CONTAMINANT TRANSPORT MODELING

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Topics to be covered in this lecture

- ✓ GW contaminants
- ✓ Mechanism and transport of contaminants
- ✓ Numerical transport modeling
- ✓ Modeling using MT3D
- ✓ Case study

GW Contaminants

Contaminant refers to an undesirable constituent which is introduced directly or indirectly as a result of anthropogenic activity.

Groundwater contamination is defined as changes in the *physico-chemical* and *microbiological characteristics* or in the *radio-nuclide content* of water as a result of anthropogenic activities which render it less useful for human needs.

Anthropogenic groundwater contamination

- **Direct anthropogenic contamination** is due to the direct input of substances from *agricultural* (NO3 , PO4 , salinity etc), *industrial* (salinity, heavy metals etc.) or *urban* (sewage, improper waste disposal etc.) activities as well as from *accidents* (e.g. oil spills). *Certain anthropogenic activities are capable of changing geochemical conditions in subsurface thus potentially mobilizing hazardous geogenic substances*. e.g. arsenic, which may be mobilized by variations in redox conditions due to groundwater abstraction for drinking water production, irrigation, etc.
- **Indirect anthropogenic contamination** e.g. in coastal aquifers, overdraft may lead to saline intrusion, which increases Na and Cl concentrations in coastal aquifers.

GW Contaminants

Groundwater contaminants may exist in many forms such as

- inorganic
- organic
- radionuclides
- particulates

GW Contaminants

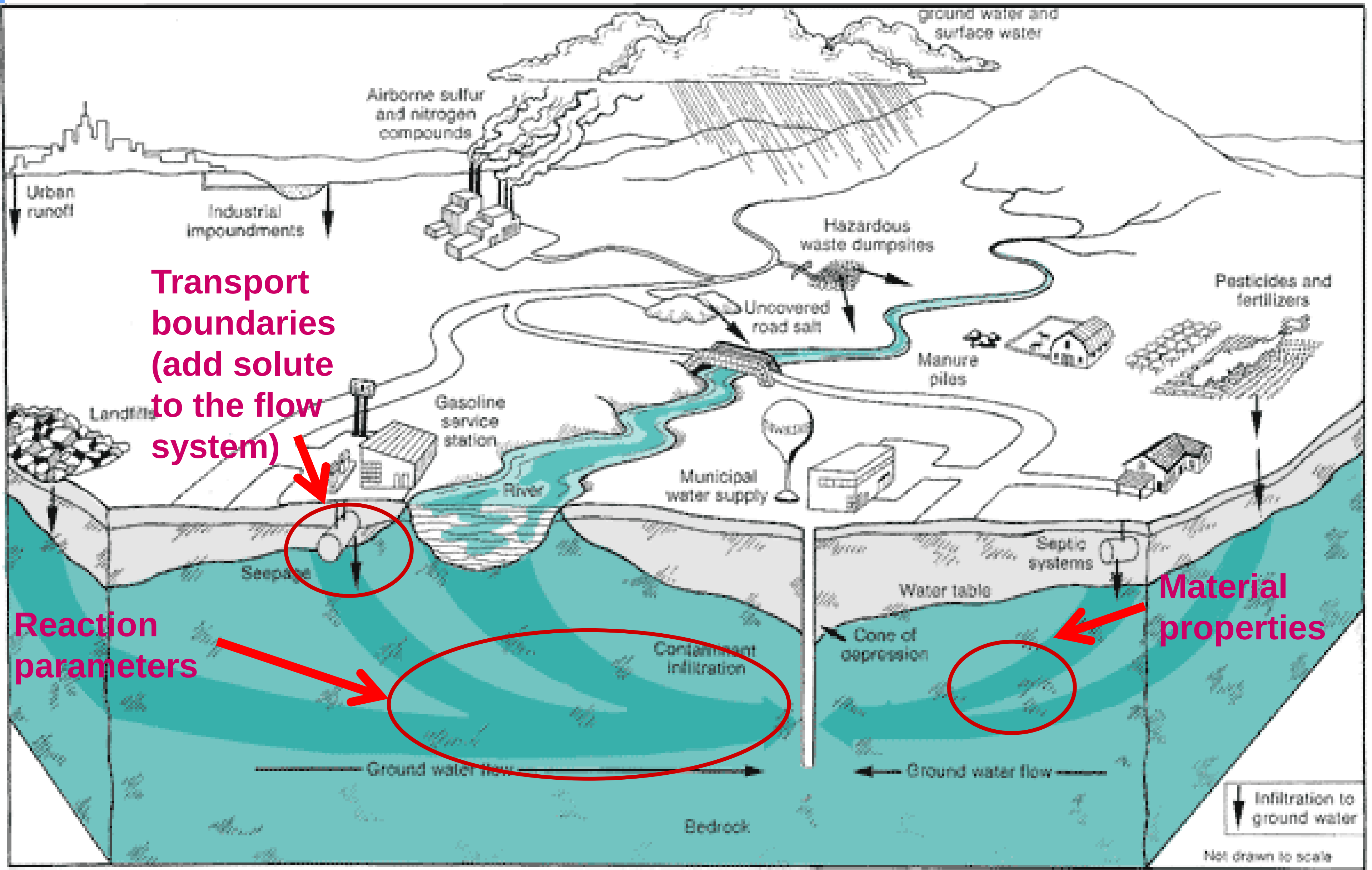
Inorganic contaminants - salts like sodium, calcium, chloride and sulphate (from waste products, fertilizer applications, seawater intrusion etc) - heavy metals like arsenic and lead etc. (arsenic geogenic origin or from ore refining, metal producing, electroplating industries).

Organic contaminants - pesticides & petroleum products.

Radionuclides sources - natural or anthropogenic like nuclear power plants, industrial & pharmaceutical radionuclide applications etc.

Particulate contaminants – airborne materials and microorganisms like bacteria and viruses.

GW Contamination



Types of contaminant sources

(a) Point source

(b) Non-point or diffuse source, and

(c) Line source.

Types of contaminant sources

Point sources - entry of contaminant can be identified to a specific site or location e.g., solid waste disposal sites.

