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
L29 – Water Quality Modeling

Topics Covered


Keywords: Water quality modeling, Hydrodynamics, Mathematical/numerical modeling, Groundwater transport.

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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

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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 -

- Dissolved
  - hydrodynamically neutral (tracer)
- Emulsified
  - hydrodynamically active (change in $\eta$, $\rho$)
  - drops, bubbles
- Particles
  - suspended material
  - bed material, sediment

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Water Quality Modeling - Considerations

- Governing laws -

**Conservation Laws**

- Mass
- Momentum
- Substances in water
- Energy/heat

**Elementary CV - Micro**

\[ dz \]
\[ dx \]
\[ dy \]

**CV - Macro scale**

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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
  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. \( \rho = \text{const.} \Rightarrow \frac{\partial \rho}{\partial t} = 0 \))

  \[
  \frac{\partial v_x}{\partial x} + \frac{\partial v_y}{\partial y} + \frac{\partial v_z}{\partial z} = \text{div} \; \vec{v} = 0
  \]

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Water Quality Modeling - Hydrodynamics

- Conservation of Momentum – Navier-Stokes equations

\[
\begin{align*}
\frac{\partial v_x}{\partial t} + v_x \frac{\partial v_x}{\partial x} + v_y \frac{\partial v_x}{\partial y} + v_z \frac{\partial v_x}{\partial z} &= -g \frac{\partial h}{\partial x} + \nu \left[ \frac{\partial^2 v_x}{\partial x^2} + \frac{\partial^2 v_x}{\partial y^2} + \frac{\partial^2 v_x}{\partial z^2} \right] \\
\frac{\partial v_y}{\partial t} + v_x \frac{\partial v_y}{\partial x} + v_y \frac{\partial v_y}{\partial y} + v_z \frac{\partial v_y}{\partial z} &= -g \frac{\partial h}{\partial y} + \nu \left[ \frac{\partial^2 v_y}{\partial x^2} + \frac{\partial^2 v_y}{\partial y^2} + \frac{\partial^2 v_y}{\partial z^2} \right] \\
\frac{\partial v_z}{\partial t} + v_x \frac{\partial v_z}{\partial x} + v_y \frac{\partial v_z}{\partial y} + v_z \frac{\partial v_z}{\partial z} &= -g \frac{\partial h}{\partial z} + \nu \left[ \frac{\partial^2 v_z}{\partial x^2} + \frac{\partial^2 v_z}{\partial y^2} + \frac{\partial^2 v_z}{\partial z^2} \right]
\end{align*}
\]
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 $D_m$.

**Fick’s First Law:**

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

**Mass transport equation**

\[
\left( v_x \frac{\partial c}{\partial x} + v_y \frac{\partial c}{\partial y} + v_z \frac{\partial c}{\partial z} \right) - D_m \left( \frac{\partial^2 c}{\partial x^2} + \frac{\partial^2 c}{\partial y^2} + \frac{\partial^2 c}{\partial z^2} \right) = -\frac{\partial c}{\partial t}
\]
Turbulent flow: **Nature of turbulence:** irregular (characterized by variations with respect to time); intensive mixing; rotation; dissipative (increased losses of energy)

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

**velocity**  
\[
v = \bar{v} + v' 
\]

**pressure**  
\[
p = \bar{p} + p' 
\]
Water QM- Hydrodynamics & Transport

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

\[
\left( \frac{\partial \bar{V}_x}{\partial z} + \frac{\partial \bar{V}_y}{\partial y} + \frac{\partial \bar{V}_z}{\partial z} \right) = 0
\]

\[
\frac{\partial \bar{V}_x}{\partial t} - \nu_y \frac{\partial \bar{V}_x}{\partial x} + \nu_z \frac{\partial \bar{V}_x}{\partial z} = -g \frac{\partial h}{\partial x} + \frac{1}{\rho} \frac{\partial}{\partial x} \left( \eta \frac{\partial \bar{V}_x}{\partial x} - \rho \nu_x^2 \right) + \frac{1}{\rho} \frac{\partial}{\partial y} \left( \eta \frac{\partial \bar{V}_x}{\partial y} - \rho \nu_x \nu_y \right) + \frac{1}{\rho} \frac{\partial}{\partial z} \left( \eta \frac{\partial \bar{V}_x}{\partial z} - \rho \nu_x \nu_z \right)
\]

Reynolds number:

\[
Re = \frac{\nu d}{\eta / \rho} = \frac{\text{inertial reaction}}{\text{viscosity force}}
\]

