Module 7 – (L27 – L30): “Management of Water Quality”:

Water quality and pollution, types and Sources of pollution, water quality modeling, environmental guidelines for water quality

WATERSHED MANAGEMENT

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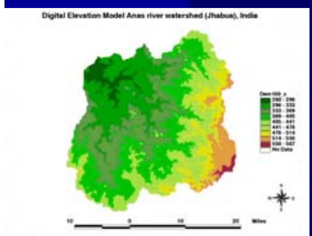
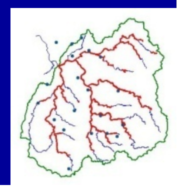
Lecture No - 29 Water Quality Modeling

L29– Water Quality Modeling

- **Topics Covered**
- Water quality, protection, quality goals, Hydrodynamics, Transport processes, Oxygen regime, Mathematical modeling, Governing equations, numerical modeling, Groundwater transport modeling.
- Keywords: Water quality modeling, Hydrodynamics, Mathematical/ numerical modeling, Groundwater transport.





Introduction - Water Quality Modeling

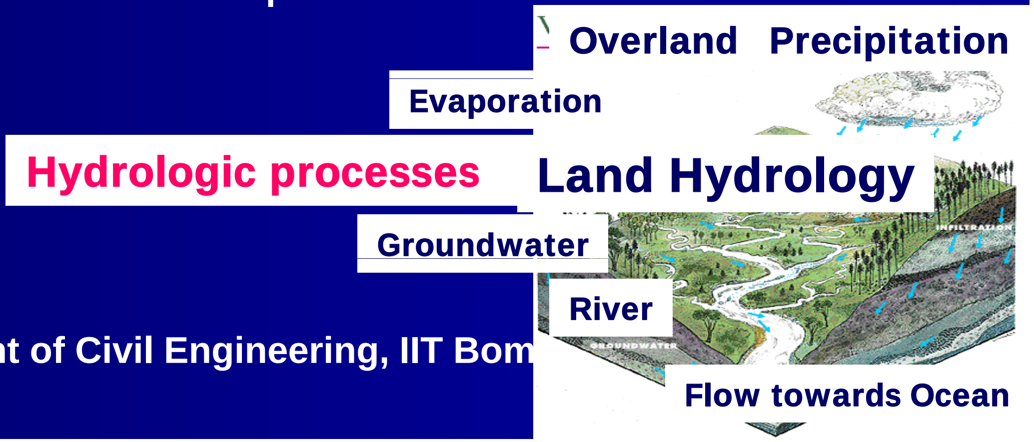
- Water quality models simulate the fate of pollutants & state of selected water quality variables in water bodies
- Incorporates variety of physical, chemical, & biological processes which control the transport and transformation of these variables
- Temperature, solar radiation, wind speed, pH, and light attenuation coefficients – important parameters
- Watershed pollutant loading
- Each water quality model has its own set of characteristics and requirements- (some models can be applied to several types of water bodies and some models only for particular water bodies)

Types of Water Quality Modeling

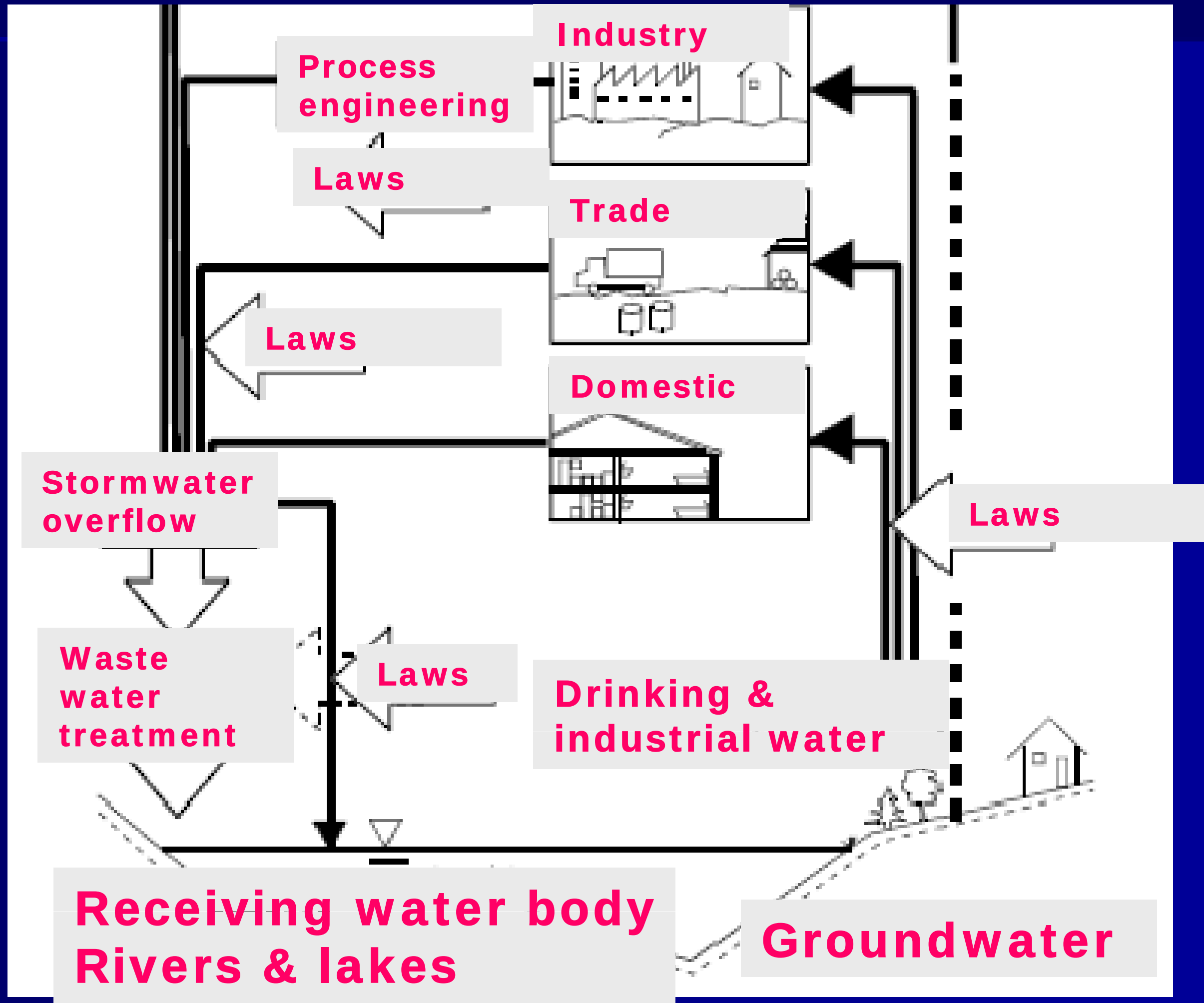
- Water quality is modeled by one or more of the following formulations:
- Advective transport formulations;
- Dispersive transport formulation;
- Heat budget formulation;
- Dissolved oxygen saturation; Reaeration
- Carbonaceous deoxygenation, Sediment, BOD, pH, Alkalinity, Nutrients, Algae, Microorganism etc

