

# Groundwater Quality Assessment and Modeling

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## INTRODUCTION

Groundwater is generally considered to be good source of drinking water; because of the filtering properties of the soil matrices; it is also used for other domestic uses, irrigation and industrial purposes. In many arid and semi-arid areas, it is the main source of water. Although groundwater is more protected than surface waters, but it is also subject to pollution due to the human interference and natural phenomena. Once the groundwater is polluted or contaminated, it is very expensive and difficult to restore its quality. The phenomenon of pollution is defined as a modification of the physical, chemical and biological properties of water, restricting or preventing its use in the various applications.

In the protection and improvement of groundwater quality, two challenging problems are to be addressed: for uncontaminated aquifers, it is required to assess the potential dangers of pollution and methods to be evolved as to how the aquifers can be prevented from the expected dangers; for contaminated aquifers, it is required to draw up remediation measures for cleaning the aquifers from the pollution. In both situations, we need a tool to predict the pollutant distribution in groundwater. Obviously, field experiments alone cannot serve the purpose but would help as a database. The only tool that we can use is mathematical modeling.

When confronted with a groundwater-pollution problem, the people responsible for its solution will ask several questions:

- (1) *What is the nature of the pollution:*
  - *is it miscible or not to the water ?*
  - *what are its physical and chemical properties ?*
  - *what sort of danger does it present ?*
  
- (2) *What is the scale of pollution:*
  - *what is the total amount of pollution ?*
  - *what is the strength of the pollution source ?*
  - *what are the dimensions and the geometrical characteristics of the pollution source ?*
  - *what is the invaded volume of soil ?*
  - *what is the duration of the pollution ?*

Answers to these questions are necessary to formulate the problem and to develop predictive model. A model is a conceptualization of reality that is represented by mathematical equations, which are interpreted to get the insight of the problems.

## ORIGINS OF GROUNDWATER POLLUTION

Groundwater pollution is usually traced back to four main origins: industrial, domestic, agricultural and environmental pollution, each family has continuous and incidental types of sources.

- (i) Industrial pollution is carried to the aquifer by:
  - rain infiltrating through waste disposals,
  - accidents like the breaking of a pipe line.
- (ii) Domestic pollution is carried to the aquifer by:
  - rain infiltrating through sanitary landfills,
  - accidental breaking of septic tanks.
- (iii) Agricultural pollution is due to irrigation water or rain carrying away fertilizers, minerals, salts, herbicides and pesticides.
- (iv) Environmental pollution is mainly due to seawater intrusion in coastal aquifers.

### TRANSPORT MECHANISMS

There are many processes, which govern the transport mechanism in a porous medium. These processes may be physical, chemical biological or combination of them. The principal processes, which are predominant and most often used by groundwater modelers, are: advection, diffusion and dispersion, sorption, biodegradation, sources and sinks, and radioactive decay. Let us look into the transport mechanisms first.

The movement of a chemical species in groundwater is different than that of in channel flow and can be examined by investigating movement in flumes in laboratory or in fields. Figure 1 shows the comparison of such motions and emphasizes that contaminant moves like plumes and these plumes are elliptical in shape and grow in direction of flow. Figure 2 shows how the spreading of contaminant due to the non-uniformity of the microscopic flow velocity of the solid matrices is caused. While Fig. 3 depicts the processes of longitudinal and transverse dispersion of contaminant through the soil pores.

Let us define the terminologies of contaminant transport to a common language to appreciate the transport process more precisely.

**Advection:** is the bodily movement of contaminants along with flowing groundwater at the seepage velocity in the porous medium.

**Diffusion:** on account of molecular mass transport process by which the solutes move from areas of higher concentration to areas of lower concentration.

**Dispersion:** on account of mixing process due to variation of velocity in porous media.

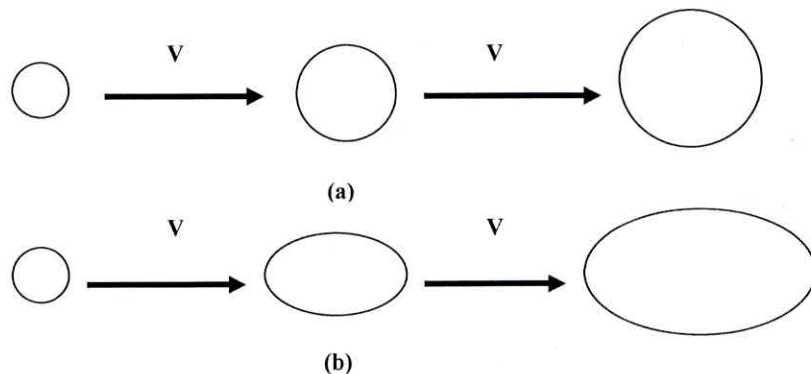


Fig. 1 Iso-concentrations in (a) uniform laminar fluid motion, and (b) uniform groundwater motion.