Landfill sites

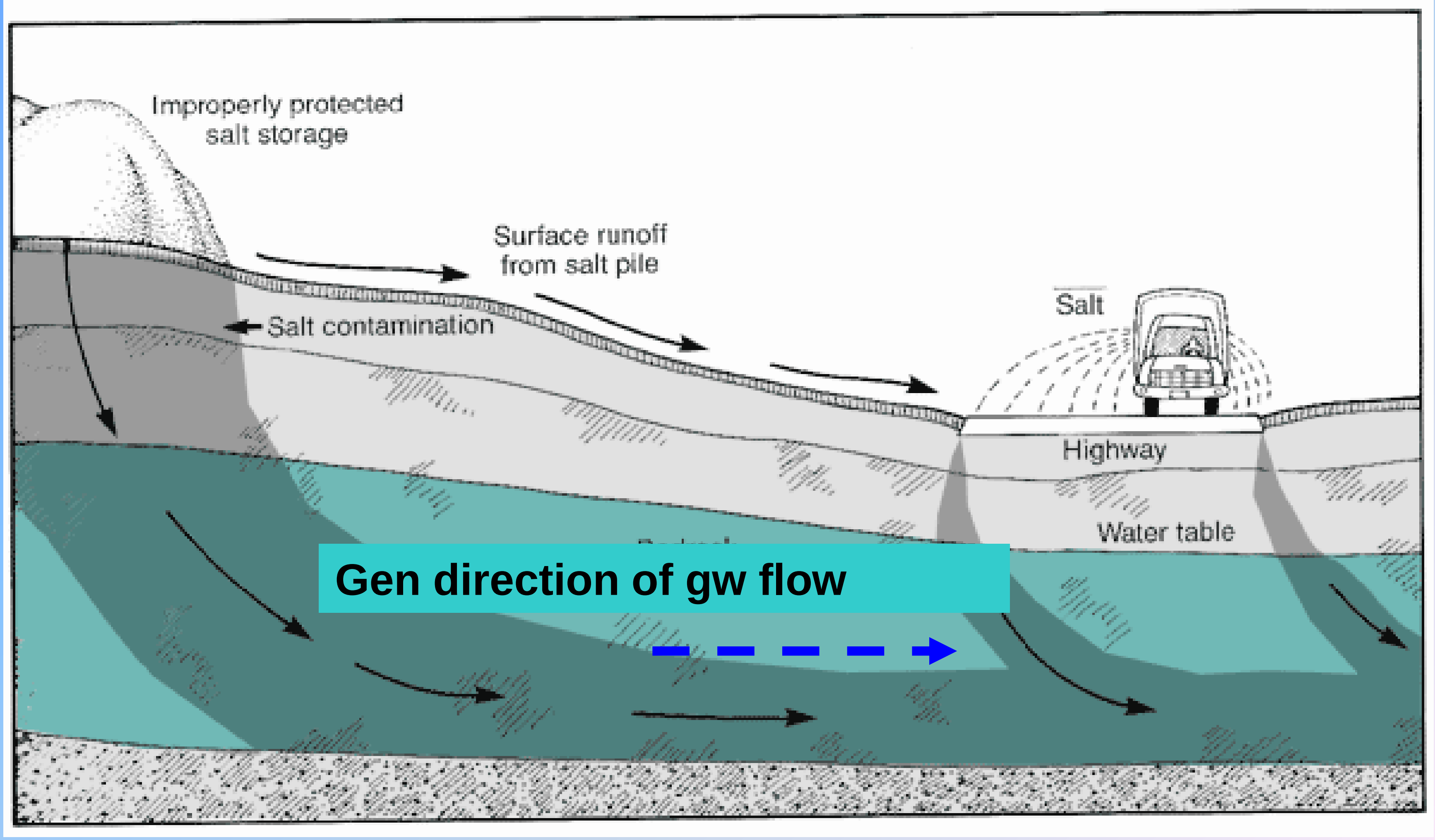
Types of contaminant sources

Non-point or diffuse sources - contaminant entry is spread over a considerable area, e.g., irrigation return flow from a field.

Line source - falls between above two categories, e.g., waste effluent discharged in an unlined drain that seeps underground all along its course before joining a river course.

Mechanism of GW contamination

Contaminant plume normally migrates through unsaturated zone before reaching the saturated zone in which it moves along the hydraulic gradient.



Transport of GW contaminants

In saturated zone, migration of contaminants is governed by

- hydraulic gradient,
- aquifer parameters,
- aquifer heterogeneity,
- distance of the contaminant source to discharge/extraction site etc.

Contaminant Transport Processes

Dissolved toxic chemicals or contaminants are transported in porous media by advection, dispersion, sorption, and degradation.

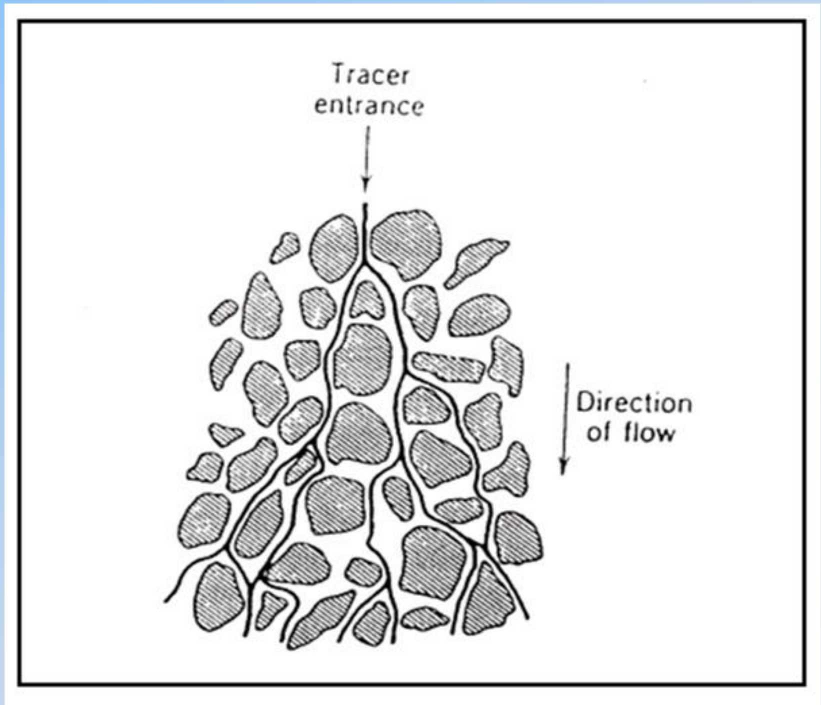
- **Advection** of contaminants is the movement caused along with flowing groundwater at the seepage velocity in porous media.
- **Dispersion** is a mixing process, in which the solute is seen to spread out from the flow path.

Changes in contaminant concentration

(1) Advective transport - dissolved chemicals move with flowing gw;

(2) Dispersive transport - small-scale-variations in flow velocity through porous media cause paths of dissolved molecules/ions to diverge from average flow direction;

Tortuous flow paths in porous media that spread a tracer/solute and create dispersion.



Contaminant Transport Processes

(3) Sorption describes the chemical processes in which the contaminant mass is either entrained into soil or leaches out from the soil.

