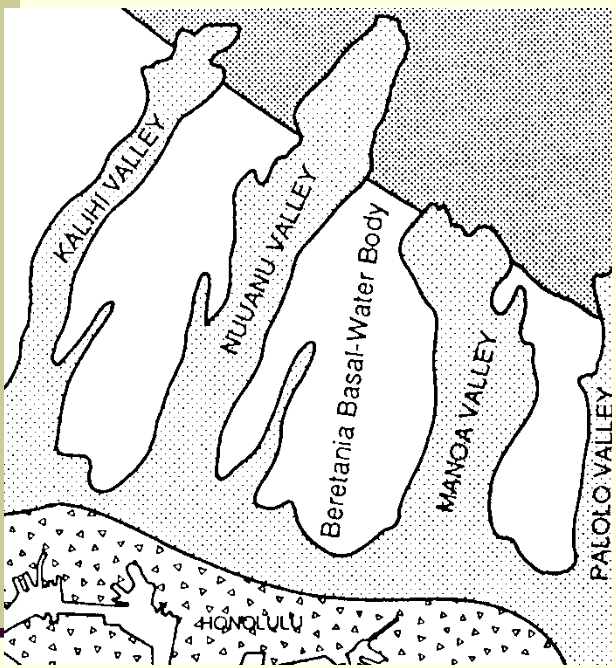
Reference: Liu, C.C.K., Loague, K.M. and Feng, J.S. 1991. Fluid Flow and Solute Transport in Unsaturated Heterogeneous Soils: Numerical Experiments, Journal of Contaminant Hydrology, 7:261-283

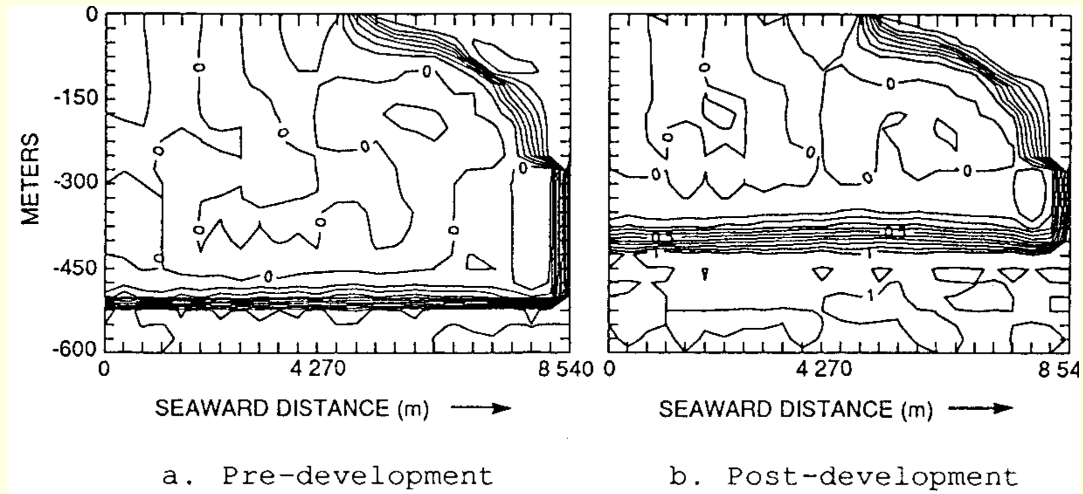
2D Groundwater Modeling of Southern Oahu Aquifer



- **2D Pearl Harbor Aquifer Flow Model (Liu, Lau and Mink, 1983).**
- **2D Beretania Aquifer Flow and Transport Model (Liu, Ewart, Huang, 1991).**

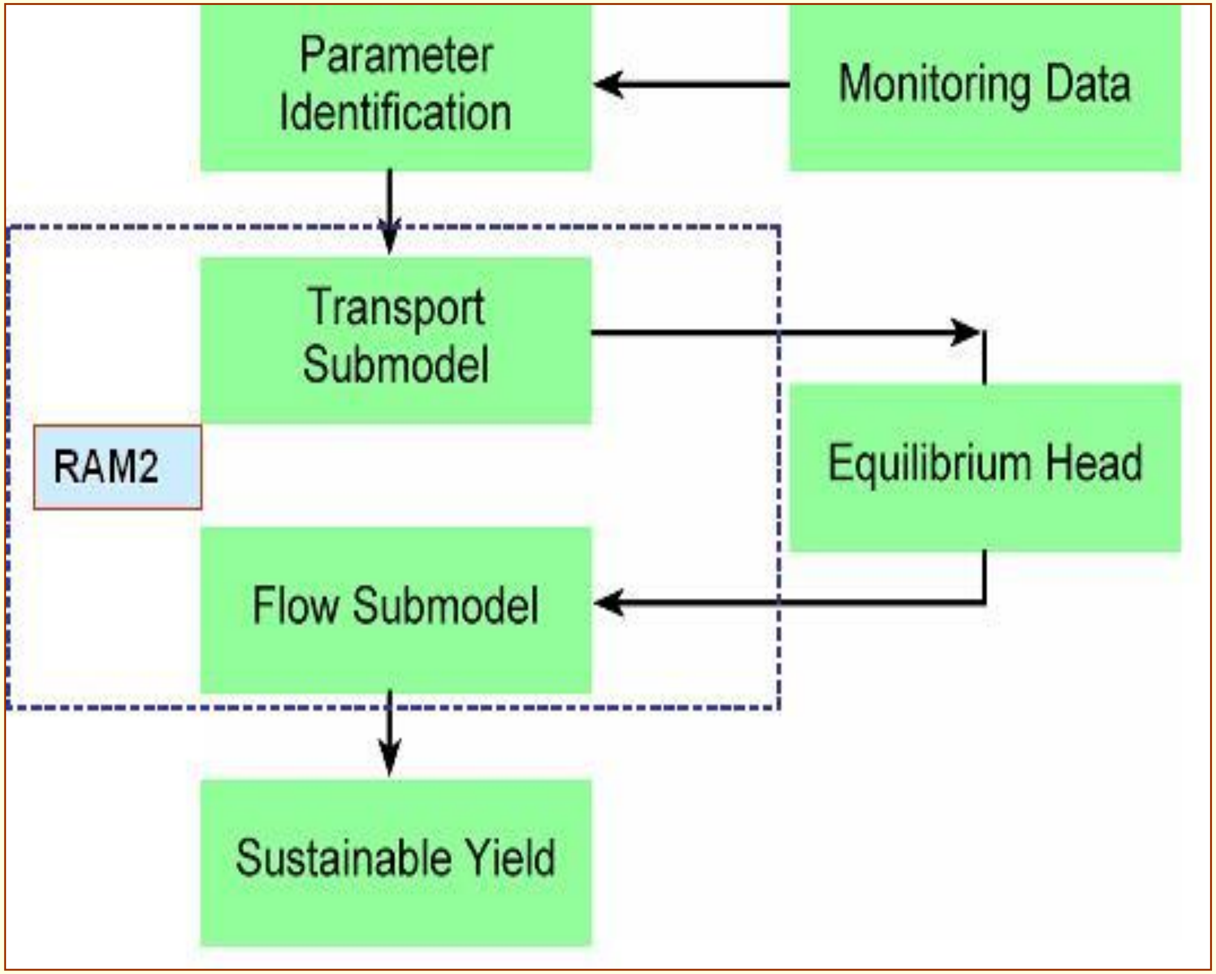
2D Flow and Transport Modeling of Beretania Aquifer, Oahu, Hawaii



