CE 3354 Engineering Hydrology

Lecture 24: Subsurface Contaminant Hydrology and Aquifer Numerical Modeling

Outline

- Subsurface Contaminant Hydrology
  - Advection-Dispersion Equation
  - Selected Analytical Solutions

- Capture Zones

- Aquifer Numerical Modeling (Introduction)
  - Numerical Generation of Flownets

Contaminant Hydrology

* Water unsuitable for a particular use is called polluted (contaminated)

* Sources of pollution
    * Natural processes
    * Runoff processes
    * Waste disposal practices
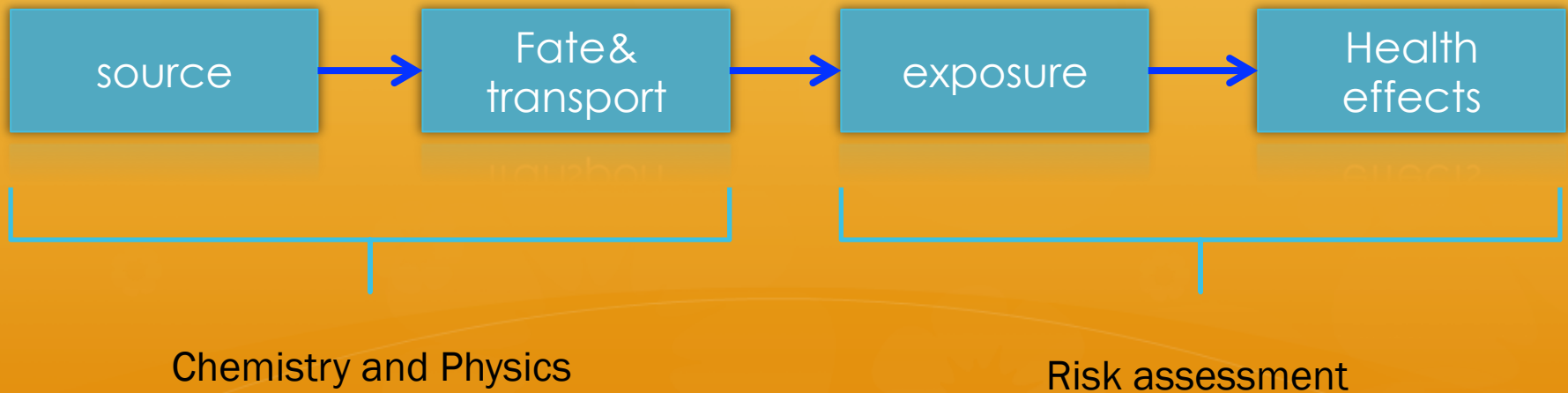   * Accidental spills and leaks

Contaminant Hydrology

* Impacts
    * Characteristics of pollutants (fate&transport)
    * Probability of exposure (Risk)
    * Probability of adverse impact from exposure (Toxicology)

* Categories:
    * Organic chemicals – solubility, density
    * Metals – solubility, oxidation state
    * Radionuclides – solubility, oxidation state, decay rate
    * Inorganics – solubility, oxidation state

Contaminant Hydrology

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┌──────────┐      ┌──────────┐      ┌──────────┐      ┌──────────┐
│  source  │ ──▶  │  Fate&   │ ──▶  │ exposure │ ──▶  │  Health  │
│          │      │transport │      │          │      │ effects  │
└──────────┘      └──────────┘      └──────────┘      └──────────┘
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Chemistry and Physics

Risk assessment

* One goal is to relate source concentration to exposure concentration.

* Expressed as a dilution-attenuation-factor

Mass Transport Concepts

* Solvent phase (soil,air,water) that contains the solute (pollutant)

* Amount of solute suspended, dissolved, or otherwise contained in the solvent is usually expressed as a concentration

* Common concentration units in flow and transport models are volumetric (mg/L) and massic (ppm).

  * Radioactive: disintegrations per second/L

  * Certain reactions: equivalents/L

Non-reactive pollutants

* Do not undergo changes, exchanges, or reactions while traversing the region of interest (conservative)

* Solutes do not form a distinct mobile phase from the host phase

  * O_2 in water; oil dispersed in water, dissolved soilds in water.

  * Oil-slick on water is two phases (oil and water) and forms a distinct mobile phase

Transport Mechanisms

✿ Advection

　✿ Transport of solutes by motion of the host fluid

　　✿ If host fluid is driven by density gradients the transport is called natural convection

　　✿ If host fluid is driven by pressure gradients the transport is called forced convection.

✿ Diffusion

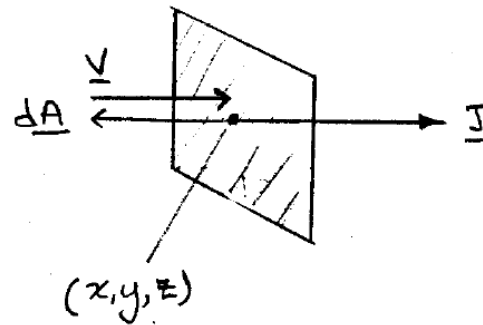　✿ Mixing of solutes by Brownian-motion type processes. Net transport is proportional to concentration gradients.