Water Quality – Hydrological Cycle

- Emissions: (Ex = out of) from the user's point of view (community, factory, etc.)
- Avoidance and reduction of pollution into the environment - sanitary engineering
- Immissions: (In = into) - from the water body's point of view: consequences of pollution, injections, etc.
- Environmental fluid mechanics: flow and transport in surface waters (rivers and lakes); flow and transport in soil and groundwater; flow & transport in the atmosphere



Water Quality Modeling – Water Cycle



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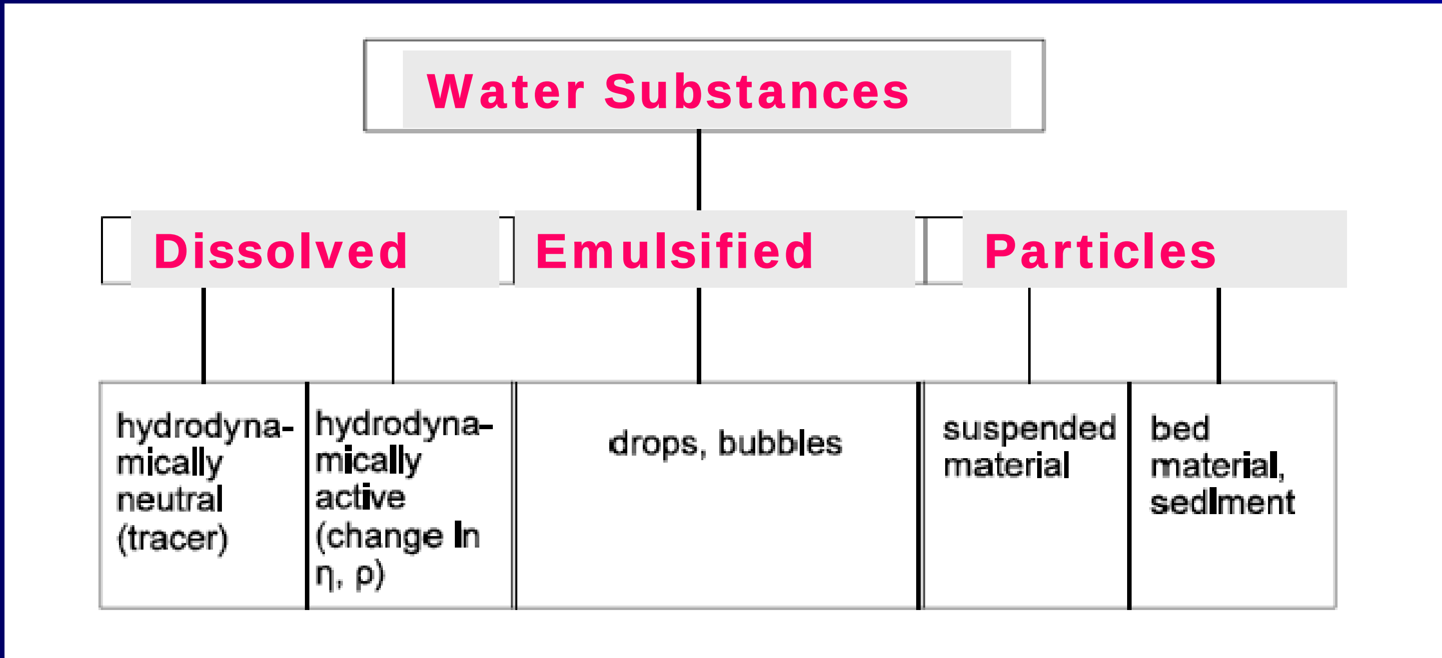
Water Quality Protection– Goals

- Water quality protection - ensure the quality of water which guarantees the preservation of environmental goods.
- **Environmental Goods:**
- functions of the river as water resource; community of aquatic living; fishing; irrigation of farm land
- leisure and recreation; focus on contamination
- substances from inland & suspended solids & sediments; drinking water supply
- **Quality goals:** given as a concentration of a substance - show condition of river with regard to the environmental goods - function as an instrument for decisions, protection & improvement of water quality; derived from effective values & law

Water Quality Modeling - Considerations

- Water Substances -



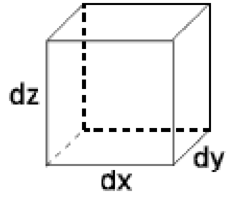
Water Quality Modeling - Considerations

- Governing laws -

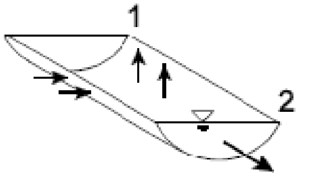
Conservation Laws

Mass | Momentum | Substances in water | Energy / heat

Elementary CV - Micro



CV – Macro scale



Water Quality – Mathematical Modeling

- The prediction of water pollution using mathematical simulation techniques.
- A typical water quality model consists of a collection of formulations representing physical mechanisms that determine position and momentum of pollutants in a water body.
- Models are available for individual components of the hydrological system such as surface runoff
- Models addressing hydrologic transport and for ocean and estuarine applications.

Water Quality Modeling - Hydrodynamics

- Conservation of Mass:

Mass balance in a CV fixed in space with the density $\rho = \rho(x,y,z,t)$ and the velocity $v = v(x,y,z,t)$:

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

- Incompressible fluids

(i.e. ρ = const. $\Rightarrow \partial\rho/\partial t = 0$)

$$\frac{\partial v_x}{\partial x} + \frac{\partial v_y}{\partial y} + \frac{\partial v_z}{\partial z} = div\ \vec{v} = 0$$

Water Quality Modeling - Hydrodynamics

- Conservation of Momentum – Navier-Stokes equations

$$\frac{\partial v_x}{\partial t} + v_x\frac{\partial v_x}{\partial x} + v_y\frac{\partial v_x}{\partial y} + v_z\frac{\partial v_x}{\partial z} = -g\frac{\partial h}{\partial x} + \nu[\frac{\partial^2 v_x}{\partial x^2} + \frac{\partial^2 v_x}{\partial y^2} + \frac{\partial^2 v_x}{\partial z^2}]$$

$$\frac{\partial v_y}{\partial t} + v_x\frac{\partial v_y}{\partial x} + v_y\frac{\partial v_y}{\partial y} + v_z\frac{\partial v_y}{\partial z} = -g\frac{\partial h}{\partial y} + \nu[\frac{\partial^2 v_y}{\partial x^2} + \frac{\partial^2 v_y}{\partial y^2} + \frac{\partial^2 v_y}{\partial z^2}]$$

$$\frac{\partial v_z}{\partial t} + v_x\frac{\partial v_z}{\partial x} + v_y\frac{\partial v_z}{\partial y} + v_z\frac{\partial v_z}{\partial z} = -g\frac{\partial h}{\partial z} + \nu[\frac{\partial^2 v_z}{\partial x^2} + \frac{\partial^2 v_z}{\partial y^2} + \frac{\partial^2 v_z}{\partial z^2}]$$

Water QM- Hydrodynamics & Transport

- Diffusive processes: Molecular diffusion; Turbulent diffusion & dispersion
- Molecular diffusion is a transport process that originates from molecular activity (Brownian movement). The driving force for molecular diffusion is a concentration gradient.
- The molecular diffusion is described by the molecular diffusion coefficient Dm.