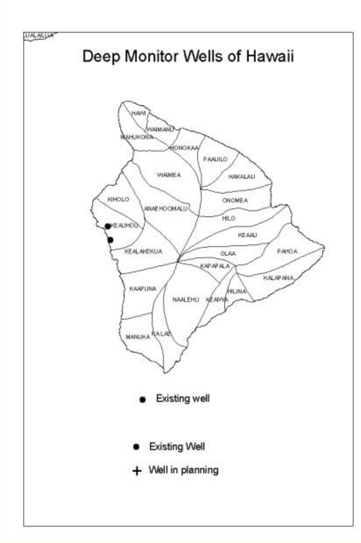


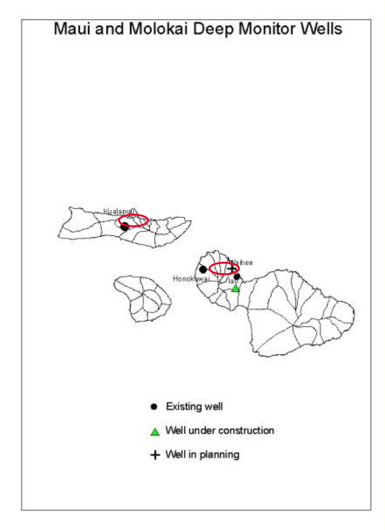
Reference: Liu, C.C.K., Ewart, C. and Huang, Q. 1991. Response of a Basal Water-Body to Forced Draft, In ASCE Book: <u>Ground Water in the Pacific Rim Countries</u>, J.Peters (ed.), American Society of Civil Engineers (ASCE), pp.36-42.

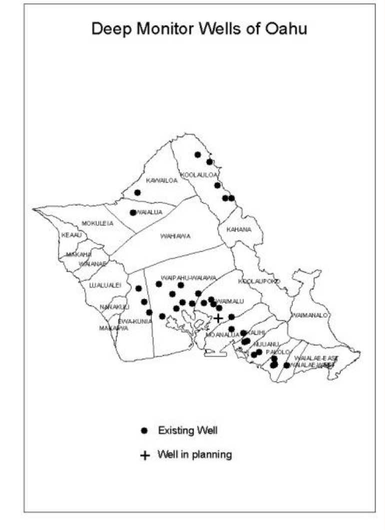
Estimating the Sustainable Yield of Hawaii Basal Aquifers by a Simple Model RAM2