Geochemical processes/reactions - adsorption-desorption & its role

adsorption: sticking of contaminant onto the grains of aquifer during conc. build-up stage; desorption: release of adsorbed contaminant during conc. depletion stage

A first order decay reaction is where solute gain or loss is proportional to its concentration

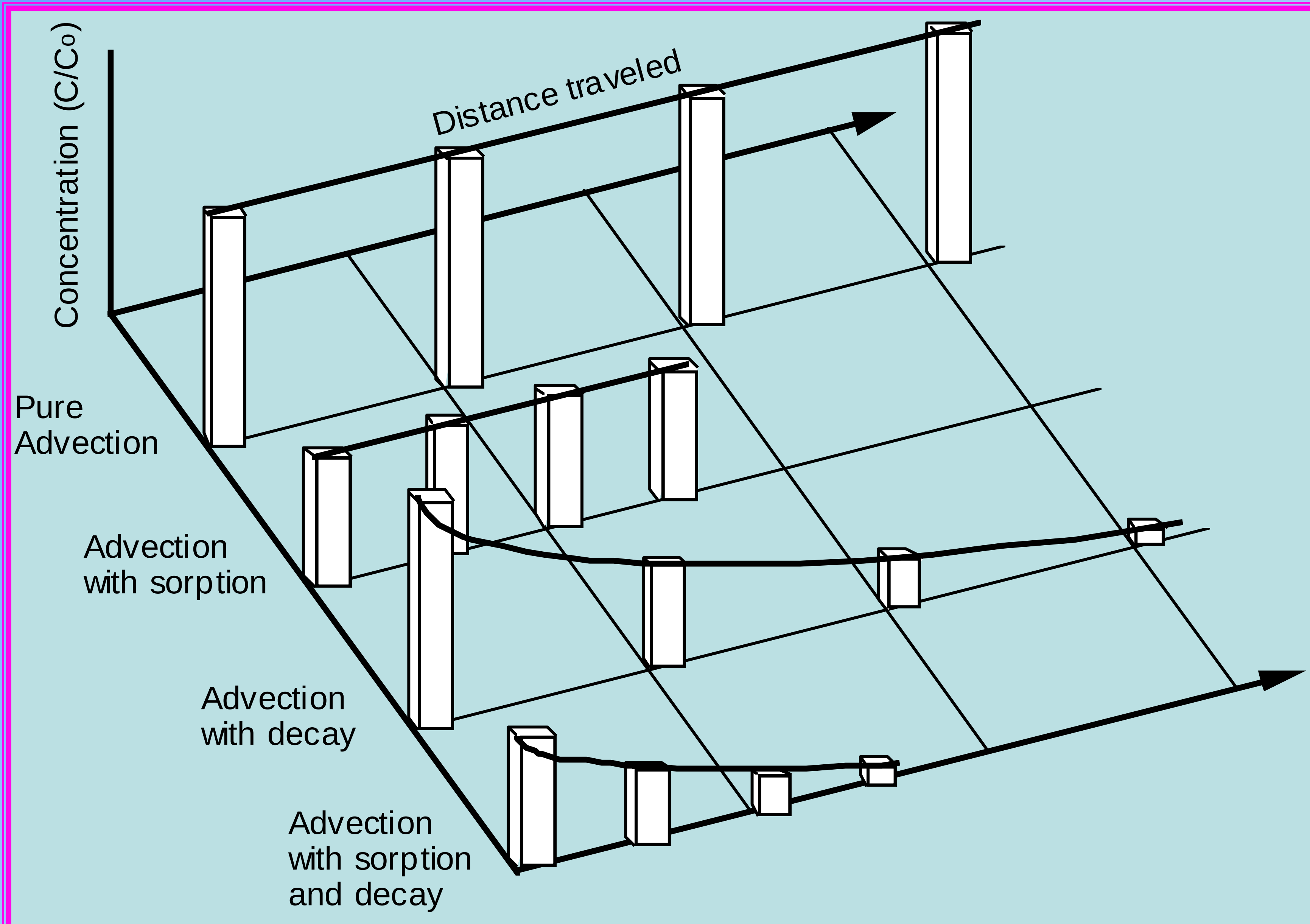
$$\frac{\mathrm{d}C}{\mathrm{d}t} = -\lambda C = \sigma = \text{source or sink}$$

(4) Fluid sources - water of one composition is introduced into and mixed with water of different composition.

Plug Flow models

- Movement is taken to be only due to advection
- Processes of sorption and degradation still may be included
- How could this assumption be reasonable?
  - Typically don’t have data on magnitude of dispersion for media.
  - Better to be explicit with lack of knowledge rather than making a wild guess
  - If the solute is distributed relatively uniformly (as in nitrogen), then dispersion and diffusion are not big players
  - If we don’t care about position, but just about final loading

Plug flow description of processes



Need for contaminant transport modeling

Increasing incidents of GW contamination - unplanned GW development, improper waste disposal practices, excessive use of fertilizers/pesticides in agriculture, & lack of public awareness in general.

GW mathematical modeling is an indispensable tool to manage increasing GW quality problems and successfully apply appropriate remediation programs.

Mathematical models

Deterministic mathematical models

- analytical (which require highly idealized parameters and boundaries),
- lumped-parameter (in which porous-media properties are treated as lumped parameters), or
- distributed parameter models (which allow representation of more realistic distribution of system properties).

Distributed parameter models

Mathematical solute-transport models require numerical solution of at least two PDEs:

- Flow eq - GW flow velocities
- Transport eq - chemical concentration in GW

Eqs solved sequentially, if water properties remain constant.

Eqs solved simultaneously, if water properties are affected significantly by changes in solute concentration.

Governing Eqs

Flow eq.

$$\frac{\partial}{\partial x_i}\left(K_i \frac{\partial h}{\partial x_i}\right) + q_s = S_s \frac{\partial h}{\partial t}$$

Solute transport eq.

$$\frac{\partial(\theta C)}{\partial t} = \frac{\partial}{\partial x_i}\left(\theta D_{ij} \frac{\partial C}{\partial x_j}\right) - \frac{\partial}{\partial x_i}\left(\theta v_i C\right) + q_s C_s$$

Transport eq. is related to flow eq. through Darcy's Law

$$v_i = \frac{q_i}{\theta} = -\frac{K_i}{\theta} \frac{\partial h_i}{\partial x_i}$$

Governing Eqs

Dispersion coefficient

$$D_{xx} = \alpha_L \frac{v_x^2}{|v|} + \alpha_T \frac{v_y^2}{|v|} + \alpha_T \frac{v_z^2}{|v|} + D^*$$

$$D_{xy} = D_{yx} = (\alpha_L - \alpha_T)\frac{v_x v_y}{|v|}$$

Other components D_{yy}, D_{zz} D_{zy}, D_{zx}, D_{yz}, D_{yx}, D_{xz}, D_{xy}

Numerical Modeling of Contaminant Transport in Groundwater Aquifers

Projection of the spatial and temporal distribution of the concentration for the given forcing function, ICs, BCs and parameters