Transport Mechanisms

* Dispersion

  * Mixing of solutes by small and large variations in the velocity field causes by shear flow, turbulent fluctuations, and braided flow paths.

  * Net transport is proportional to concentration gradients

    * Shear induced – open channel and pipe flow

    * Turbulent induced – open flows (all types)

    * Hydrodynamic – porous media

Transport Mechanisms

❋ Flux – amount of a quantity that passes a point in space per unit area per unit time

J   flux vector

V   velocity vector

dA   area vector

β   quantity per unit volume of interest

Transport Mechanisms

❀ Mass flux is the mass per unit time per unit area that passes the point (x,y,z)

❀ Flux models:

advective flux : $\dfrac{c \underline{v} \cdot \underline{dA}}{\underline{dA}} = \underline{J}$ $J = \wp U$ (mass flux)

$= CU$ (contaminant flux)

diffusive flux : $\underline{J} = -D \left(\dfrac{\partial c}{\partial x}\underline{i}, \dfrac{\partial c}{\partial y}\underline{j}, \dfrac{\partial c}{\partial z}\underline{k} \right) = -D \nabla C$

dispersive flux: $\underline{J} = -\underline{D}_h \left(\dfrac{\partial c}{\partial x}\underline{i}, \dfrac{\partial c}{\partial y}\underline{j}, \dfrac{\partial C}{\partial z}\underline{k} \right) = -\underline{D}_h \cdot \nabla C$

Transport Mechanisms

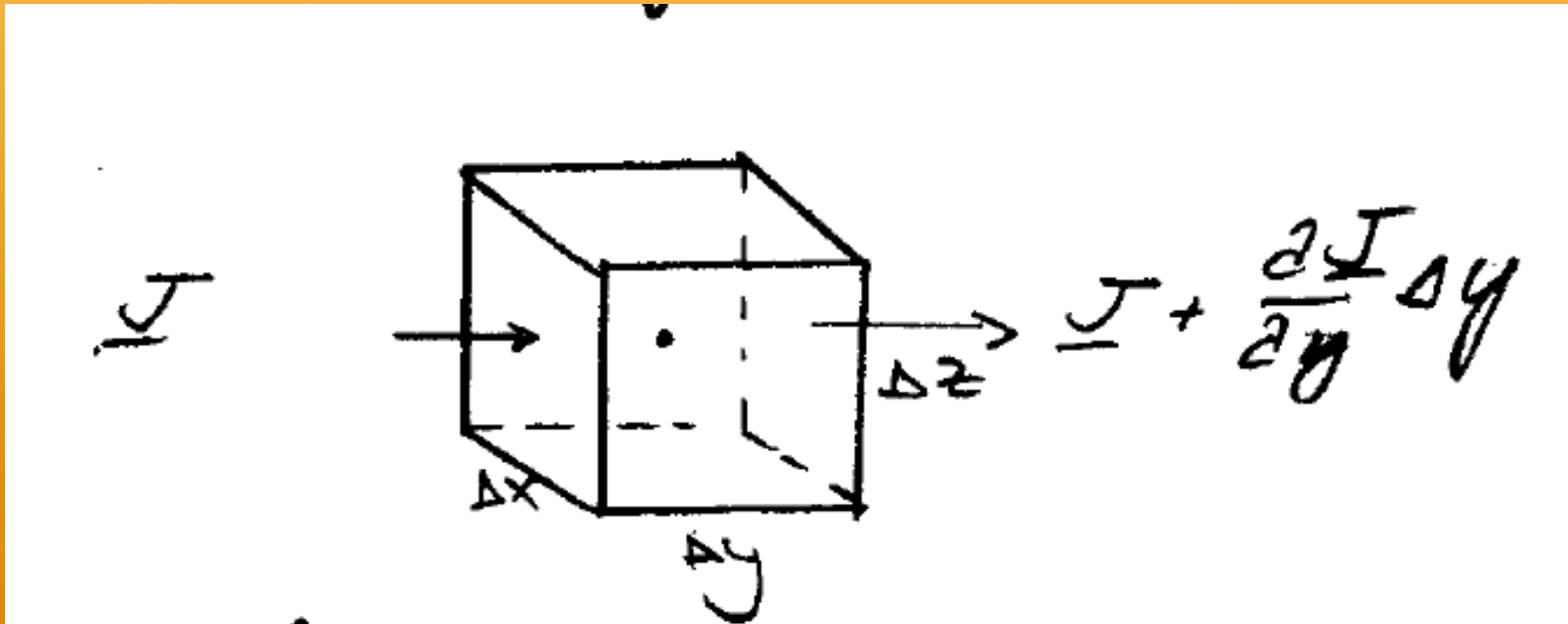❀ Usually the Diffusive and Dispersive Flux terms are combined as:

$$\underline{J} = -\underline{D} \cdot \nabla C$$

$$\underline{D} = \begin{pmatrix} D_{xx} & D_{xy} & D_{xz} \\ D_{yx} & D_{yy} & D_{yz} \\ D_{zx} & D_{zy} & D_{zz} \end{pmatrix} \longleftarrow \text{Dispersion matrix and the individual elements are dispersion coefficients}$$

Advection

- Consider an element in space – only mechanism is advection:

- Apply Reynold's Transport Theorem:

Advection

$$0 = \frac{\partial}{\partial t} \int_{cv} c \, d\forall + \int_{c.s.} C \, (\underline{V} \cdot dA)$$

Observe that $\int_{c.s.} C(\underline{V} \cdot d\underline{A})$ is identical to

$$0 = \frac{\partial c}{\partial t} \Delta x \Delta y \Delta z + \left(\frac{\partial J}{\partial x} + \frac{\partial J}{\partial y} + \frac{\partial J}{\partial z}\right) \Delta x \Delta y \Delta z$$

$$\int_{c.s.} \underline{J} \cdot d\underline{A}$$

This principle is fundamental to linking the Reynold's Transport theorem to pollutant transport.

$$\therefore \quad \frac{\partial c}{\partial t} = -\nabla \cdot \left(c \underline{V}\right)$$

OR $\quad \underline{0 = \frac{\partial c}{\partial t} + \nabla \cdot c \underline{V}}$ $\longleftarrow$ Fundamental equation of advective transport

Diffusion/Dispersion

Similar to advection one can study an element in space and apply the transport theorem to the flux term

Diffusion/Dispersion

$$0 = \frac{d}{dt} \int_{CV} c \, dV + \int_{C.S.} \underline{J} \cdot d\underline{A}$$

$$0 = \frac{\partial c}{\partial t} \Delta x \Delta y \Delta z + \left(\frac{\partial J}{\partial x} + \frac{\partial J}{\partial y} + \frac{\partial J}{\partial z} \right) \Delta x \Delta y \Delta z$$

$$0 = \frac{\partial c}{\partial t} + \nabla \cdot \underline{J} \quad = \frac{\partial c}{\partial t} + \underbrace{\nabla \cdot \left(- D \nabla c \right)}$$

in one-dimension to illustrate
the structure we have

$$\frac{d}{dx} \left(- D \frac{\partial c}{\partial x} \right)$$

Combined Transport

✤ When the processes are combined the result is called the Advection-Dispersion equation and the NET flux is the sum of the individual process fluxes:

$$\underline{J} = c\underline{V} - \underline{D} \cdot \nabla c$$

✤ The mass balance becomes:

$$0 = \frac{d}{dt}\int_{CV} c\, dV + \int_{C.S.} \underline{J} \cdot d\underline{A}$$

$$0 = \frac{\partial c}{\partial t}\Delta x \Delta y \Delta z + \nabla \cdot \left(c\underline{V} - \underline{D} \cdot \nabla c\right)\Delta x \Delta y \Delta z$$

Dispersion Coefficients

Now why all the fluid mechanics? The dispersion coefficients usually are related to the velocity field

$$J_{shear} = -\varepsilon_{shear} \frac{\partial \overline{C}}{\partial x}$$

↳ velocity dependent

$$J_{turbulent} = -\varepsilon_{turb} \frac{\partial C}{\partial x}$$

↳ velocity dependent

$$J_{hydrodynamic} = -\varepsilon_{hydro} \frac{\partial C}{\partial x}$$

↳ $= \alpha_L U$

↳ dispersivity

Solutions to Advection-Dispersion Equations

- 1D Finite-Duration Pulse

- 2D Constant Injection

  - http://cleveland2.ce.ttu.edu/software/spreadsheets/ssants/

Capture Zones

❁ A contaminant collection technique that uses arrays of wells to pump contaminated water (pump-and-treat) out of aquifer.
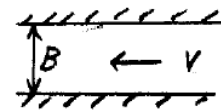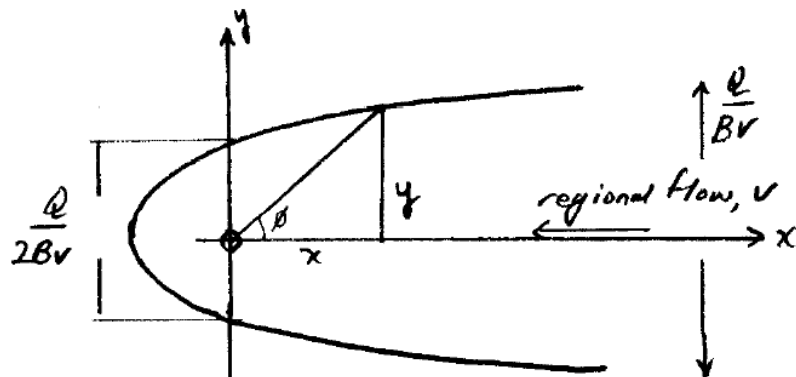

Capture Zone Calculations/design

One method to control polluted groundwater is with hydraulic capture and treatment.