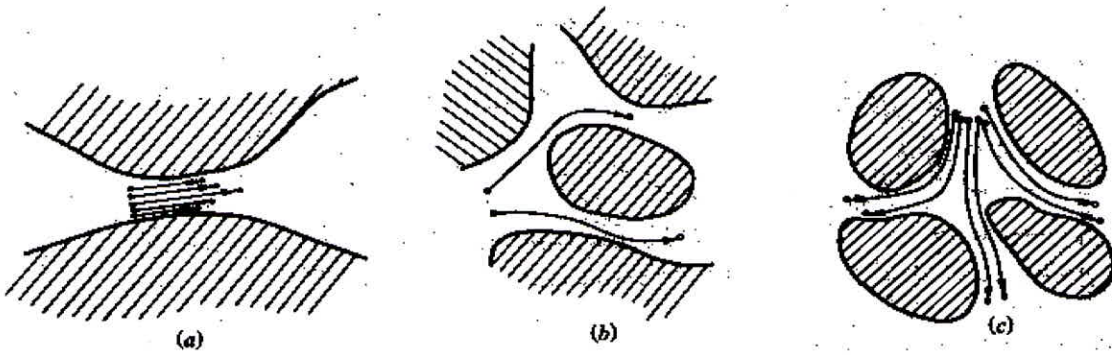


Fig. 2 Non-uniformity of the microscopic flow velocity due to the existence of solid matrices.



Fig. 3 Longitudinal and Transversal dispersion in hydrodynamic dispersion phenomena.

**Adsorption:** process of sorption, interaction of contaminant with solid, partitioning of organic contaminants from soluble phase into the soil matrix.

**Bio-degradation:** transformation of certain organic species to simple CO<sub>2</sub> and water in the presence of microbes in the subsurface.

**Sources and sinks:** the solute may enter or leave the porous area through sources or sinks. Discrete and distributed pollutant sources, wells, discharge ditches and recharge wells are examples of solute sources and sinks.

**Radioactive decay:** the radioactive components within the fluid decrease the concentration as a result of decay over time.

**Advective Process**

The contaminant moves with the flowing groundwater at a velocity equal to the seepage velocity in the porous medium, and the seepage velocity is determined using Darcy's law, as:

$$v_s = \frac{K}{n} \frac{dh}{dl} \tag{1}$$

where  $v_s$  = average linear velocity ( $LT^{-1}$ ),  $K$  = hydraulic conductive of the aquifer ( $LT^{-1}$ ),  $n$  = effective porosity of the soil matrix (dimensionless), and  $h$  = potential difference of head between length  $l$ , (L).

If advection is the only form of transport, then water with a concentration,  $C_0$ , moves as a plug into the aquifer when injected from some time  $t_0$  onward, Fig. 4. In reality, the front moves slower than the groundwater due to the chemical reactions that take place between solutes and solid particles; the reduction of velocity is called retardation.

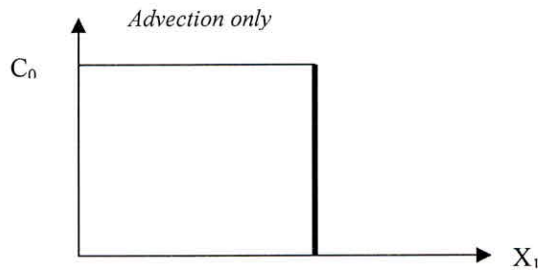


Fig. 4 Advection of fluid flow with a constant concentration source of  $C_0$  : front moves a distance  $X_1 = v_s t$ , where  $v_s$  = seepage velocity and  $t$  = elapsed time.

### Diffusion and Dispersion

Diffusion and dispersion take place in two different types of domain. The domain of diffusion is the scattering of particles by random or turbulent motion in microscopic scale. The domain of dispersion is the scattering of particles or cloud of contaminants by the interaction of differential advection and diffusion of materials in heterogeneous porous media in a greater scale. Diffusion is a component of dispersion.