Fick's First Law:

specific mass flux: $q = -D_m \frac{\partial c}{\partial x}$

Mass transport equation

$$\left(v_x \frac{\partial c}{\partial x} + v_y \frac{\partial c}{\partial y} + v_z \frac{\partial c}{\partial z} \right) - D_m \left(\frac{\partial^2 c}{\partial x^2} + \frac{\partial^2 c}{\partial y^2} + \frac{\partial^2 c}{\partial z^2} \right) = -\frac{\partial c}{\partial t}$$

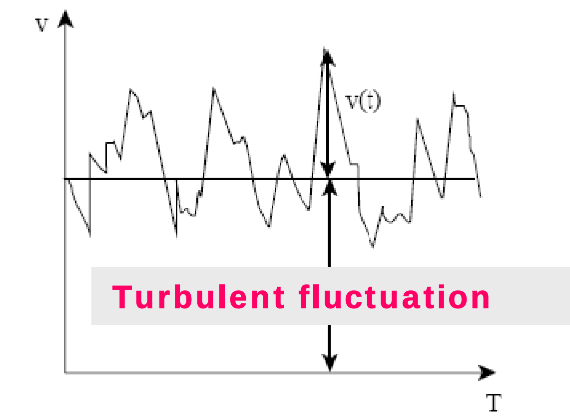
Water QM – Hydrodynamics & Transport

Heat transfer equation

$$\left(v_x \frac{\partial T}{\partial x} + v_y \frac{\partial T}{\partial y} + v_z \frac{\partial T}{\partial z} \right) - D_T \left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2} \right) = -\frac{\partial T}{\partial t}$$

- Turbulent flow: **Nature of turbulence:** irregular (characterized by variations with respect to time); intensive mixing; rotation; dissipative (increased losses of energy)

velocity	$v = \bar{v} + v'$
pressure	$p = \bar{p} + p'$



Water QM- Hydrodynamics & Transport

- Turbulent flow: Continuity & momentum (x-dir.)

$$\left(\frac{\partial \overline{v_x}}{\partial z} + \frac{\partial \overline{v_y}}{\partial y} + \frac{\partial \overline{v_z}}{\partial z}\right) \equiv 0$$

$$\frac{\partial \overline{v_x}}{\partial t} + \overline{v_x}\frac{\partial \overline{v_x}}{\partial x} + \overline{v_y}\frac{\partial \overline{v_x}}{\partial y} + \overline{v_z}\frac{\partial \overline{v_x}}{\partial z} = -g\frac{\partial \overline{h}}{\partial x} + \frac{1}{\rho}\frac{\partial}{\partial x}\left(\eta\frac{\partial \overline{v_x}}{\partial x} - \rho\overline{v_x'^2}\right) + \frac{1}{\rho}\frac{\partial}{\partial y}\left(\eta\frac{\partial \overline{v_x}}{\partial y} - \rho\overline{v_x' v_y'}\right) + \frac{1}{\rho}\frac{\partial}{\partial z}\left(\eta\frac{\partial \overline{v_x}}{\partial z} - \rho\overline{v_x' v_z'}\right)$$

unknown

Reynolds number:

$$Re = \frac{v_{ch} L_{ch}}{\eta/\rho} = \frac{\text{inertial reaction}}{\text{viscosity force}}$$

		lower $Re_{critical}$
Pipe flow d: diameter of the pipe	$Re = \frac{vd}{\eta/\rho}$	~ 2000
Open Channel flow y: water depth	$Re = \frac{vy}{\eta/\rho}$	~ 500

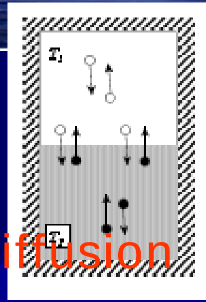
The kinematic viscosity is defined as:

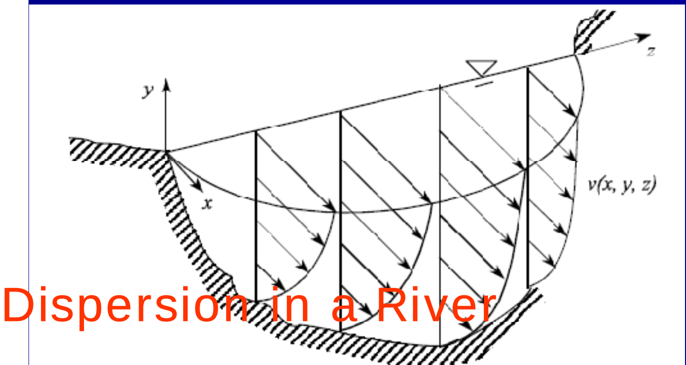
$$\nu = \frac{\text{dynamic viscosity } \eta}{\text{density } \rho}$$

Ref: Lecture notes on Environmental Fluid Mechanics, Prof. H. Kobus, Dept. Civil Engg., Uni. Stuttgart, Germany

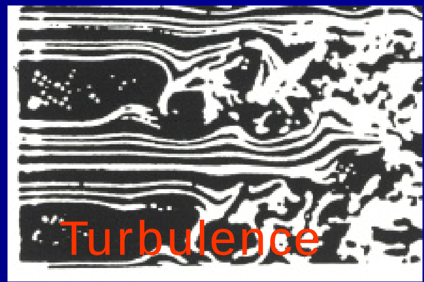
Water Quality Modeling

Molecular diffusion:	$q = -D_m \dfrac{\partial c}{\partial x}$
Turbulent diffusion:	$q = -\varepsilon_D \dfrac{\partial c}{\partial x}$
Dispersion:	$q = -K \dfrac{\partial \bar{c}}{\partial x}$
Momentum flux:	$\tau = -\rho \nu \dfrac{\partial v_x}{\partial y}$
Turbulent momentum exchange :	$\tau = -\rho \nu_t \dfrac{\partial \bar{v}_x}{\partial y}$
Heat flux:	$q_T = -\rho c_p D_T \dfrac{\partial T}{\partial x}$