Goal is to capture, extract, treat & serve polluted groundwater. Design problem is where to locate extraction wells and what pumping rates

regional flow, no wells

well operating, area draining to well is capture zone

Capture Zones

Simplest model to construct capture zone curves is

$$y = \pm \frac{Q}{2Bv} - \frac{Q}{2\pi Bv} \tan^{-1}\left(\frac{y}{x}\right)$$

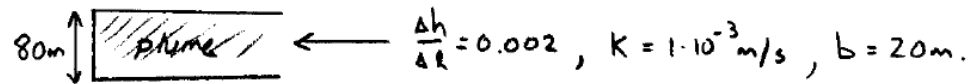$$\tan \phi = \frac{y}{x} \qquad \text{so} \qquad y = \frac{Q}{2Bv}\left(1 - \frac{\phi}{\pi}\right)$$

We can use these relationships to specify Q and location of well relative to plume. (1) Well(s) is located so that computed capture zone just encloses plume. (2) Well is located as close as possible to plume, without violating rule (1).
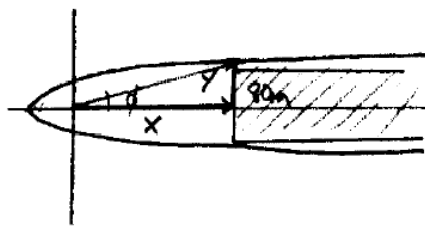
Capture Zones

Example

Locate an extraction well at $Q = 0.004 \, m^3/s$ to capture plume.

80m | plume | ← | $\frac{\Delta h}{\Delta \ell} = 0.002$, $K = 1 \cdot 10^{-3} \, m/s$, $b = 20m$.

① determine regional specific discharge

$$\frac{Q}{A} = K \frac{\Delta h}{\Delta \ell} = 1 \cdot 10^{-3} \, m/s \, (0.002) = 2 \cdot 10^{-6} \, m/s$$

② Find critical dimension of capture zone.

$$\frac{Q}{2Bv} = \frac{0.004 \, m^3/s}{2 \cdot 20 \cdot 2 \cdot 10^{-6} \, m/s} = 50m$$

∴ well cannot be located at leading edge, but $\frac{Q}{Bv} = 100m$ which is big enough to capture plume

③

find x when $y = 40m$ (half plume width)

$$y = \frac{Q}{2Bv}\left(1 - \frac{\phi}{\pi}\right) = 40m = 50m\left(1 - \frac{\phi}{\pi}\right) \Rightarrow \phi = 0.2\pi$$

$$\therefore \quad x = \frac{y}{\tan\phi} = \frac{40}{\tan(0.2\pi)} = 55m$$

④ locate well 55m downgradient of plume.

Capture Zones
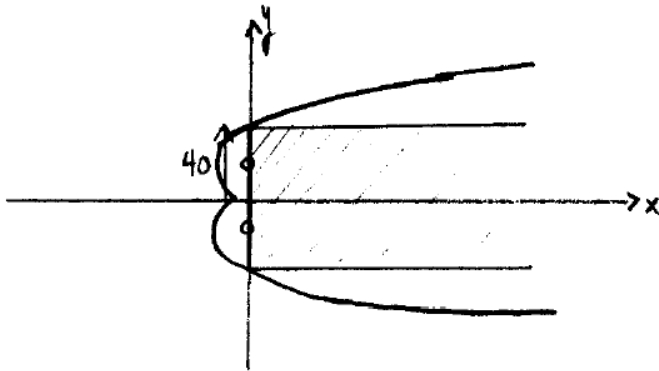
For multiple wells the following equations are used

$$y = \frac{Q}{2Bv}\left(n - \frac{1}{\pi}\sum_{i=1}^{n}\phi_i\right)$$ and optimal well spacing is

$$n=2, \quad \frac{Q}{\pi Bv}$$

$$n=3, \quad \frac{(2^{\frac{1}{3}})Q}{\pi Bv}$$

Example – 2 wells, same problem

$$\frac{2Q}{2vB} = 80 = \frac{Q}{vB} \quad \therefore \quad Q = 80(20)(2\cdot10^{-6}\,m/s)$$

$$= 0.0032\,m^3/s \text{ each well}$$

optimal spacing $= \dfrac{8Q}{\pi} = 25.5m$

Capture Zone Type-Curves

Capture-Zone Type Curves: A Tool for Aquifer Cleanup

by Iraj Javandel and Chin-Fu Tsang[2]

ABSTRACT

Currently a common method of aquifer cleanup is to extract the polluted ground water and, after reducing the concentration of contaminants in the water below a certain level, the treated water is either injected back into the aquifer, or if it is environmentally and economically feasible, released to a surface-water body. The proper design of such an operation is very important, both

The NPL identifies the targets for long-term action under the "Superfund" law (CERCLA, 1980). This list has been continuously growing since October 1981 when EPA first published an interim priority list of 115 sites. In addition, as of October 1984, EPA has inventoried more than 19,000

Major questions to be answered for the design of such projects include the following:

1. What is the optimum number of pumping wells required?

2. Where should the wells be sited so that no contaminated water can escape between the pumping wells?

3. What is the optimum pumping rate for each well?

4. What is the optimum water treatment method?

5. Where should one reinject the treated water back into the aquifer?

The purpose of this paper is to introduce a simple method for answering four of the above questions which are of hydraulic nature.