Hawaii Basal Aquifers with Deep Monitoring Wells

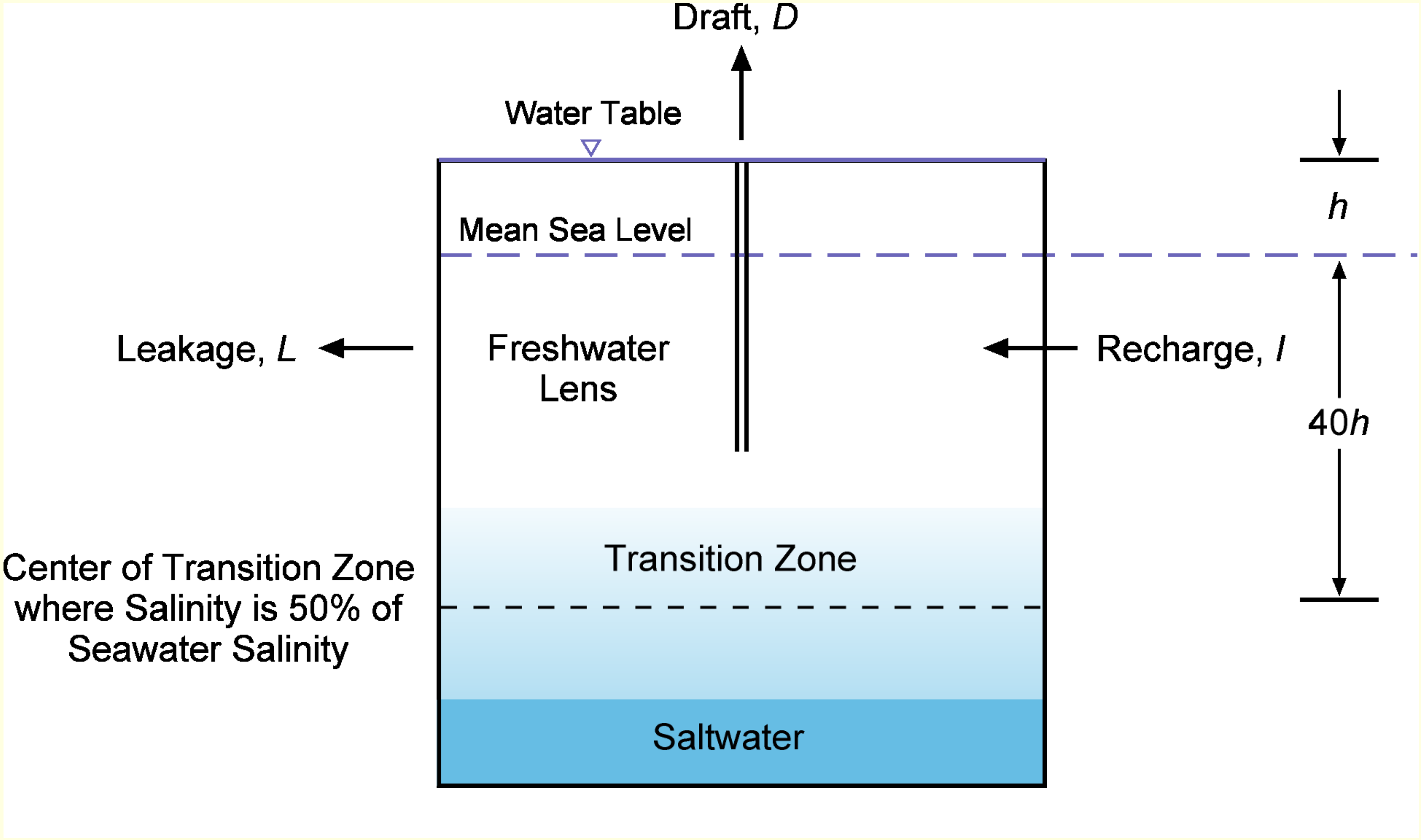




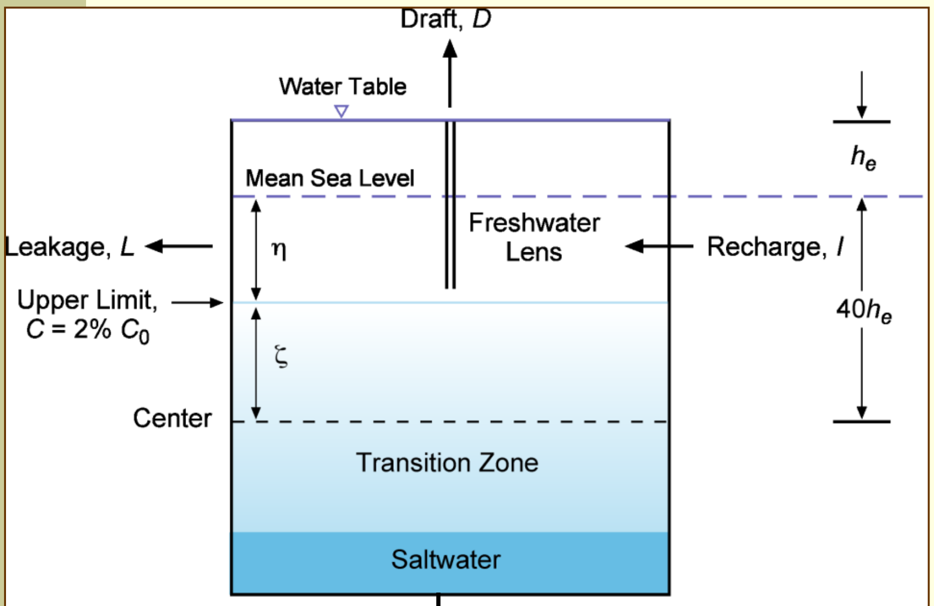


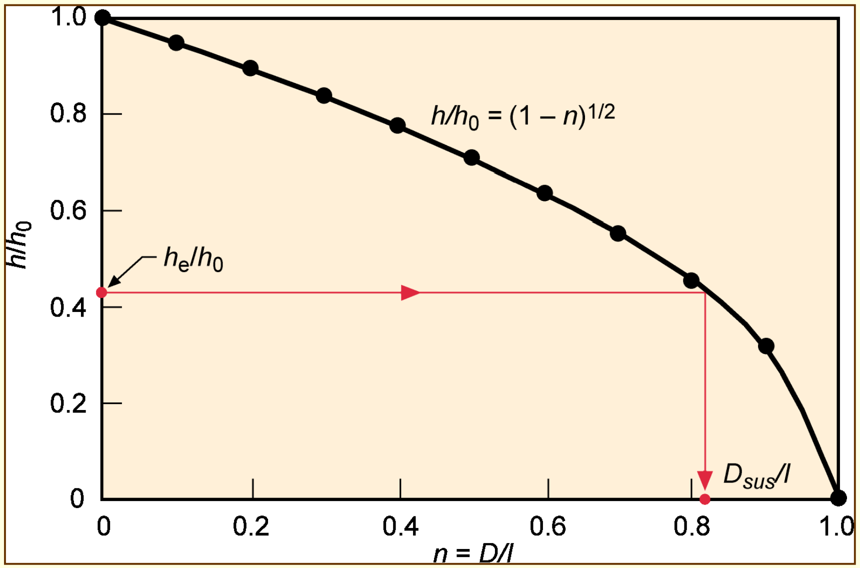
Island	Project Aquifers
Oahu	Ewa-Kunia, Waipahu-Waiawa, Waimalu, Moanalua, Kalihi, Nuuanu, Palolo, Waialae-West, Waialua, Kawailoa, Koolauloa,
Maui	Iao, Honokowai, Waihee (available within two years)
Hawaii	Keauhou,
Molokai	Kualapuu