Basic Strategy: MT3D

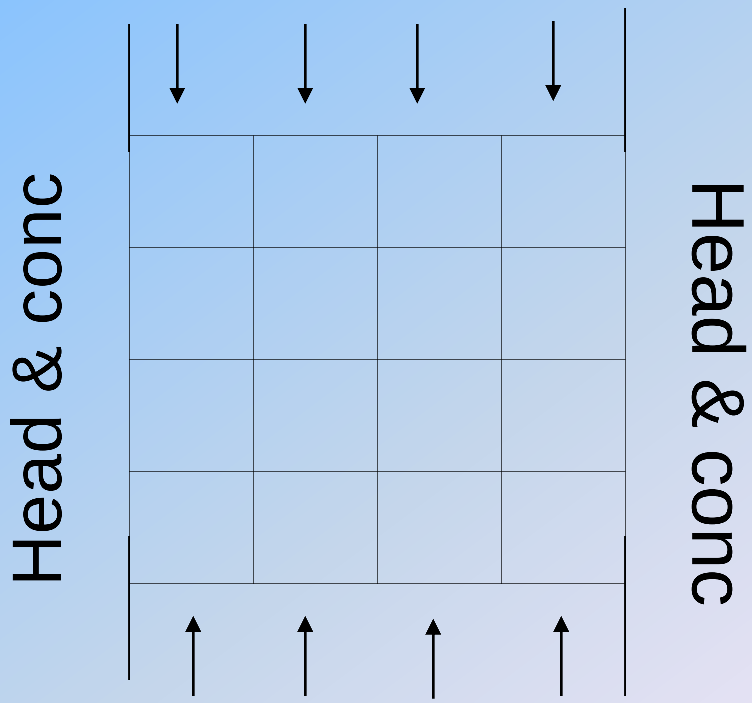
- FD grid is superposed over the study area
- Time domain is discretized by finite number of time levels
- Start from an initial time level (known heads and conc.) and set up an advanced time level
- Solve the flow eq to estimate nodal heads at advanced time level (by FDM - using MODFLOW)
- Compute flow velocities, using pre-computed heads and invoking Darcy’s law

Basic Strategy: MT3D (contd.)

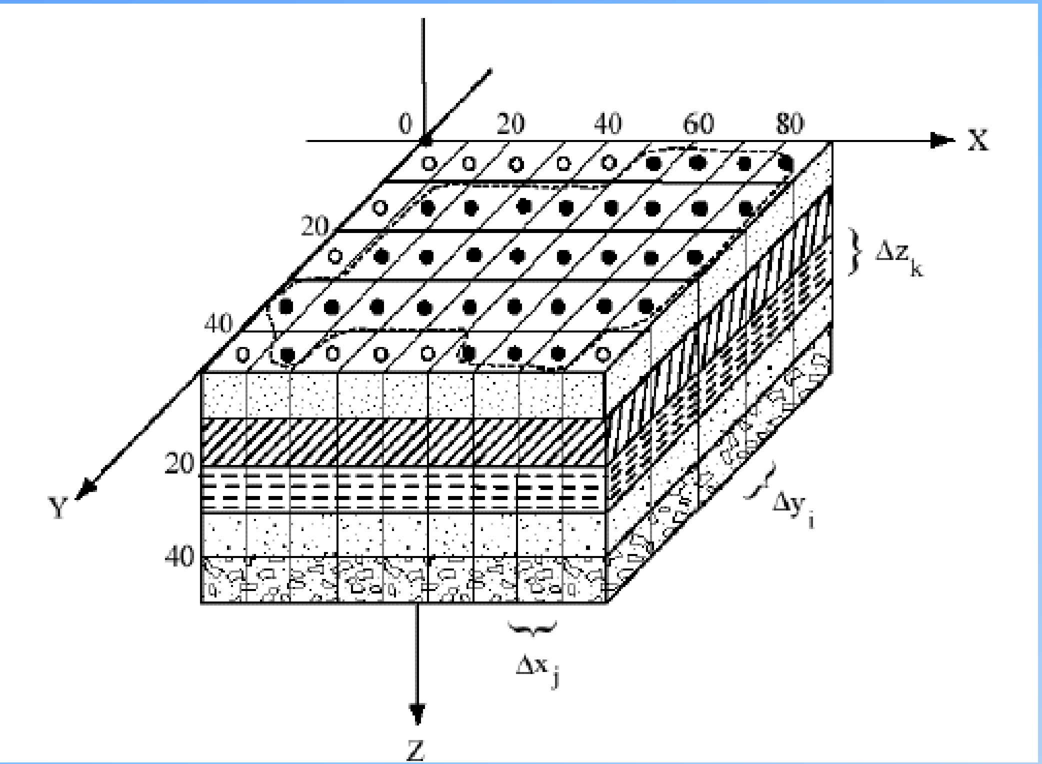
- Solve the transport eq to estimate nodal concentrations at advanced time level
- March in the time domain
- Compute the resultant nodal concentrations at *all* the advanced time levels

Initial & Boundary Conditions

- IC: Nodal heads & conc. at zero time level
- Flow BC: Heads or flow rates
- Transport BC: Conc. or fluxes
- Forcing Function: Lateral fluxes from across the boundary, vertical fluxes



Spatial discretization



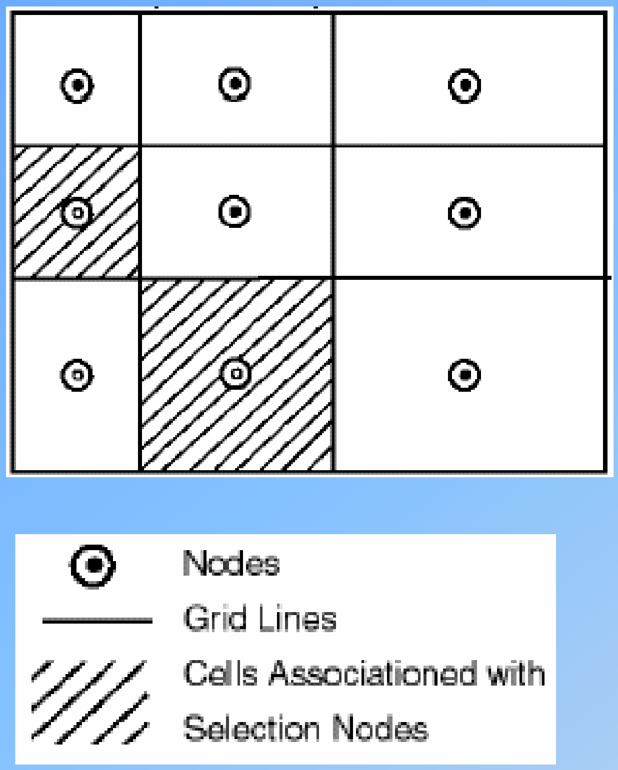
Aquifer is discretized into a mesh of blocks/cells using suitable number of rows (I), columns (J), and layers (K).