1-Well Array
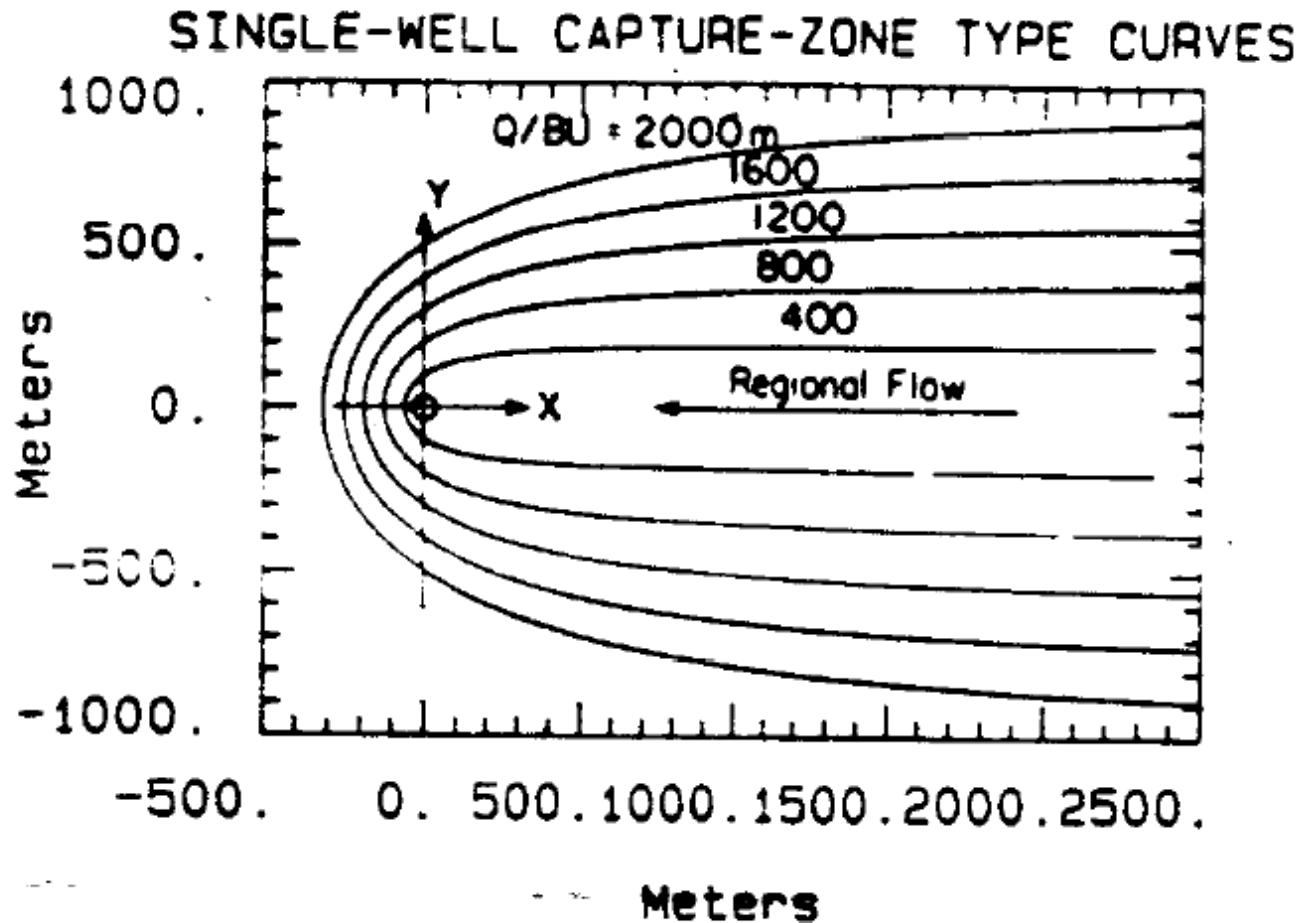

SINGLE-WELL CAPTURE-ZONE TYPE CURVES

Fig. 1. A set of type curves showing the capture zones of a single pumping well located at the origin for various values of (Q/BU).