Conceptual formulation of RAM2 model



Estimating the Sustainable Yield of a Basal Aquifer by RAM2

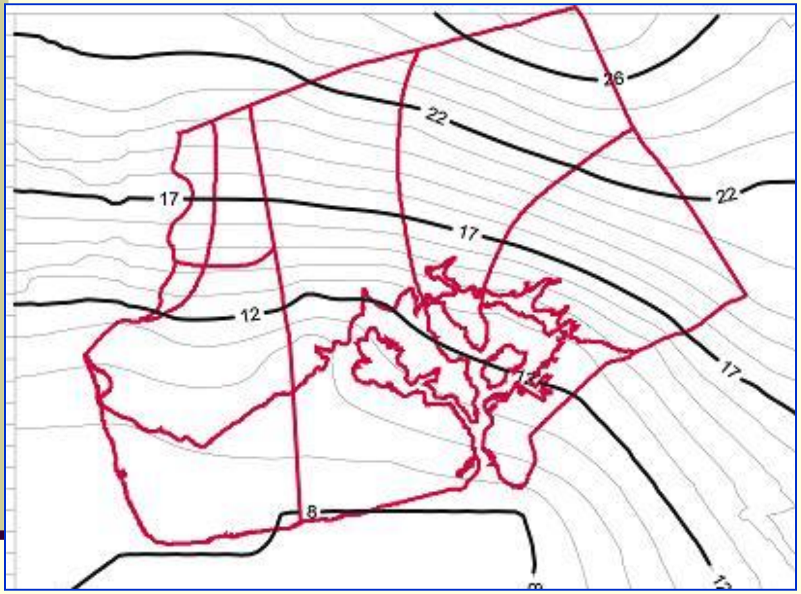


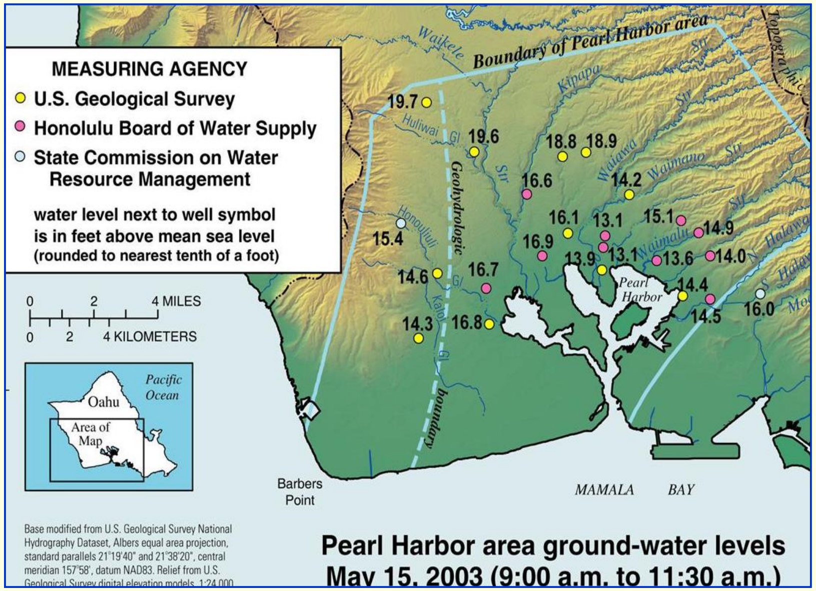


Estimate equilibrium hydraulic head, h_e

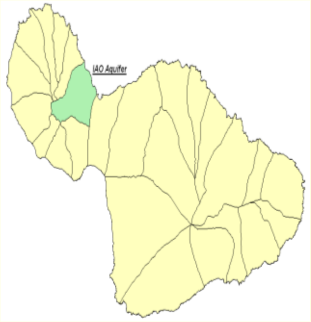
Estimate sustainable yield

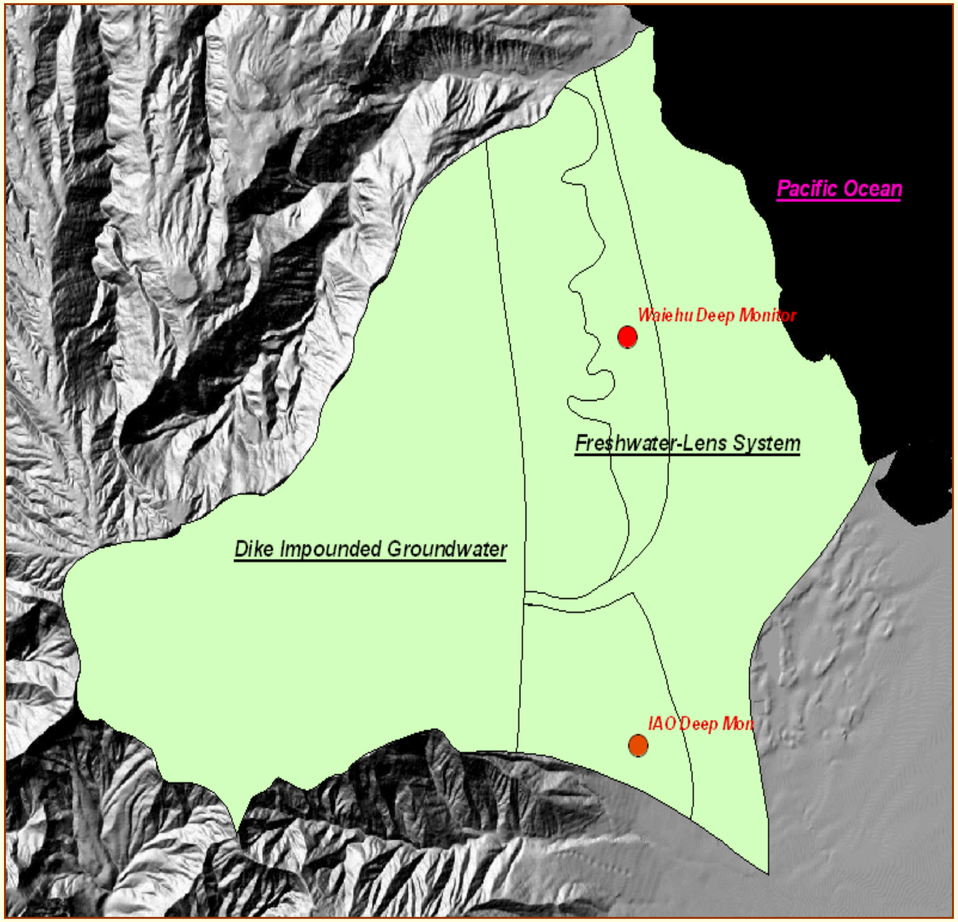
Simulated hydraulic head contours in Pearl Harbor using SHARP model and observed hydraulic heads