- - - - - Aquifer boundary

• Active cell

o Inactive cell

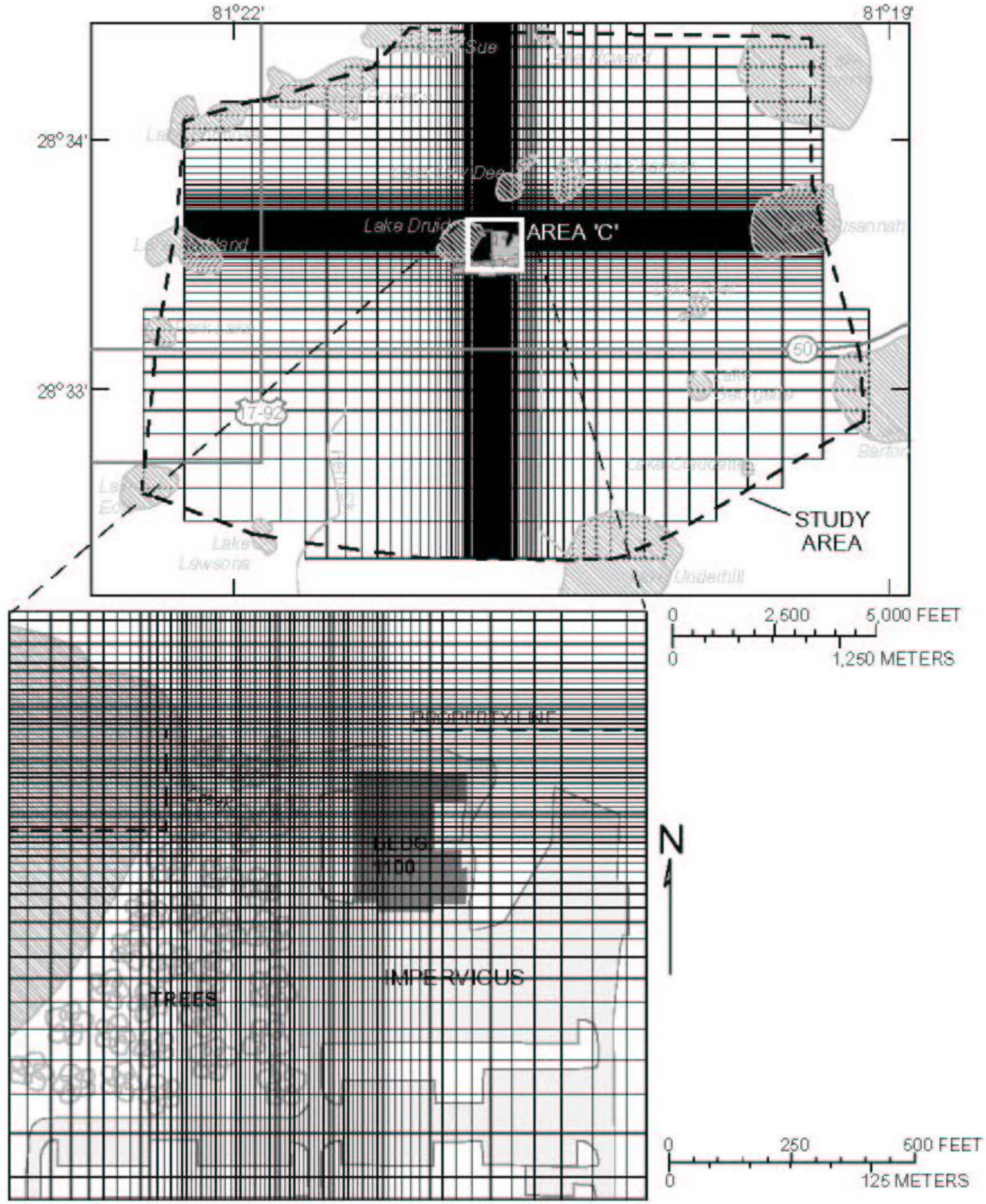
Spatial/Parameter discretization



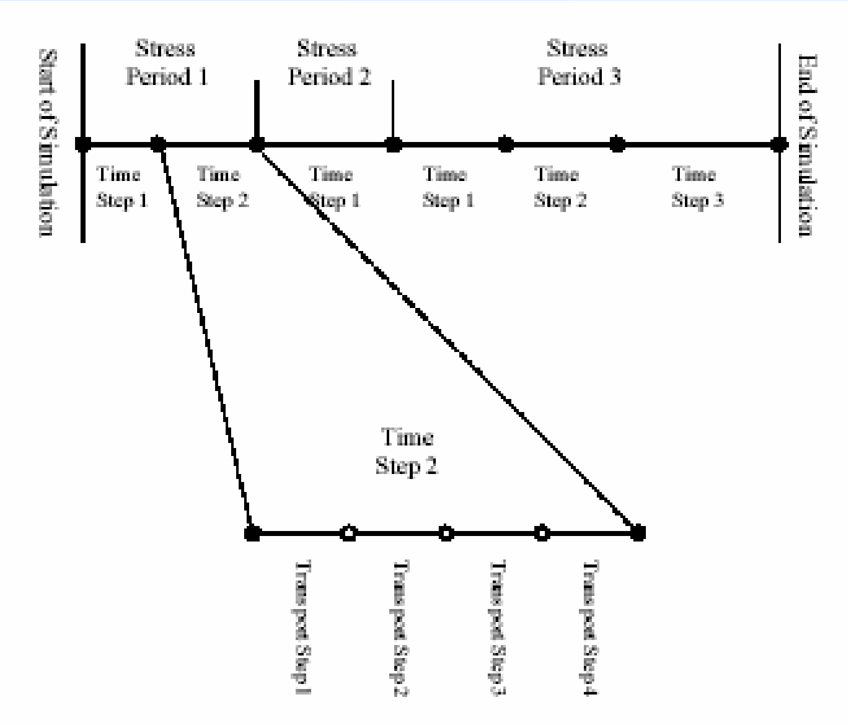
The hydraulic and chemical parameters (such as K or D) are assumed to be uniform over the extent of a cell.

Concentration or hydraulic head is calculated at the centre (node) of a cell.

Variably spaced FD grid allows good discretization of remediation area, while allowing model to go to hydrologic boundaries.



Temporal discretization



In MODFLOW, simulation time is divided into stress periods, which are in turn divided into time steps.