2-Well Array

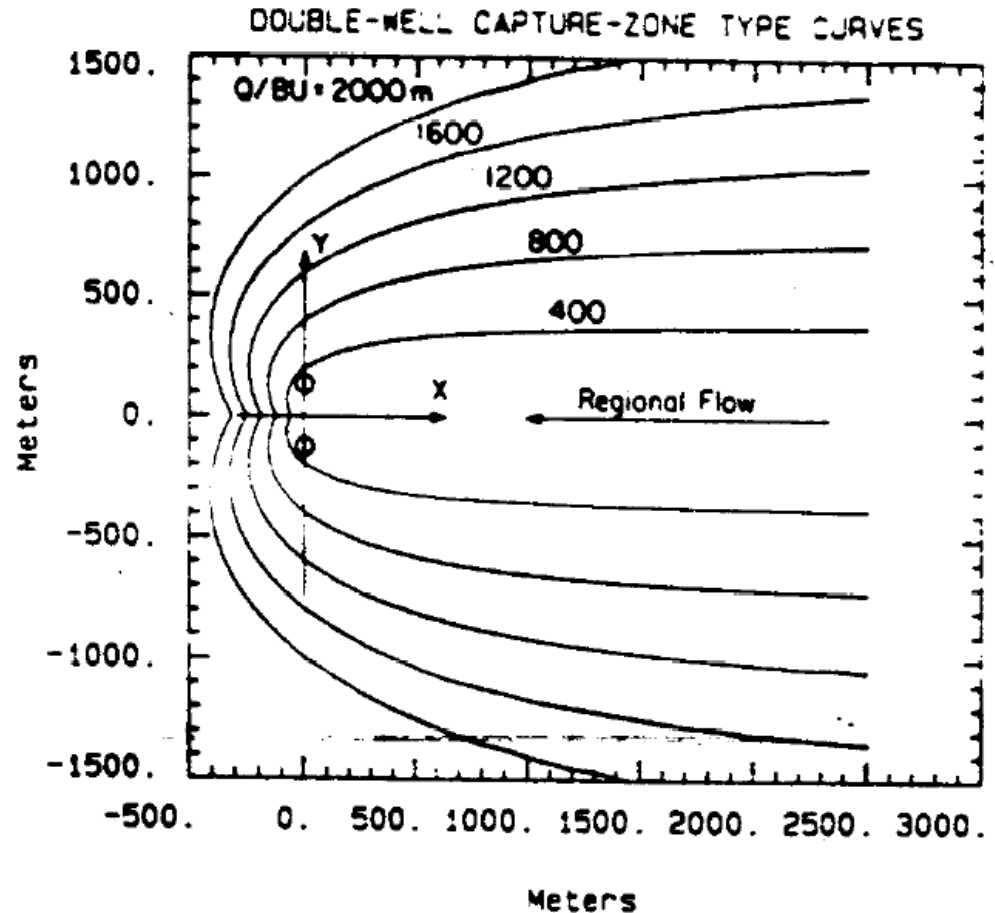Well Spacing = $Q/\pi BU$

DOUBLE-WELL CAPTURE-ZONE TYPE CURVES

Fig. 5. A set of type curves showing the capture zones of two pumping wells located on the y-axis for various values of (Q/BU).

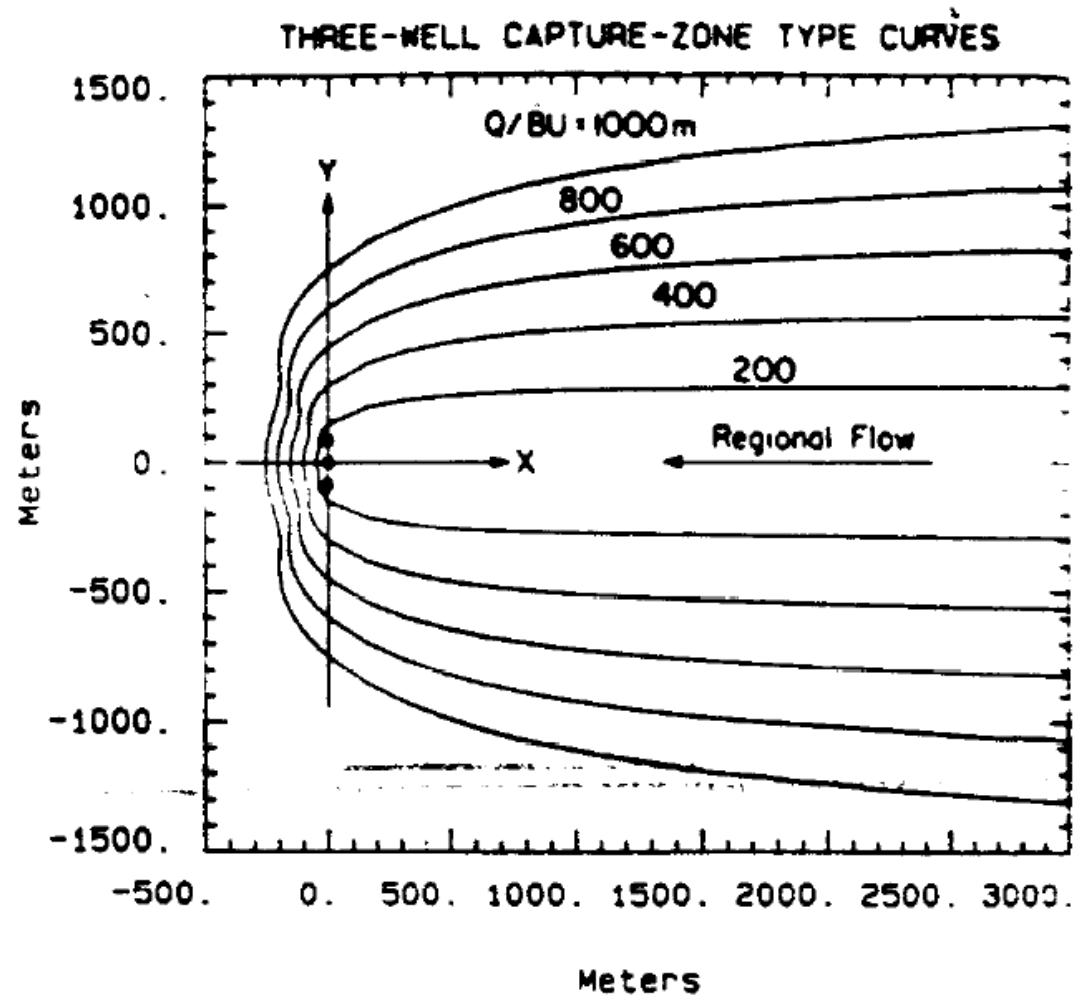# 3-Well Array

Well Spacing $= [2^{1/3}]Q/\pi BU$

Fig. 6. A set of type curves showing the capture zones of three wells all located on the y-axis for various values of (Q/BU).