Diffusion



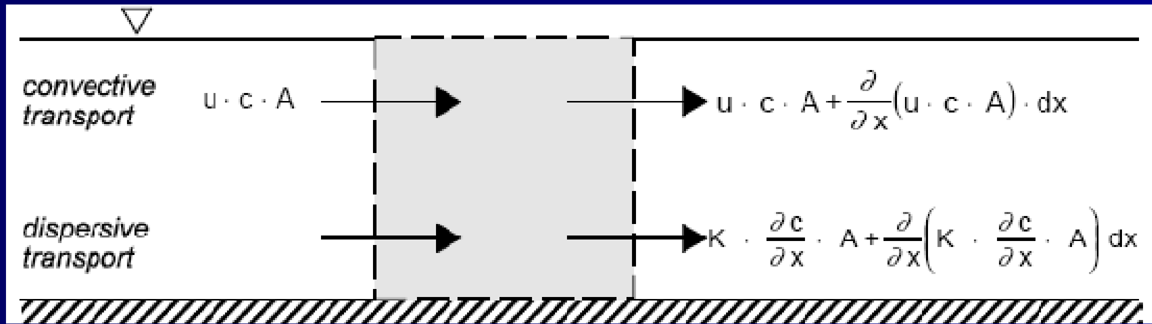
Dispersion in a River


Turbulence

Ref: Lecture notes on Environmental Fluid Mechanics, Prof. H. Kobus, Dept. Civil Engg., Uni. Stuttgart, Germany

WQM- Transport in Rivers & Canals

- One dimensional transport:



size of section	microscopic	macroscopic
distribution process	diffusion	dispersion
velocity distribution	$v = v(x, y, z)$	$v = \bar{v}(z)$
concentration distribution	$C = C(x, y, z)$	$C = \bar{C}(z)$
mass balances	$\frac{\partial C}{\partial t} + v(x, y, z)\frac{\partial C}{\partial x} = \frac{\partial}{\partial x}\left[D\frac{\partial C}{\partial x}\right] + \frac{\partial}{\partial y}\left[D\frac{\partial C}{\partial y}\right] + \frac{\partial}{\partial z}\left[D\frac{\partial C}{\partial z}\right]$ D: diffusion coefficient	$\frac{\partial \bar{C}}{\partial t} + \bar{v}(z)\frac{\partial \bar{C}}{\partial x} = K\frac{\partial^2 \bar{C}}{\partial x^2}$ K: dispersion coefficient

Ref: Lecture notes on Environmental Fluid Mechanics, Prof. H. Kobus, Dept. Civil Engg., Uni. Stuttgart, Germany

WQM- Transport in Rivers & Canals

- **One dimensional transport equation**

$$\frac{\partial \bar{c}}{\partial t} + v_x \frac{\partial \bar{c}}{\partial x} = K \frac{\partial^2 \bar{c}}{\partial x^2} + I$$

v_x	mean velocity in x-direction
$\bar{c}$	concentration averaged over the cross section
I	sink or source term, describes the reaction of the substance with its environment

- **Two dimensional transport equation**

$$\frac{\partial \bar{c}}{\partial t} + \left(v_x \frac{\partial \bar{c}}{\partial x} + v_y \frac{\partial \bar{c}}{\partial y} \right) = \left(K_x \frac{\partial^2 \bar{c}}{\partial x^2} + K_y \frac{\partial^2 \bar{c}}{\partial y^2} \right) + I$$

- **Three dimensional transport equation**

$$\frac{\partial \bar{c}}{\partial t} + \left(v_x \frac{\partial \bar{c}}{\partial x} + v_y \frac{\partial \bar{c}}{\partial y} + v_z \frac{\partial \bar{c}}{\partial z} \right) = \left(K_x \frac{\partial^2 \bar{c}}{\partial x^2} + K_y \frac{\partial^2 \bar{c}}{\partial y^2} + K_z \frac{\partial^2 \bar{c}}{\partial z^2} \right) + I$$

Ref: Lecture notes on Environmental Fluid Mechanics, Prof. H. Kobus, Dept. Civil Engg., Uni. Stuttgart, Germany

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WQM- Oxygen regime of Rivers

Streeter- Phelps Equation for oxygen regime

The combination of oxygen deficit and reaeration is combined in the Streeter-Phelps-equation:

Assumptions:
- oxygen transfer only over water-air interface
- upstream effects are not taken into account

Governing differential equation:

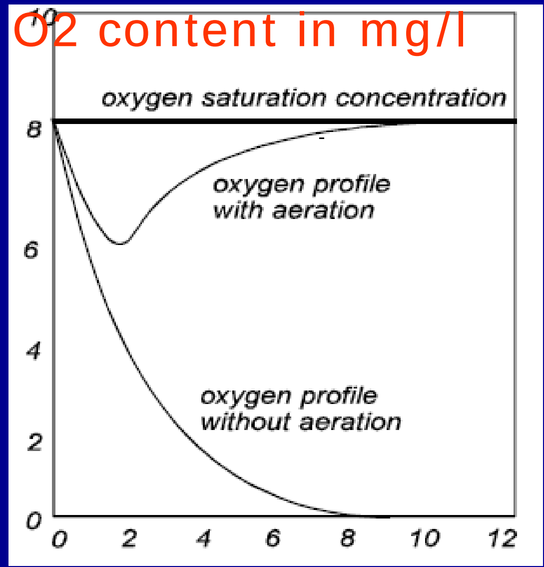
$$\frac{\partial(c_S - \bar{c})}{\partial t} = K_d L - K_a(c_S - \bar{c})$$

Boundary condition:

$$\bar{c}(t = 0) = \bar{c}_0$$

$$L(t = 0) = L_0 = \frac{BOD_5}{1 - e^{-(5d)K_a}}$$

O2 content in mg/l



Time in days

$$\bar{c}_S - \bar{c}(t) = \frac{K_d L_0}{K_a - K_d}\left[e^{-K_d t} - e^{-K_a t}\right] + (\bar{c}_s - \bar{c}_0)\, e^{-K_a t}$$

L	biological oxygen demand [mg/l]
L_0	biological oxygen demand at the time t = 0 [mg/l]
BOD_5	biochemical oxygen demand after 5 days [mg/l]
K_a	coefficient of reaeration [1/d]
	K_L = r/y (y = depth of the water)
K_d	decay coefficient [1/d]
c_S	oxygen saturation concentration, const. (= r, for first order decay)

Ref: Lecture notes on Environmental Fluid Mechanics, Prof. H. Kobus, Dept. Civil Engg., Uni. Stuttgart, Germany

Groundwater Transport Modeling

- 2D non-homogeneous confined aquifer-Flow Equation

$$\frac{\partial}{\partial x}\left(T_x \frac{\partial h}{\partial x}\right) + \frac{\partial}{\partial y}\left(T_y \frac{\partial h}{\partial y}\right) = S\frac{\partial h}{\partial t} + Q_w \delta(x - x_i)(y - y_i) - q_s$$