For transport solution, each time step of head solution is divided further into smaller transport time steps, during which heads are considered constant.

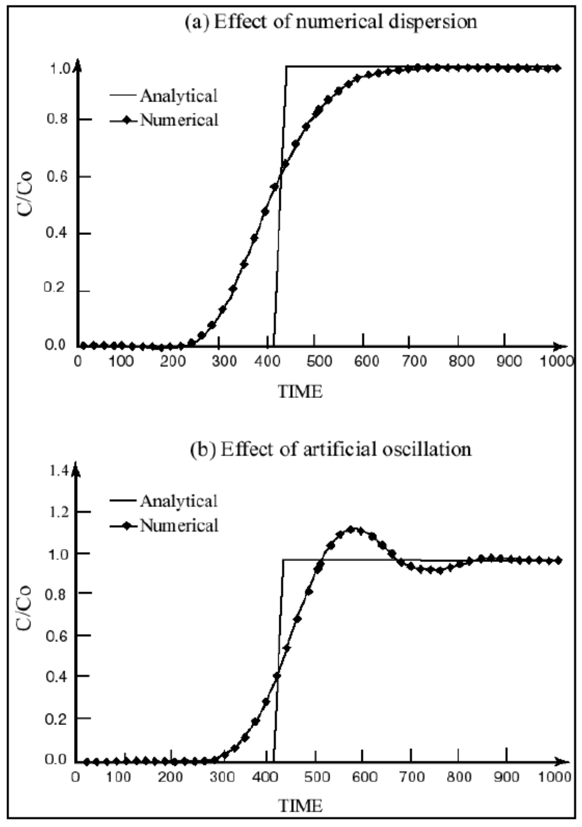
Transport Eq Sol: Numerical Techniques

Advection dominated problems $P_e = \frac{|v|L}{D}$

Pe >> 1 advection dominates; Pe << 1 diffusion dominates

Two types of numerical problems:

- Numerical dispersion (when physical dispersion is small or negligible)
- Artificial oscillation (overshoot & undershoot)



<u>Standard FDM method suitable</u> when

(1) physical dispersivity is large, or

(2) grid spacing is sufficiently fine.

MASS BUDGET CALCULATIONS

At the end of each transport step, mass budget is calculated to find out the total mass into or out of the GW flow system:

$$DISCREPANCY(\%) = \frac{(IN - OUT)}{0.5(IN + OUT)} \times 100$$

Model Calibration, Validation, Sensitivity Analysis

- Calibration – process of making the model match real-world data. Involves making several model runs, varying parameters until the 'best fit' is achieved.
- Validation – process of confirming validity of calibration by using the model to fit an independent set of data.
- Sensitivity analysis – process of changing parameters to see the effect on model results. The most sensitive parameters need to be checked for accuracy to ensure the best model.

List of packages included in MT3D

Package Name **Abbreviation** **Package Description**

Basic Transport **BTN** Handles basic tasks; specification of BC & IC, determination of stepsize, printout of simulation results.

Flow Model Interface **FMI** Interfaces with a flow model. FMI Package prepares heads and flow terms in the form needed by MT3D.

Advection **ADV** Solves the concentration change due to advection

Dispersion **DSP** Solves the concentration change due to dispersion

List of packages included in MT3D

Package Name **Abbreviation** **Package Description**

Sink & Source Mixing **SSM** Solves the concentration change due to sink/source mixing explicitly or formulates the coefficient matrix of all sink/source terms for the matrix solver.

Chemical Reactions **RCT** Solves concentration change due to reaction explicitly or formulates the coefficient matrix of the reaction term for the matrix solver.

Generalized Conjugate Gradient Solver **GCG** Solves the matrix equations resulting from the implicit solution of the transport equation.

Utility **UTL** Contains utility modules that are called upon by primary modules to perform such general-purpose tasks as input/output of data arrays.

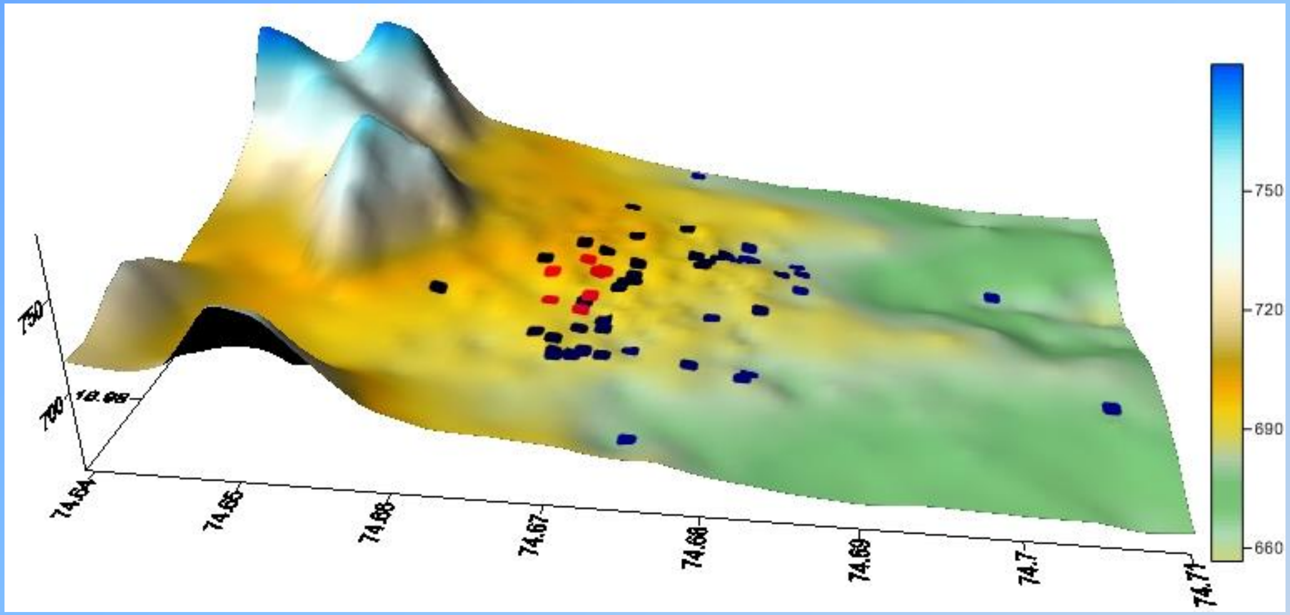
Making Regulatory Decisions

- What models can do:
  - Predict trends and directions of changes
  - Improve understanding of the system and phenomena of interest
  - Estimate a range of possible outcomes or system behavior in the future.