4-Well Array

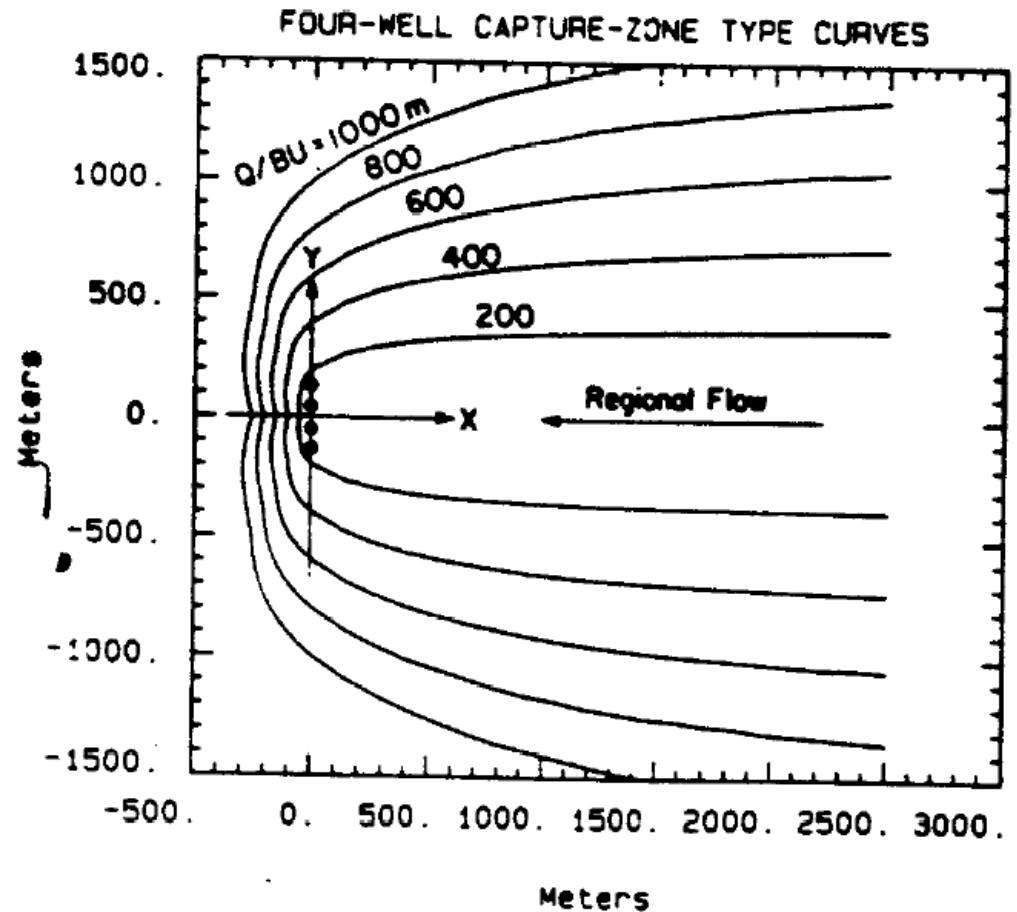- Well Spacing
  $= 1.2 \, Q/\pi BU$

Fig. 7. A set of type curves showing capture zones of four pumping wells, all located on the y-axis for several values of (Q/BU).

Example

EXAMPLE

This example is designed to illustrate the use of this technique for aquifer cleanup. It is assumed that leakage from a faulty injection well has contaminated a confined aquifer with trichloroethylene (TCE). A thorough investigation of the site has identified the TCE concentration distribution as given in Figure 8. Hydrologic studies have revealed the following data: aquifer thickness, 10 m; regional hydraulic gradient, 0.002; aquifer hydraulic conductivity, 10^{-4} m/s; effective porosity, 0.2; storage coefficient, 3×10^{-5}; and permissible drawdown at each well, 7 m.

Suppose we want to clean the aquifer such that maximum remaining TCE concentration after the cleanup operation does not exceed 10 ppb. To optimize the aquifer cleanup operation cost we want to minimize the cost of pumping the contaminated water and treating it at the surface. Reinjection of the treated water is an option which should not be ignored.
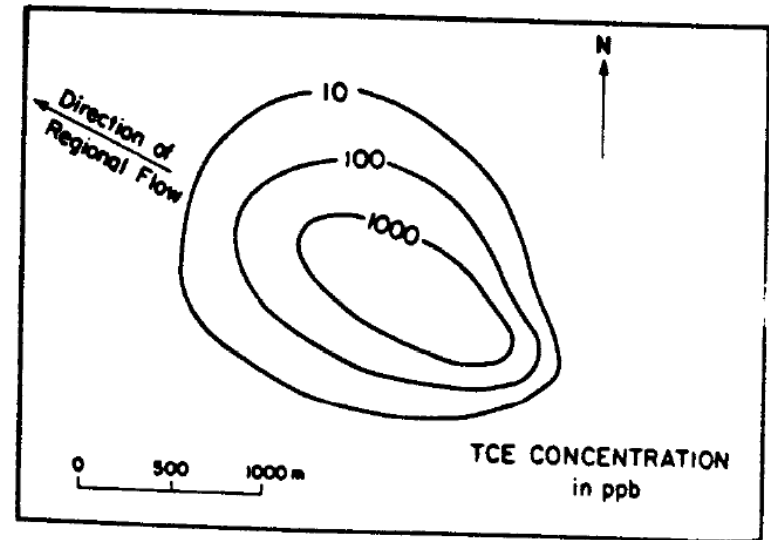

Fig. 8. Observed TCE concentration distribution.