- 2D non-homogeneous unconfined aquifer-Flow Equation

$$\frac{\partial}{\partial x}\left(K_x \frac{\partial h}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_y \frac{\partial h}{\partial y}\right) = S_y\frac{\partial h}{\partial t} + Q_w \delta(x - x_i)(y - y_i) - q_s$$

- 2D Transport equation

$$v_x = -K_x \frac{\partial h}{\partial x} \qquad v_y = -K_y \frac{\partial h}{\partial y}$$

$$R\frac{\partial c}{\partial t} = \frac{\partial}{\partial x}\left(D_{xx}\frac{\partial c}{\partial x}\right) + \frac{\partial}{\partial y}\left(D_{yy}\frac{\partial c}{\partial y}\right) - \frac{\partial}{\partial x}(V_x c) - \frac{\partial}{\partial y}(V_y c) - \frac{c'W}{nb} - R\lambda c$$

Water Quality – Numerical Modeling

- Numerical procedures- approx. sol. to most of field problems.
- Transform a complex practical problem into a simple discrete form of mathematical description
- Recreate & solve the problem on a computer, & finally reveal phenomena virtually according to requirements of analysts.
- Numerical or approximate solution for a complex problem efficiently, as long as proper numerical method is used.
- Numerical methods are used to analyze these phenomena like
  - Finite Difference Method (FDM)
  - Finite Element Method (FEM)
  - Finite Volume Method (FVM)
  - Method of Characteristics (MoC)
  - Boundary Element Method (BEM)
  - Meshfree Method (MFree)

Surface Water Quality Models

- **WASP** Water Quality Analysis Simulation Program, US EPA: Interpret & predict water quality responses to natural phenomena and manmade pollution for various pollution management decisions
- QUAL2K - river and stream water quality model
- Aquatox- simulation model for aquatic systems; predicts the fate of various pollutants, such as nutrients & organic chemicals, & effects on ecosystem
- EPD-RIV1- Riverine Hydrodynamic and Water Quality Model, a system of programs to perform 1D dynamic hydraulic & water quality simulations
- SWMM – Storm Water Management Model

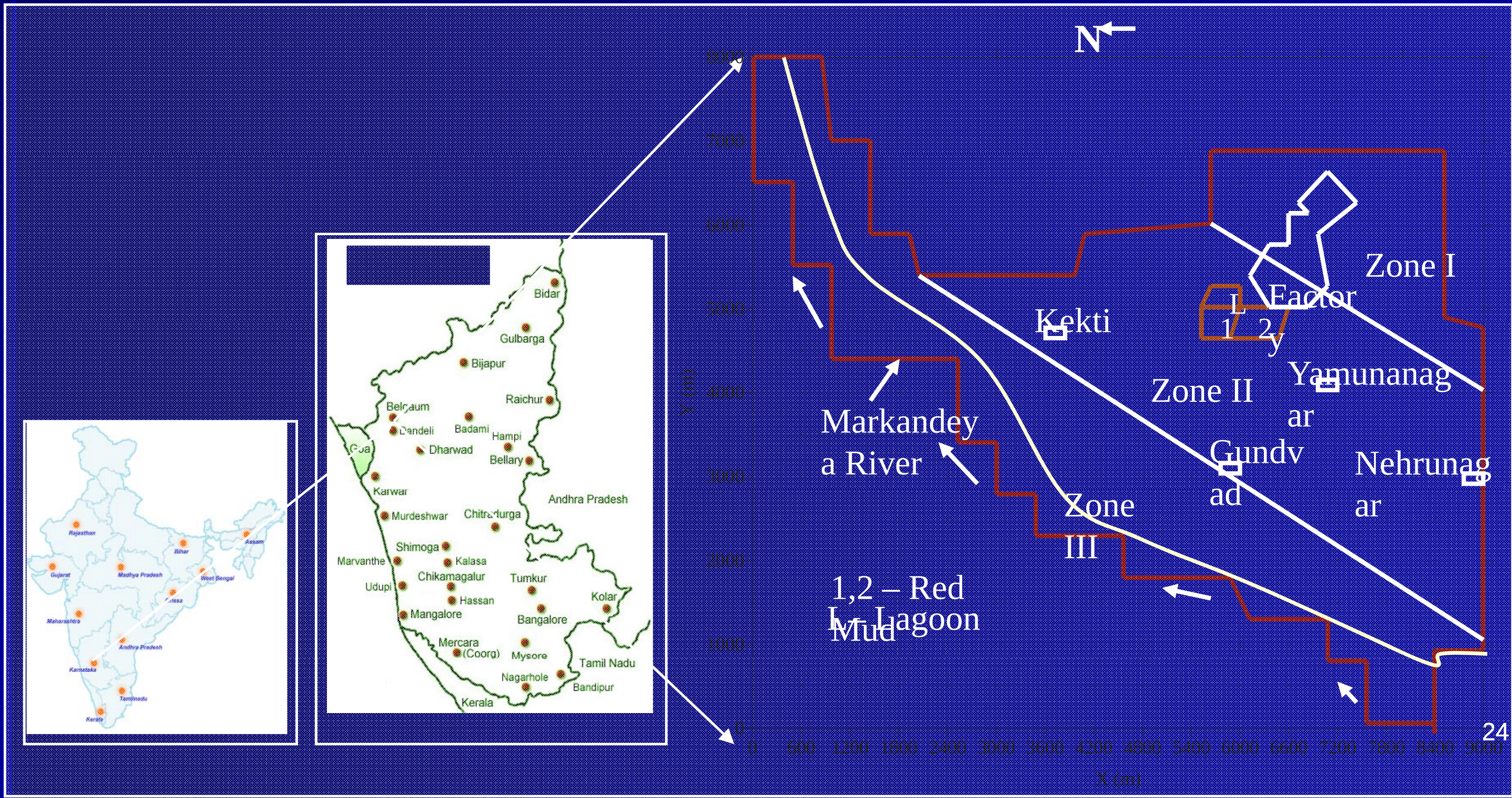
Groundwater Quality Models

- MODFLOW (1988) - USGS flow model for 3-D aquifers
- MODPATH - flow line model for depicting streamlines
- MOC (1988) - USGS 2-D advection/dispersion code
- MT3D (1990, 1998) - 3-D transport code works with MODFLOW
- RT3D (1998) - 3-D transport chlorinated – MODFLOW
- BIOPLUME II, III (1987, 1998) - authored at Rice Univ 2-D based on the MOC procedures.
- FEMWATER
- GMS package

Groundwater Transport Modeling – Case Study

Dhar et al., (1999), NGRI Report; M. Meenal & T. I. Eldho, (2012) Submitted *to Journal of Hydrologic Engineering, ASCE*

- HINDACO-Belgaum, India)



Case study..