Making Regulatory Decisions

- What models CANNOT do:
  - Simulate phenomena the model wasn’t designed for.
  - Represent natural phenomena exactly
  - Predict unpredictable future events
  - Eliminate uncertainty

Case study



3D surface map of the study area

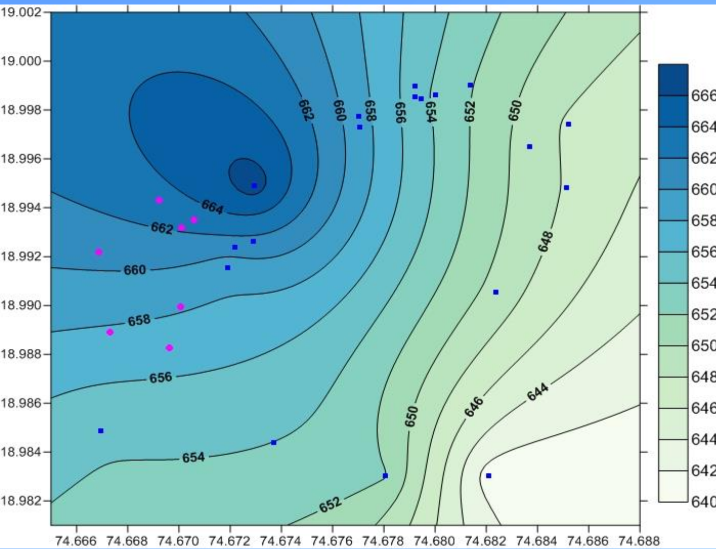
Topography of study area blue dots show sampling locations while red dots mark the depot well locations.

BTEX refers to the chemicals benzene, toluene, ethylbenzene and xylene; compounds occur naturally in crude oil

Study Domain

- Area is underlain by Deccan Trap and groundwater is extracted through both dug wells and borewells.

- Depth of dugwells varies from 8 m to 20 m in general, while the borewells extend from depths of 60 m to more than 80 m.



Water table elevation map of study area based on monitored DTWL at selected locations in June 2016 (pink color dots show the wells locations).

Monthly values of rainfall recharge

Month	Jan	Feb	Mar	Apr	May	June	July	Aug	Sept	Oct	Nov	Dec
Recharge (mm)	0	0	0	0	0	14.61	11.26	14.19	22.97	6.5	2.44	0

Aquifer Parameters

- ***Slug tests*** conducted at 3 different sites. Cooper-Papadopolus-Bredehoeft (1967) and Hvorslev slug test method (1951) have shown K in general varies around 0.05 to 2 m/d. Value of K in northern parts (lower topography) is higher compared to southern parts (Jadhav wadi region).

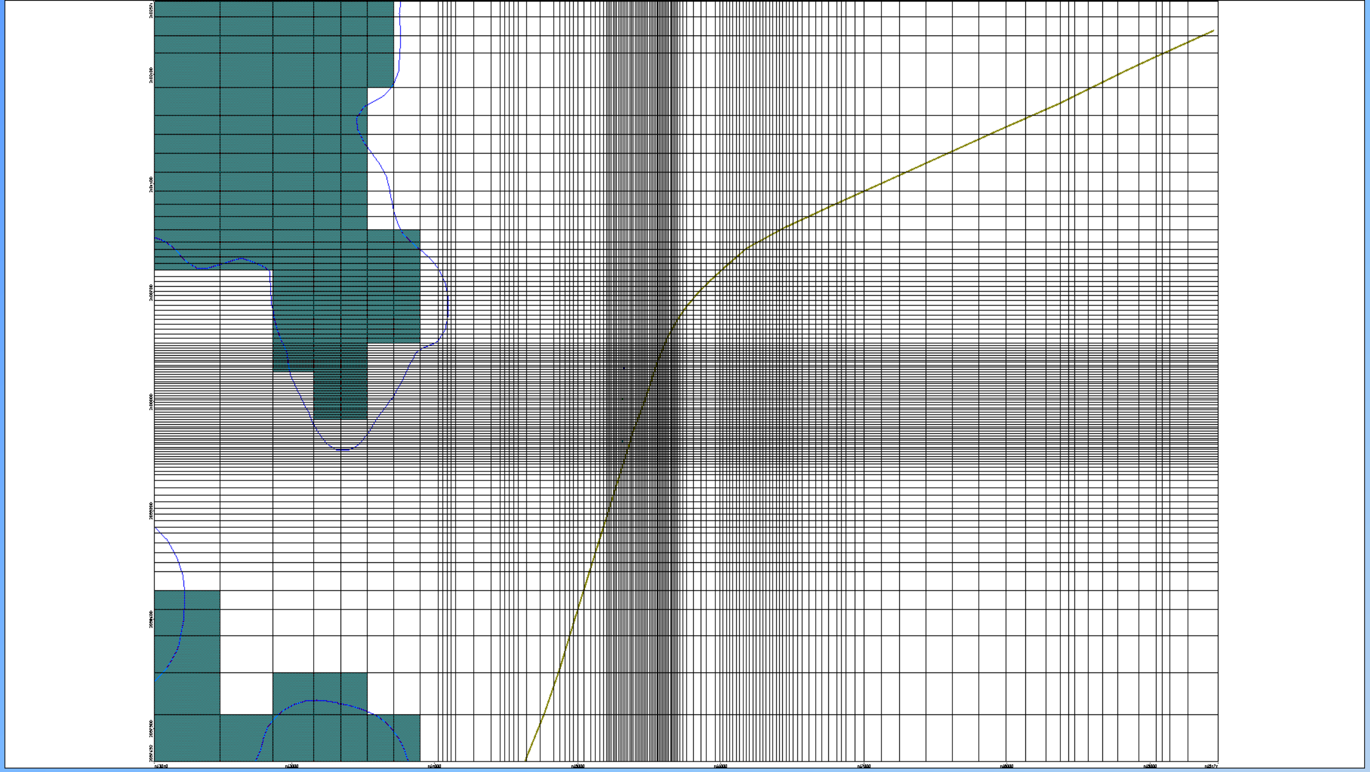
  K of volcanic rocks varies from 0.05 to 15 m/day (GEC)

- Recommended value of Sy for vesicular basalt terrain is 0.02. Effective porosity taken to be 0.22 (average total porosity of soil, based on analyses of soil samples collected from field, computed to be 44%). The value of longitudinal dispersivity was taken as 10 m.