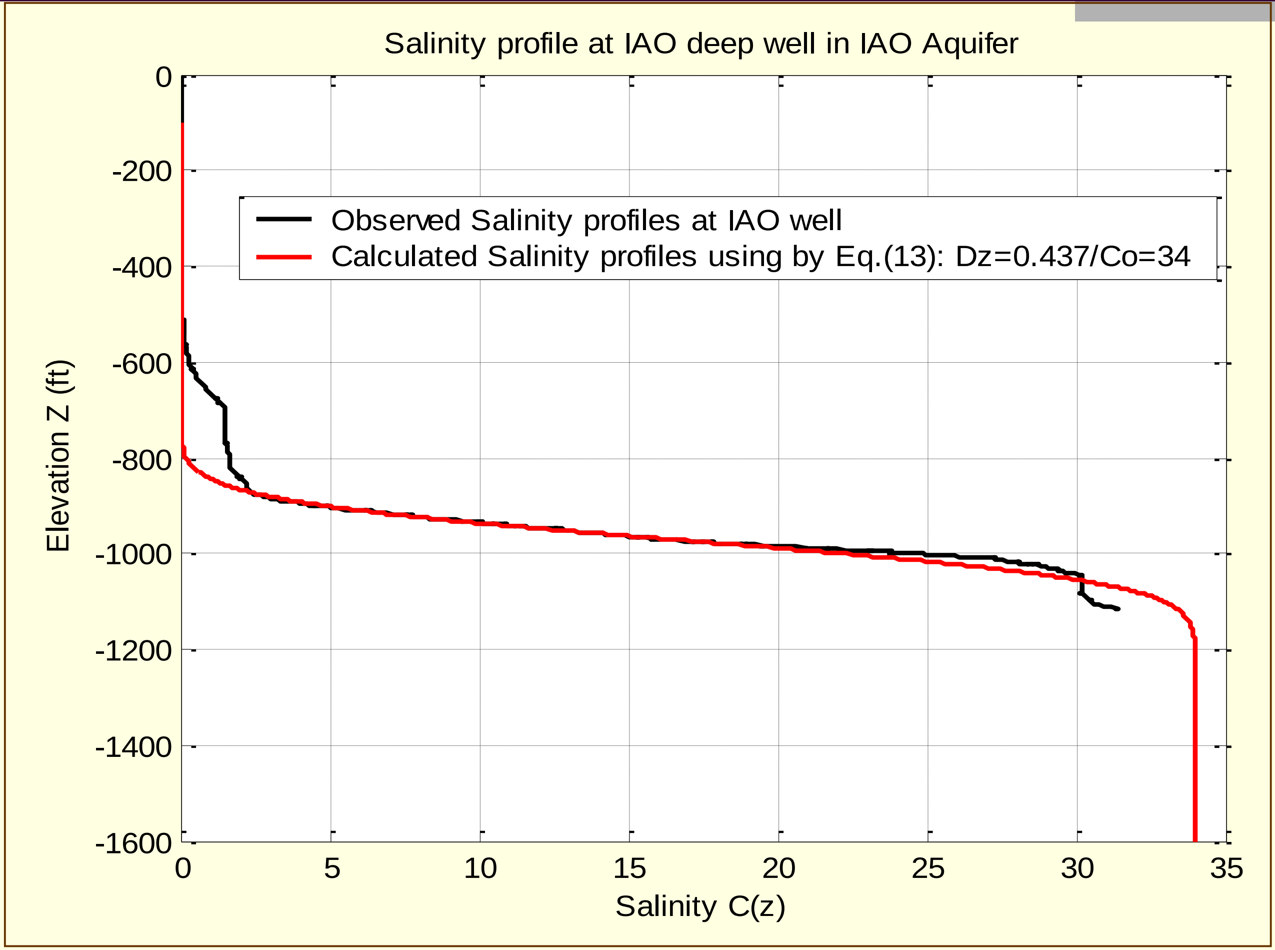


Estimation of the Sustainable Yield of Iao Aquifer



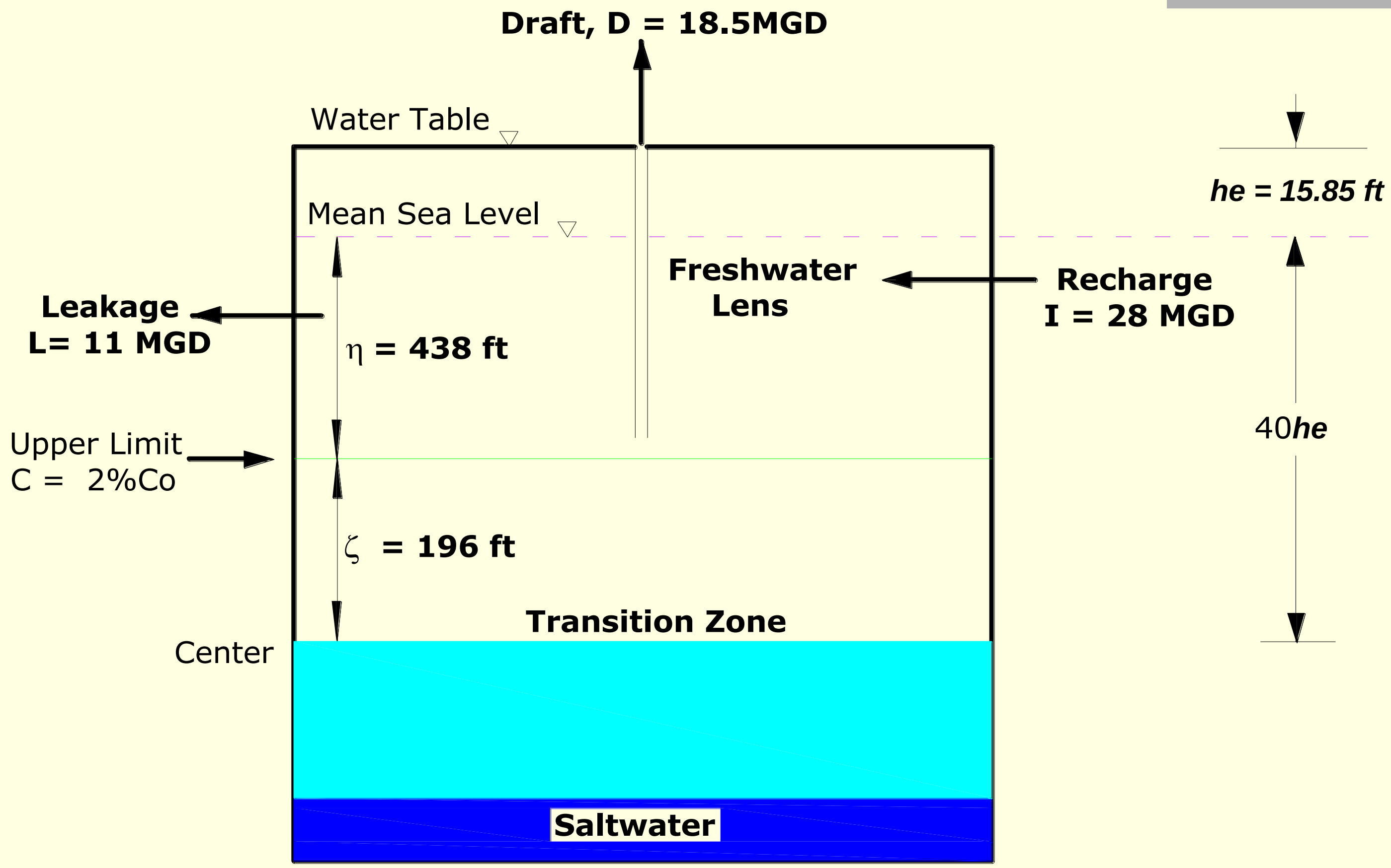


Estimating Effective Dispersion Coefficient by using Deep Monitoring Well Data



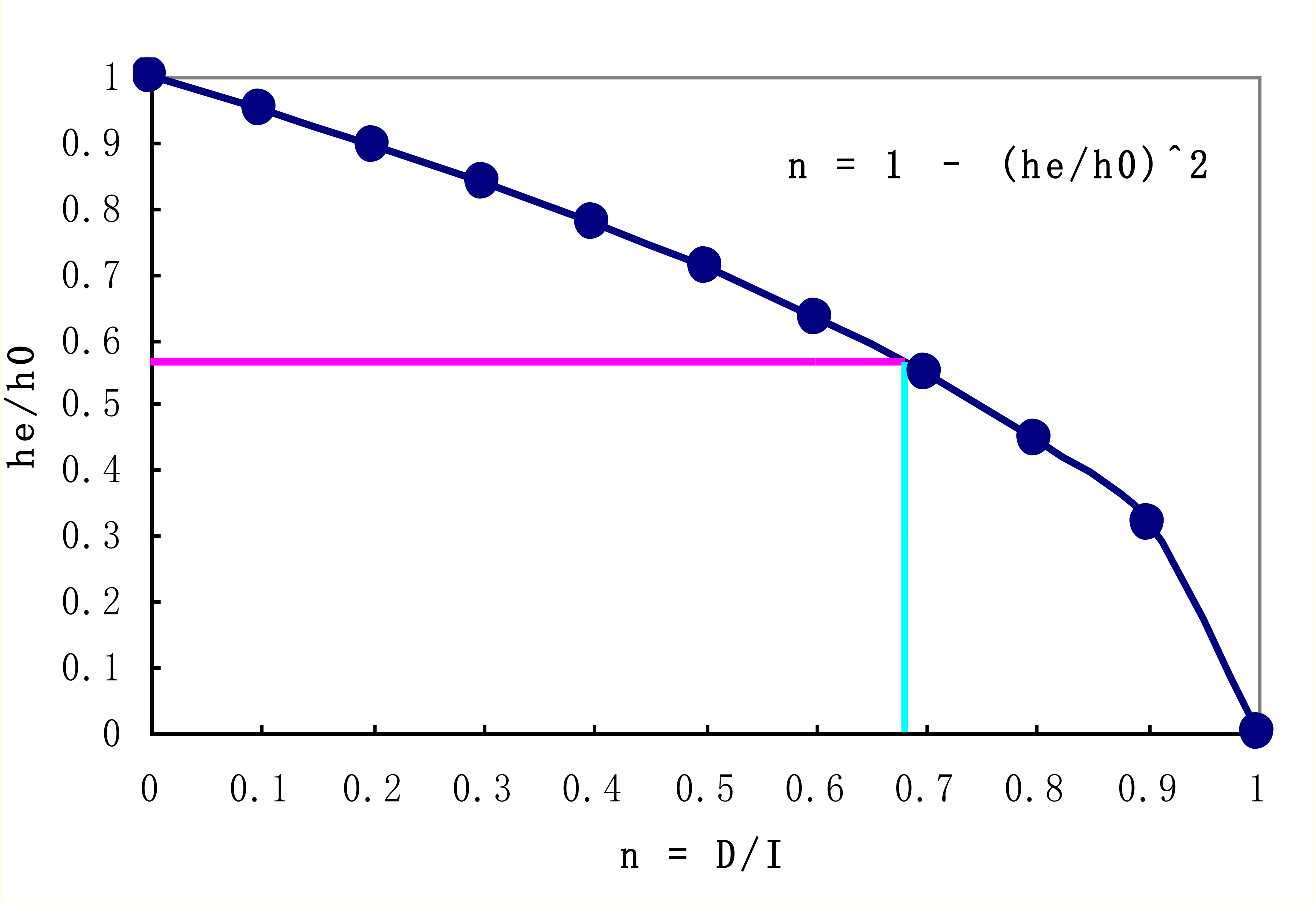
Estimated effective dispersion coefficient ~ 0.298 ft^2/d