- Watershed area- 72 sq. km, basaltic terrain on northern side of Belgaum.
- Watershed is drained by Markandeya river in the north
- Red mud- hydrous silt muddy, highly alkaline solid waste produced by physical and chemical treatments of bauxite in alumina production.
- Red mud is harmful to the ecological environment, safety of its storage has become an environmental problem of concern.
- Natural recharge of 65 mm/yr is given as input to the flow model.
- The seepage from red mud ponds is simulated as additional recharge (130 mm/yr) from the ponds.

Parameter	Value
Hydraulic Conductivity (m/day)	
Zone I	0.5
Zone II	1
Zone III	2
Longitudinal dispersivity (m)	50
Transverse dispersivity (m)	5
Specific Yield	0.2

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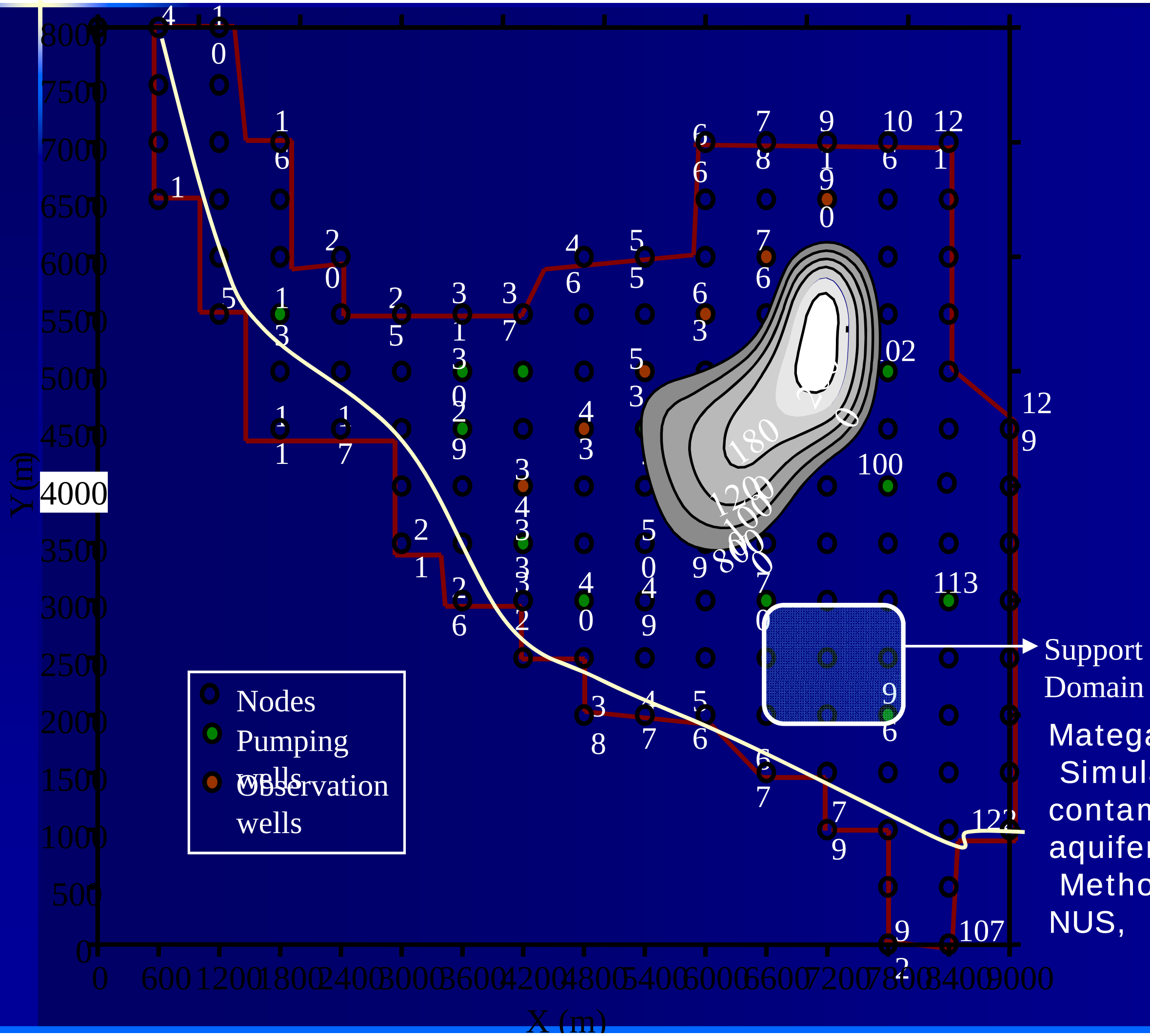
Case study..

Mategaonkar, Meenal, (2012). Ph.D. Thesis, Dept. Civil Engineering, IIT Bombay



Mategaonkar Meenal, Eldho T.I. (2011). Simulation of groundwater flow & contaminant transport in unconfined aquifer using Meshfree Point Collocation Method. IPWE -2011, Jan. 3-7, 2011- NUS, Singapore.