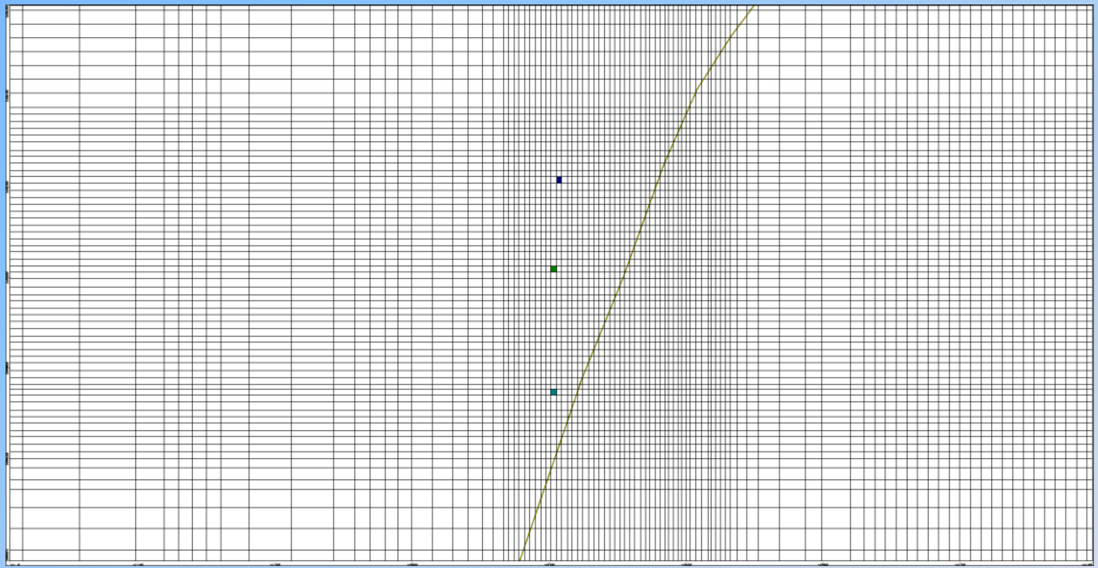
Study Domain

Study domain was extended to minimize impact of BCs on area of interest. Extended boundaries were assumed to be no-flow boundaries. Top surface of upper layer of model was taken to be topographic elevation of gs of study area.

Study domain was discretized by 105 rows and 139 columns. Near well locations and contaminant source locations, grid spacing kept smaller. Hilly area above 720 m of elevation above msl on north-west and south-west marked by inactive FD cells.



Discretization of extended study domain by finite difference cells in horizontal plane (green color shows inactive cells).



Three possible locations of contaminant sources.

These sites correspond to storage tanks locations and oil water separator site. The railway track is shown in olive color.

Simulation Runs

- Model was run for transient conditions assuming initial heads (water table elevation) corresponding to June 2016 for average values of rainfall recharge and evapotranspiration values.

- GW draft corresponding to dug/ open wells and bore wells was taken as 46 m^3/d and 518 m^3/d.

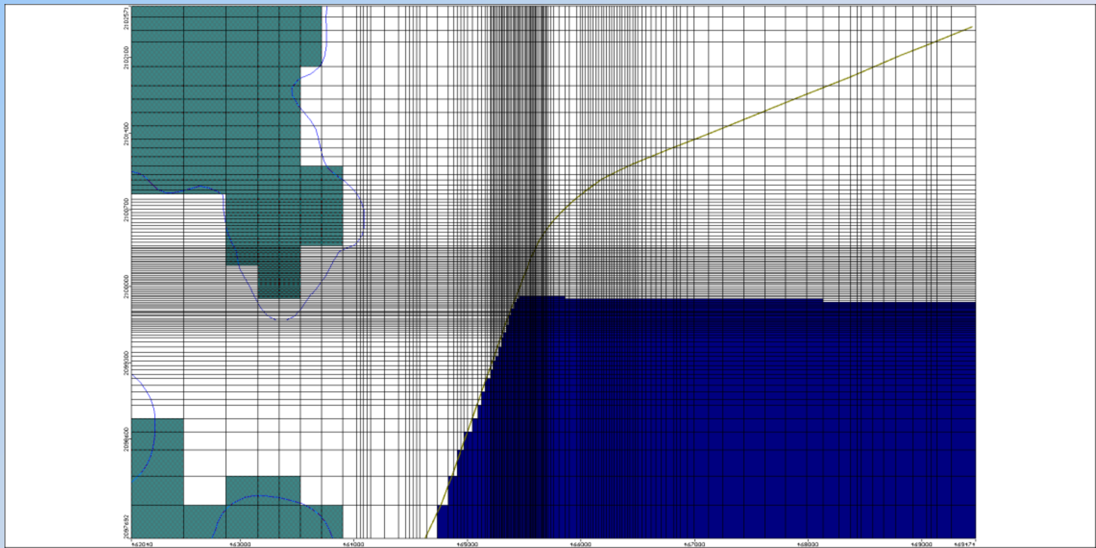
- Three separate sites (point sources) were selected as possible source of contaminant in depot premises (each site of size 9 m x 9 m) including one near oil water separator location where the fuel is offloaded and possible oil spill may occur.

- Contaminant concentration was taken as 2580 mg/l at the 3 sites which is maximum total solubility of BTEX in water. As a worst case scenario, contaminant was directly released into saturated zone of aquifer. Distribution coeff for simulating sorption process was taken as 1E-07 l/mg while first order reaction rate for dissolved phase was taken as 0.002/day.

Simulation Run Scenarios

Three scenarios were simulated based on three sets of possible values of K. Total simulation period for scenarios 1 and 2 was 3 yrs, while for scenario 3 it was 10 yrs

Scenario 1	Zone 1: Kx = Ky = 0.5 m/d, Kz = 0.05 m/d Zone 2: Kx = Ky = 0.5 m/d, Kz = 0.05 m/d
Scenario 2	Zone 1: Kx = Ky = 2.0 m/d, Kz = 0.2 m/d Zone 2: Kx = Ky = 1.0 m/d, Kz = 0.1 m/d
Scenario 3	Zone 1: Kx = Ky = 1.0 m/d, Kz = 0.1 m/d Zone 2: Kx = Ky = 0.5 m/d, Kz = 0.05 m/d



Simulation Runs

- For given values of K, contaminant plume may travel spatially on account of advection and hydrodynamic dispersion while at the same time it may get attenuated due to sorption and first order irreversible decay.

- Presence of contaminant at a depth of 8 m below its point of release shows significant attenuation. Figures show position of plume after a period of 3 years.

- Plume extent shows concentration values above 1.51 mg/l which is the permissible limit of BTEX in water by WHO.

Conclusions

- All scenarios illustrate that during a period of 3 to 10 yrs, the plume does not migrate over long distances, even though contaminant source is assumed to be releasing contaminant into aquifer at a constant rate throughout the year, whereas, during the field visits, contamination was found to be significant even in wells located as far as 800 -1000 m from the depot premises.

- WQ analyses revealed that contaminant becomes ‘not detectable’ during a period of 8 months (Nov 2015 to June 2016) in wells where its presence was significantly high in Nov 2015. This kind of contaminant degradation in field reveals that source of contaminant is not constant.

- Results discussed only an indication of field conditions.

Thank you !