Calculate Equilibrium Hydraulic Head of Iao Basal Aquifer



Equilibrium hydraulic head ~ 15.85 ft

Estimating the Sustainable Yield of Iao Basal Aquifer

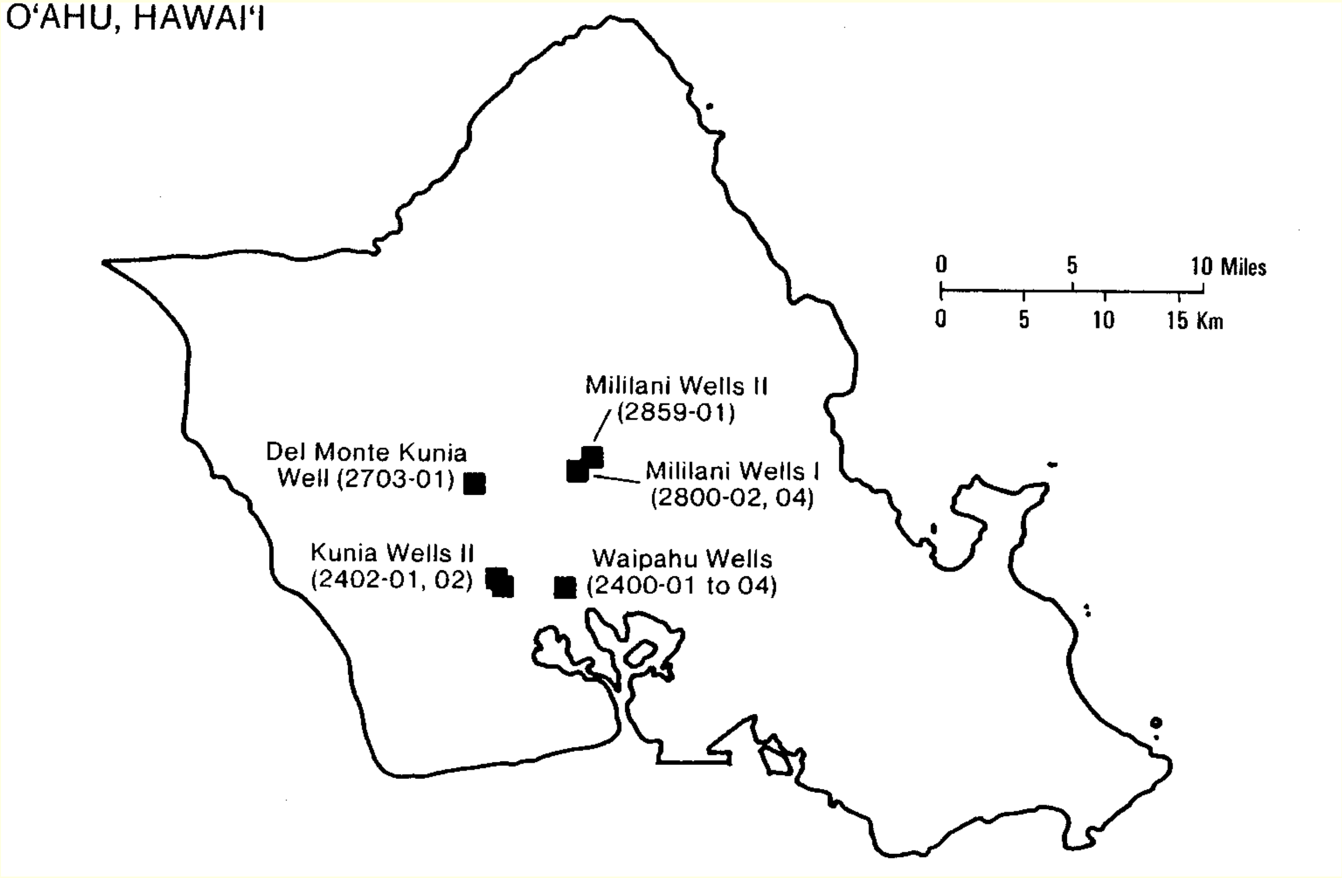


Estimated sustainable yield ~ 19 MGD

3.地下水污染的風險評估

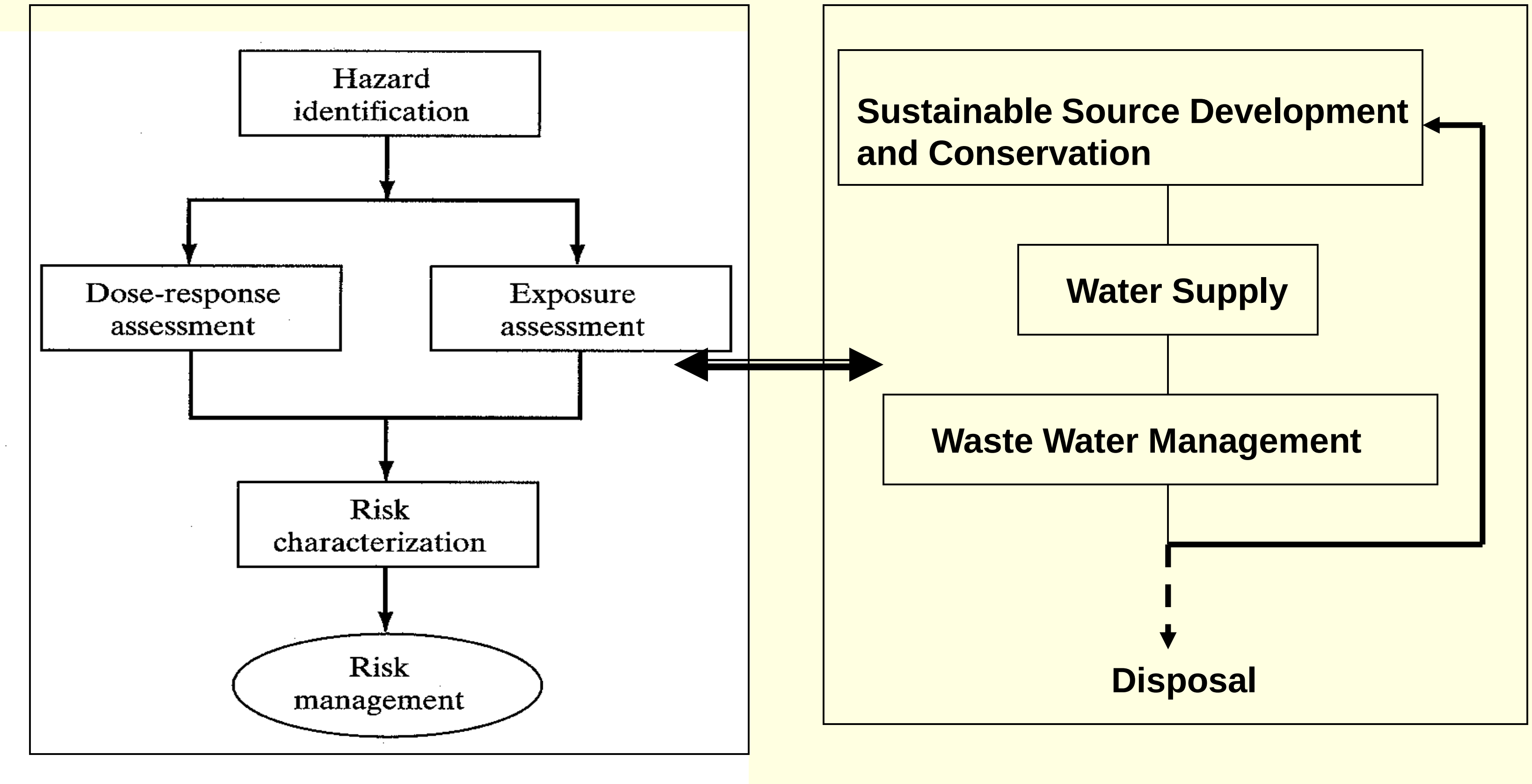
Groundwater Contamination and Risk Assessment

Closed well sites on Oahu, Hawaii in 1983

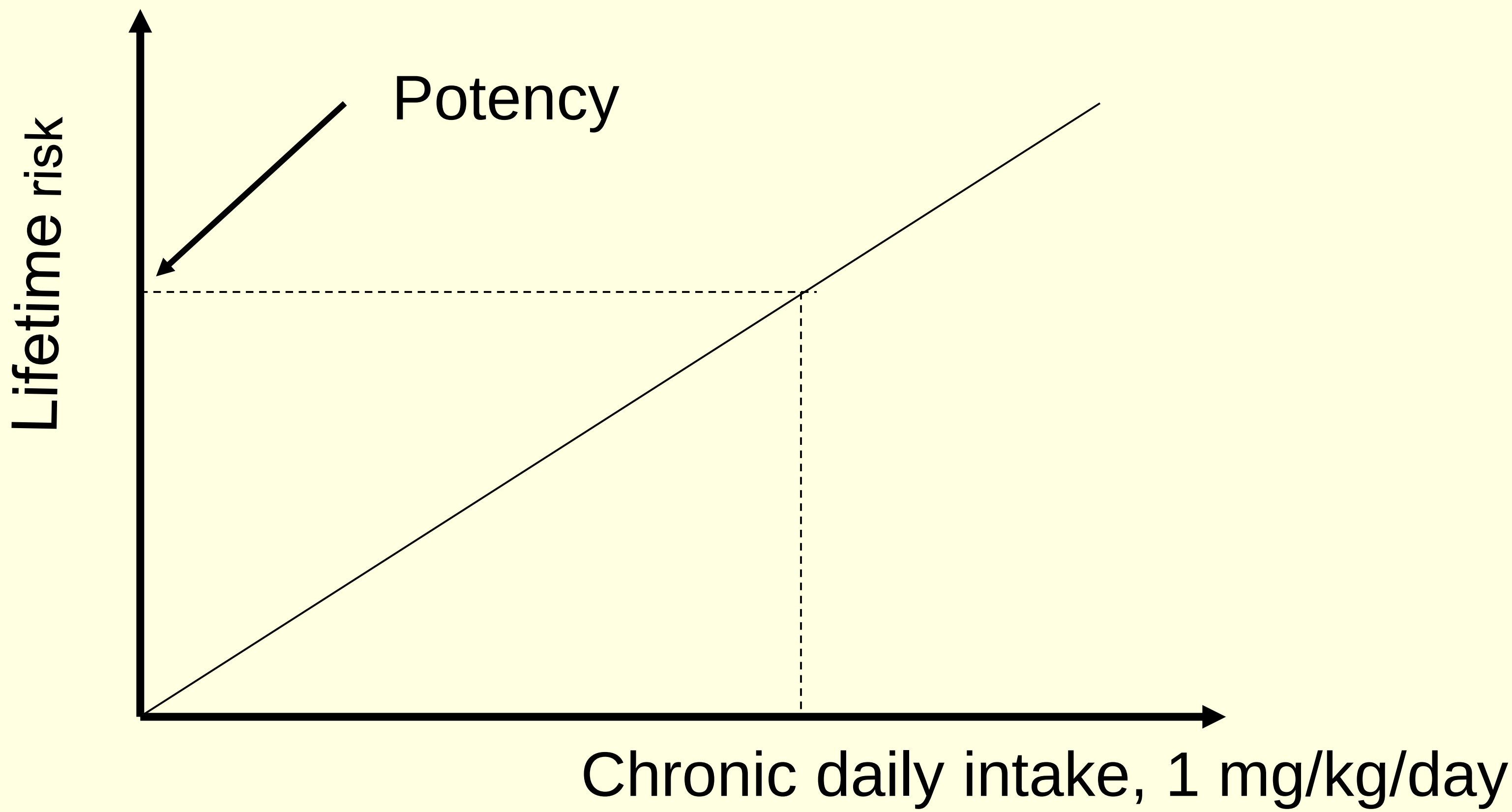


Risk Assessment and Modern Environmental Engineering

Integrated Risk Assessment *Water and Wastewater Engineering*



Carcinogen Potency Factor



Groundwater Contamination and Risk Assessment

Dose-response model (Ref. *Crouch*, *E.A.C.*, *et al 1983)*

$$R = 1 - (1-\alpha)\exp\left(-\frac{\beta D}{1-\alpha}\right)$$

If $\alpha = 0$ and D is very small

$$R \approx \beta D$$

where:

R = Risk, probability of dying with a tumor induced by a dose D

D = Chronic daily intake(CDI) (mg/kg of body weight /day)

α = Background lifetime tumor incidence

β = carcinogenic potency (kg-day/mg)