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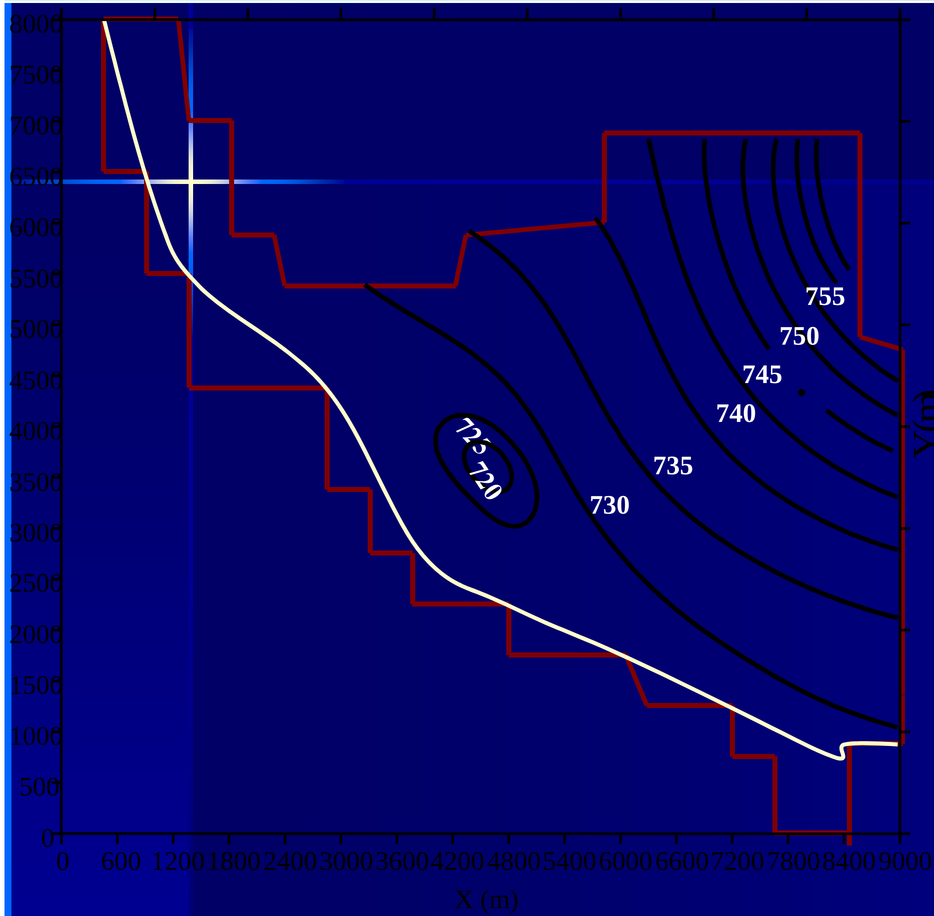
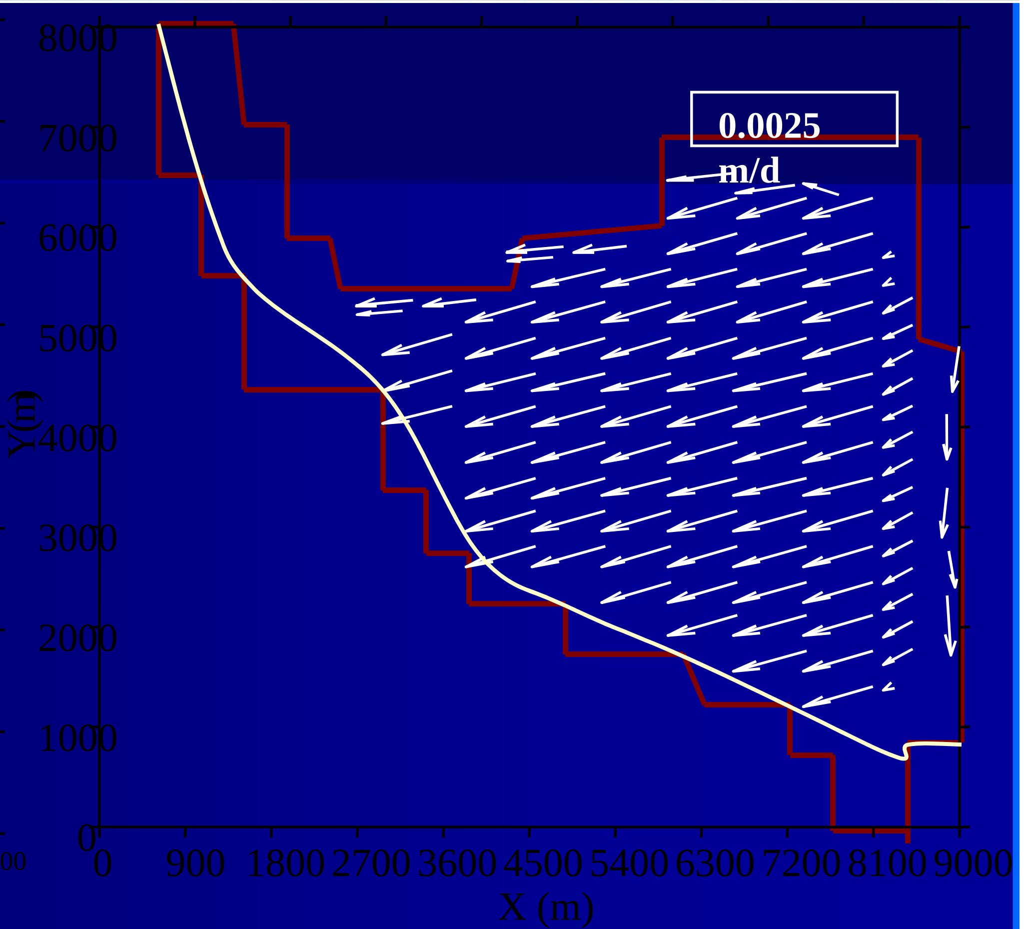
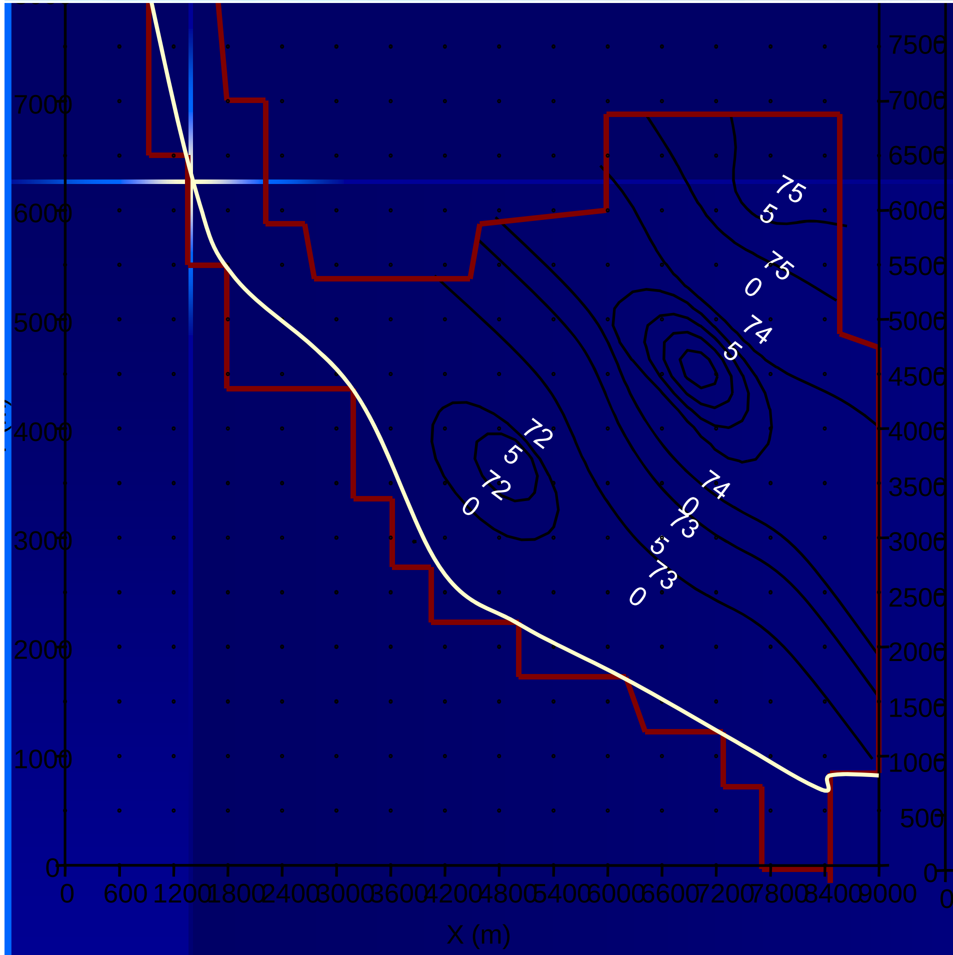