<table>
<thead>
<tr>
<th>Flow Type</th>
<th>( Re )</th>
<th>Lower ( Re_{critical} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pipe flow</td>
<td>( Re = \frac{\nu d}{\eta / \rho} )</td>
<td>(~ 2000)</td>
</tr>
<tr>
<td>Open Channel flow</td>
<td>( Re = \frac{\nu y}{\eta / \rho} )</td>
<td>(~ 500)</td>
</tr>
</tbody>
</table>

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:
\[ q = -D_m \frac{\partial c}{\partial x} \]

Turbulent diffusion:
\[ q = -\varepsilon_D \frac{\partial c}{\partial x} \]

Dispersion:
\[ q = -K \frac{\partial c}{\partial x} \]

Momentum flux:
\[ \tau = -\rho \nu \frac{\partial \nu_x}{\partial y} \]

Turbulent momentum exchange:
\[ \tau = -\rho \nu \frac{\partial \nu_x}{\partial y} \]

Heat flux:
\[ q_T = -\rho c_p D_T \frac{\partial T}{\partial x} \]

Ref: Lecture notes on Environmental Fluid Mechanics, Prof. H. Kobus, Dept. Civil Engg., Uni. Stuttgart, Germany
WQM- Transport in Rivers & Canals

One dimensional transport:

\[
\begin{align*}
\text{convective transport:} & \quad \mathbf{u} \cdot \mathbf{c} \cdot A + \frac{\partial}{\partial x} \left( \mathbf{u} \cdot \mathbf{c} \cdot A \right) \cdot dx \\
\text{dispersive transport:} & \quad K \cdot \frac{\partial \mathbf{c}}{\partial x} \cdot A + \frac{\partial}{\partial x} \left( K \cdot \frac{\partial \mathbf{c}}{\partial x} \cdot A \right) \cdot dx
\end{align*}
\]

<table>
<thead>
<tr>
<th>size of section</th>
<th>microscopic</th>
<th>macroscopic</th>
</tr>
</thead>
<tbody>
<tr>
<td>distribution process</td>
<td>diffusion</td>
<td>dispersion</td>
</tr>
<tr>
<td>velocity distribution</td>
<td>( \mathbf{v} = \mathbf{v}(x, y, z) )</td>
<td>( \mathbf{v} = \mathbf{v}(z) )</td>
</tr>
<tr>
<td>concentration distribution</td>
<td>( C = C(x, y, z) )</td>
<td>( C = \overline{C}(z) )</td>
</tr>
</tbody>
</table>
| mass balances | \[
\frac{\partial C}{\partial t} + \mathbf{v}(x, y, z) \cdot \frac{\partial C}{\partial x} = -\frac{\partial}{\partial x} \left( \frac{\partial C}{\partial x} \right) + \frac{\partial}{\partial y} \left( \frac{\partial C}{\partial y} \right) + \frac{\partial}{\partial z} \left( \frac{\partial C}{\partial z} \right)
\]
| \[ \text{D: diffusion coefficient} \] | \[
\frac{\partial \overline{C}}{\partial t} + \mathbf{v}(z) \frac{\partial \overline{C}}{\partial z} = K \frac{\partial^2 \overline{C}}{\partial z^2}
\]
| \[ \text{K: dispersion coefficient} \] |

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
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:

\[
\bar{c}(t = 0) = \bar{c}_0
\]

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

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

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

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

2D Transport equation

\[
\nu_x = -K_x \frac{\partial h}{\partial x} \quad \nu_y = -K_y \frac{\partial h}{\partial y}
\]

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

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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
- **FEMWATER**
- **GMS package**
Groundwater Transport Modeling – Case Study

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.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hydraulic</td>
<td></td>
</tr>
<tr>
<td>Conductivity (m/day)</td>
<td></td>
</tr>
<tr>
<td>Zone I</td>
<td>0.5</td>
</tr>
<tr>
<td>Zone II</td>
<td>1</td>
</tr>
<tr>
<td>Zone III</td>
<td>2</td>
</tr>
<tr>
<td>Longitudinal dispersivity (m)</td>
<td>50</td>
</tr>
<tr>
<td>Transverse dispersivity (m)</td>
<td>5</td>
</tr>
<tr>
<td>Specific Yield</td>
<td>0.2</td>
</tr>
</tbody>
</table>
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
- www.epa.gov
- http://wrmin.nic.in
- 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

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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.

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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.

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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.

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