Risk Assessment for TCP and DBCP in Water of Mililani Wells

Average cancer risk of drinking water from Mililani wells

$$\overline{\boldsymbol{R}} = 3\boldsymbol{x}10^{-5}\,\boldsymbol{[(}22\boldsymbol{x}0.045\boldsymbol{x}2\boldsymbol{)} + 0.0236\boldsymbol{x}1.7\boldsymbol{x}2\boldsymbol{)]}$$

$$= 6.18\boldsymbol{x}10^{-5}$$

Average annual excess cancer risk (individual)
(assume an average life span of 70 years)

$$\boldsymbol{R_a} = \frac{6.18\boldsymbol{x}10^{-5}}{70} = 8.8\boldsymbol{x}10^{-7}$$

Average Annual Excess Risk

Average annual excess cancer risk for the entire community of Mililani
(Based on the 1980 census, the population of Mililani was 21,400)

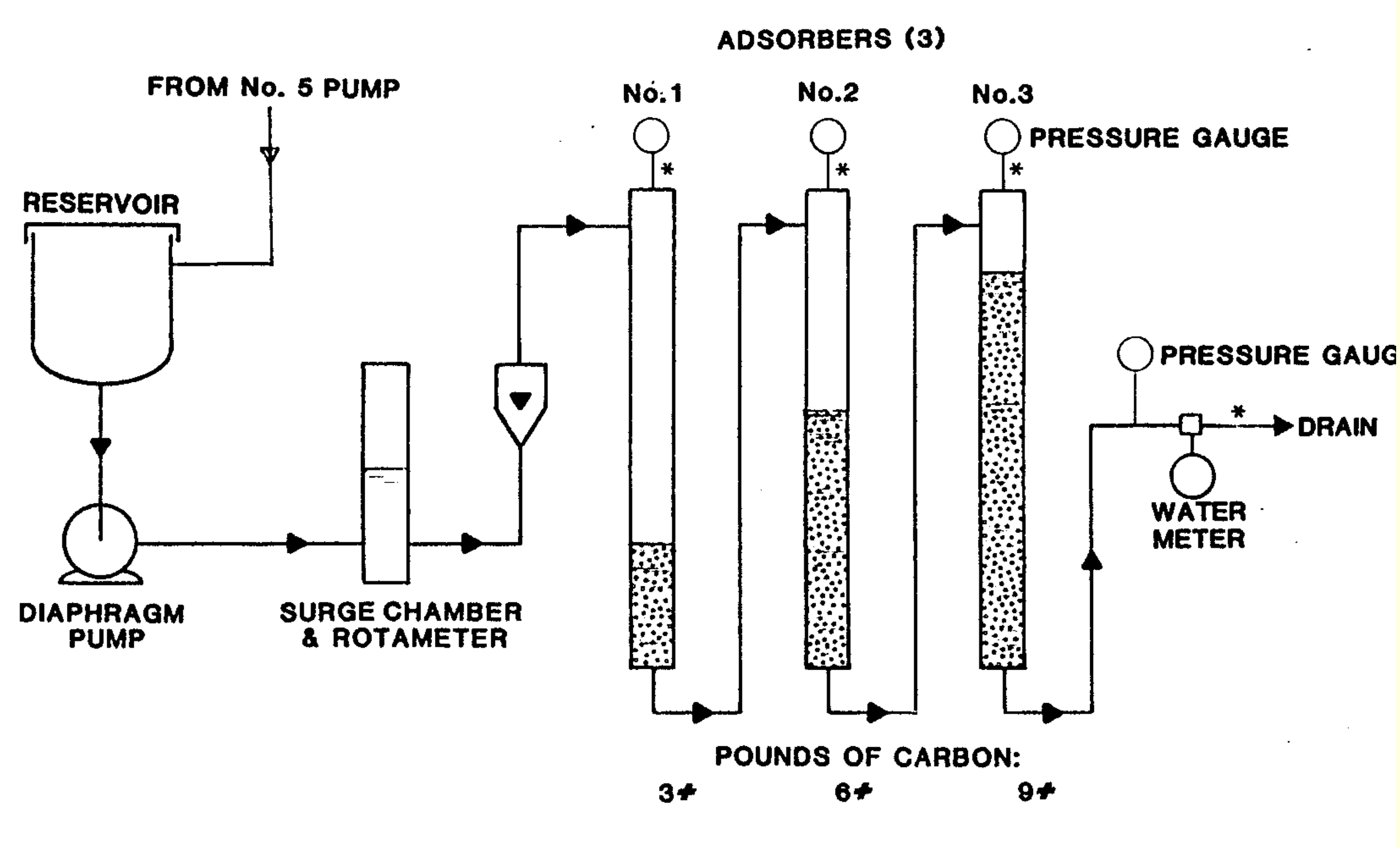
$$R_c = 8.8x10^{-7}(21{,}400)$$

$$= 1.88x10^{-2}$$

Note that, based on Hawaii Tumor Registry, the average annual number of new cancer cases in Mililani during the period of 1979-83 was 38

ECONOMIC ANALYSIS OF POLLUTION CONTROL

Schematic of the Mililani GAC facilities



Cost Estimate for the Mililani GAC facilities
(a) Capital Cost

Eight 12-foot Diameter Contactors (in place)	$ 547,200
Initial Carbon Fill (in place)	168,000
Foundation for (8) Contactors	40,000
Complete Piping and Valving for System (in place)	260,000
Instrumentation	8,000
Backwash Water Handling System	53,600
Site Preparation Work	39,000
TOTAL DIRECT COSTS	$1,115,800
Indirect costs, inclusive of: 30% contractor overhead and profit, 0.6% mobilization and 4.17% GET	$ 388,000
TOTAL CAPITAL	$1,503,800
Additional cost of force main between Sites I and II if treatment system is sited at Mililani II (not required if sited at Mililani I)	$ 822,100
TOTAL CAPITAL INCLUDING FORCE MAIN	$2,325,900

Cost Estimate for the Mililani GAC facilities (b) Operational Cost

Expressed on an annual bases for treatment of a daily average flow of 4 MGD

Carbon Usage	$ 40,940
Carbon Installation Cost	3,240
Carbon Disposal Cost*	32,400
Added Energy Cost for System	7,230
TOTAL DIRECT COST	$ 83,810
Estimated Labor Cost (One Man-year)	$ 28,500
ANNUAL OPERATIONAL COST	$112,310

Estimated average annual cost for the Mililani GAC facilities of removing residues of pesticides

1. Capital recovery cost
   (assume a life span of the treatment facilities of 50 years and an interest rate of 6%)

   $2,325,900 x 0.0344 = $147,555

2. Annual operational cost

   $112,310

3. Total average annual cost

   $259,865

Cost/benefit analysis for the Mililani GAC facilities of removing residues of pesticides

1. Average annual benefit

    - prevention of an average 0.02 cancer cases

2. Average annual cost

    - $259,865

Estimated Expenditures to Prevent a Life From being Shortened by One Year.

Program	1990 U.S. $
Childhood immunizations	Direct savings
Eliminating lead in gasoline	Direct savings
Safety rules at underground construction sites	52,000
Hemodialysis at a dialysis center	56,000
Coronary artery bypass surgery	68,000
Front seat air bags in new cars	109,000
Dioxin effluent controls at paper mills	5,570,000

Source: Kolluru (1996) based on data from the Harvard School of Public Health.