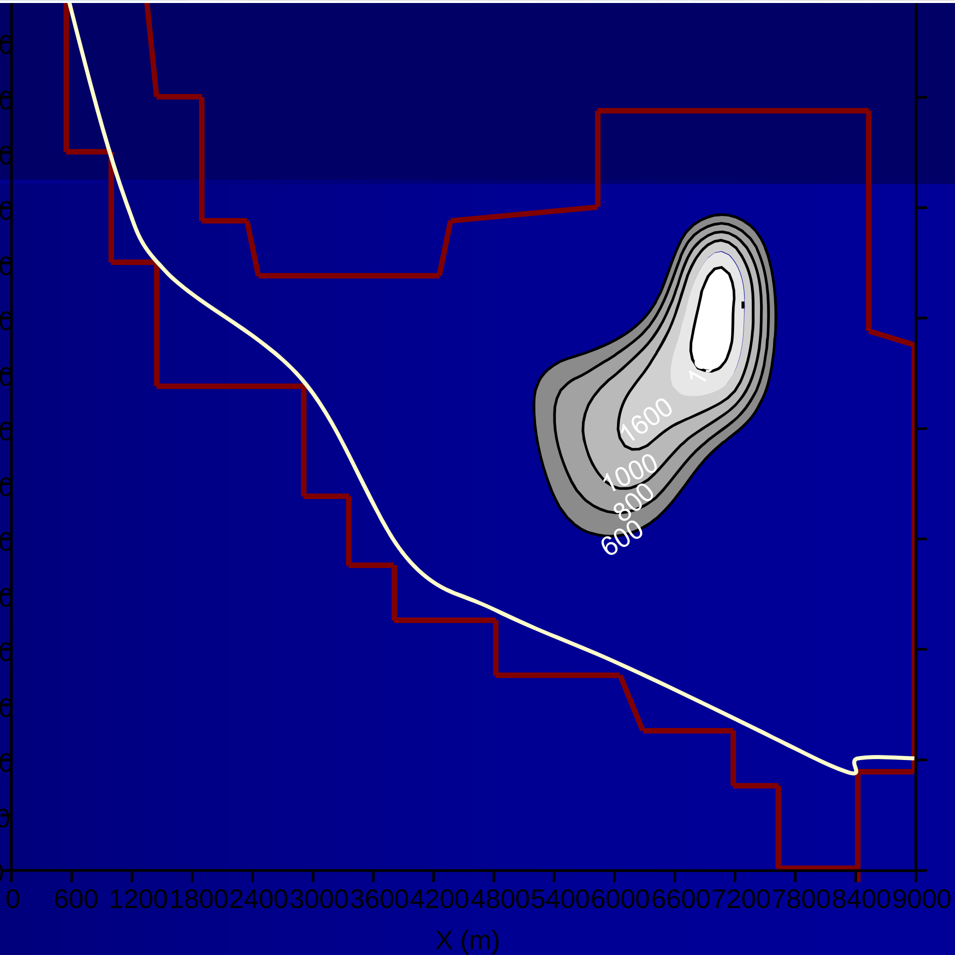


Steady state head distribution

Velocity distribution



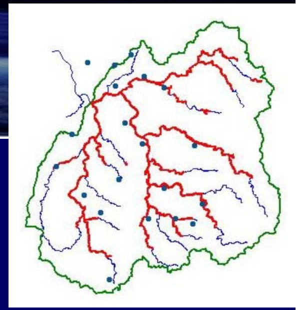
Head distribution after 20 yrs.



Concentration distribution after 20 yrs.

References

- Guidelines for Water Quality Management, Central pollution control board (CPCB)
- Website : http://www.cpcb.nic.in
- Hydrological Modeling of Small Watershed – C.T Han, H.P. Johnson, D.L. Brakensiek (Eds.), ASAE Monograph, Michigan
- Freeze, R.A. and Cherry J.A. (1979). Groundwater. Prentice Hall-INC., Englewood Cliffs, NJ
- www.epa.gov
- http://wrmin.nic.in
- Standard Methods for the Examination of Water and Wastewater; APHA, AWWA, and WEF, 21st Edition, 2005.
- http://cgwb.gov.in/

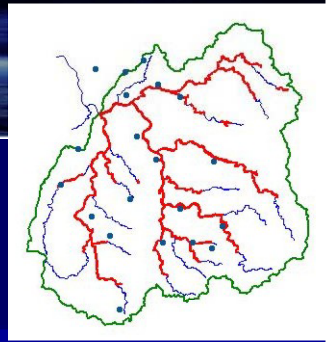


Tutorials - Question!.?.

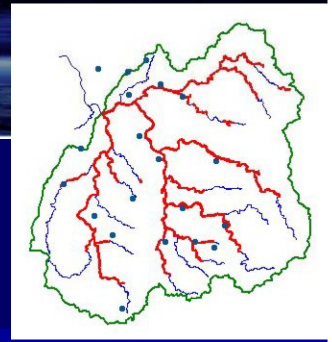
- Critically study various groundwater water and surface water quality models available in literature (details can be obtained from Internet: (eg. www.epa.gov; *www.bentley.com*)

- Study the capabilities of each model and the problems where it can be applied

Self Evaluation - Questions!.

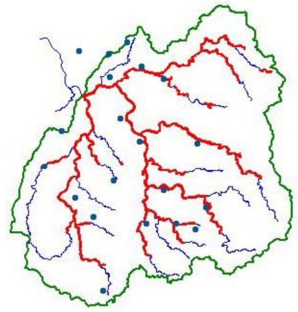


- Illustrate the different types of water quality modeling.
- Describe WQ modeling within the perspective of water cycle.
- Explain various conservation laws used in WQ modeling?.
- Describe with governing equations, the groundwater transport modeling.
- Illustrate the role of numerical modeling in WQ modeling.
- Describe various models used in groundwater quality modeling



Assignment- Questions?.

- Illustrate watershed based WQ issues within the perspective of Hydrologic cycle.
- What are the typical WQ problem goals?.
- Describe with governing equations, the surface water transport modeling.
- Illustrate the oxygen regime modeling in Rivers.
- Describe various models used in surface water quality modeling



Unsolved Problem!.

- With reference to a typical point source pollution from an industry to groundwater in your watershed area, critically study the possible water quality modeling for TDS concentration.
- Identify the possible water quality model from the open sources (from Internet sources: like MODFLOW/ MT3D).
- Collect the necessary data for the water quality modeling.
- Try to develop the model for your study area and predict the future spreading, say for next 10 years.

THANK YOU

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