B=10m
dh/dl = 0.002
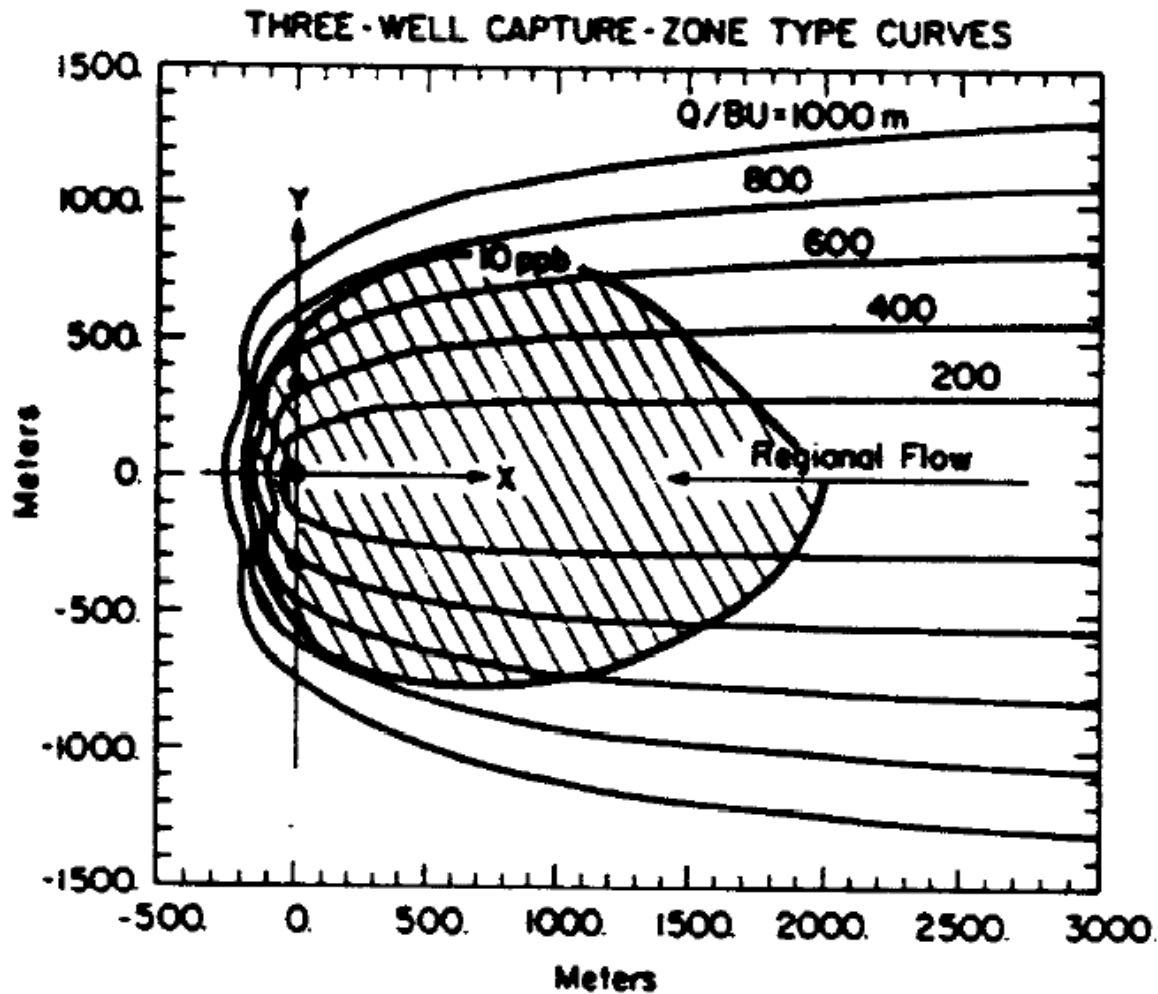K = 0.0001 m/s
n = 0.2
S =0.00003
Drawdown <= 7m

Example

Fig. 9. The 10-ppb contour line of TCE at the matching position with the capture-zone type curve of (Q/BU) = 800.

Example

❀ Apply the original aquifer properties to find the discharge/well and the maximum drawdown

The rate of discharge for each pumping well is

$$Q = 800(10)(2 \times 10^{-7}) = 0.0016 \text{ m}^3/\text{sec}$$

Drawdown in the middle well is the sum of the drawdowns of the two lateral wells in that well plus its own drawdown, which amounts to 5.7 m. If we are convinced that the total drawdown is less than 7 m or field tests indicate that, then our optimum number of wells is three and the rate of discharge from each one is 0.0016 m³/sec. One of these wells is on the origin and the other two are at $(0, \pm 320)$ as shown in Figure 9.

Next Time

❀ DONE!