As flow takes place, the solute spreads in all directions at a molecular scale on account of concentration gradients and random motion on account of diffusion. The solute moves from regions of higher concentration to areas of lower concentration due to diffusion, and the diffusive transport also occurs in absence of velocity of flow. Fick's law of diffusion describes the diffusive flux, as:

$$f_x = -D_m \frac{dc}{dx} \quad (2)$$

where,  $f_x$  = mass flux of contaminant per unit area per unit time ( $ML^{-2}T^{-1}$ ),  $D_m$  = molecular diffusion coefficient ( $L^2T^{-1}$ ), typical value of  $D_m$  = range between  $1 \times 10^{-9}$  to  $2 \times 10^{-9}$   $m^2/s$  at  $25^\circ C$ , and  $dc/dx$  = concentration gradient in the direction of flow ( $ML^{-3}L^{-1}$ ).

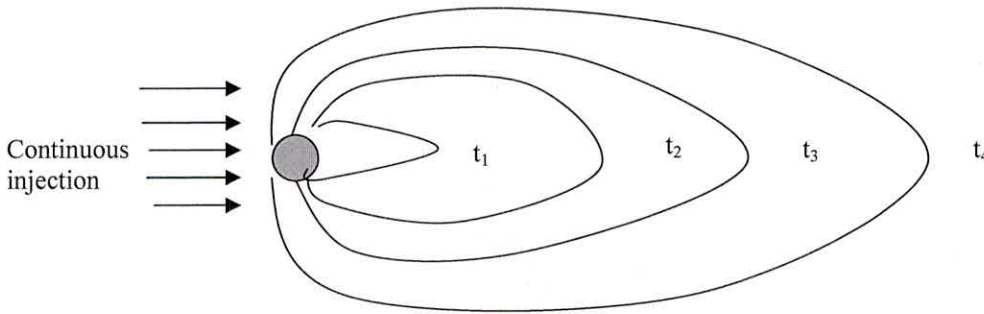
Dispersion results from the simultaneous action of both a purely mechanical phenomenon and a physicochemical phenomenon. The mechanical dispersion is caused due to the velocity variation of a fluid flowing through a porous medium, while the physicochemical dispersion is molecular diffusion, which results from the chemical potential gradient. The combined result of mechanical phenomenon and molecular or physicochemical phenomenon is known as *hydrodynamic dispersion* and it is a macroscopic phenomenon. Hydrodynamic dispersion is the process in which solutes spread out and are diluted compared to simple advection alone.

The illustrated examples 1 and 2 exhibit effects of dispersion on the distribution of concentration of a tracer as it moves along the groundwater flow.



**Example 1**

Consider continuous injection of a tracer into a well situated in a uniform one-dimensional flow field in the x-direction. One would observe a gradual spreading of the tracer around the well, and the extent at which the tracer spreads would be larger than the region as one expects from an average flow alone. It would not only spread longitudinally along the mean flow direction, but would also expand transversely. There exists a transition zone rather than an abrupt interface between the tracer-containing solution and the original fluid around the well as shown in Fig.5. Without dispersion, the tracer would move in accordance with the mean flow velocity.

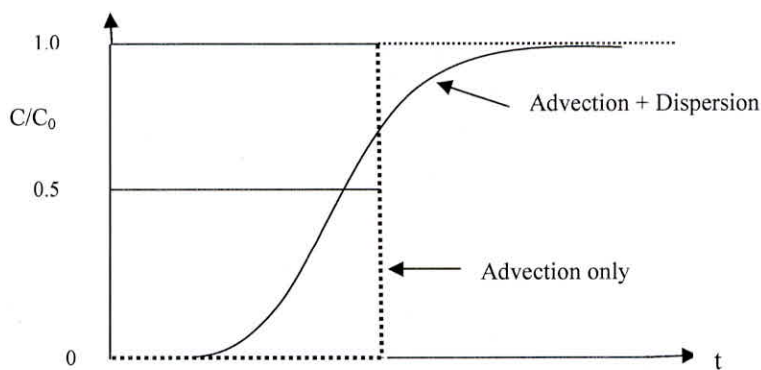


**Fig. 5** Tracer distribution in a one-dimensional flow field with a continuously injected point source.

**Example 2**

Consider a steady flow in a homogeneous sand column saturated with water. At a certain time, the water with a tracer concentration  $C_0$  starts to replace the original water. If the concentration at the other end of the column,  $C$ , is monitored, and a curve of relative concentration  $C/C_0$  versus time  $t$  is drawn, the curve, one will get, is shown in Fig. 6. This curve is called the *breakthrough curve*.

If there is no dispersion, the breakthrough curve should be of the shape shown by dashed line in Fig.6, that is, there should be an abrupt concentration interface moving at the mean flow velocity. For dispersion, the curve would be the solid line as show in the figure. If movement of the tracer is monitored along the direction of flow on space, the influence of advection plus dispersion, and advection plus dispersion plus retardation due to adsorption would be as shown in Figs. 7(a) and (b).



**Fig. 6** Schematic breakthrough curve in one dimension.

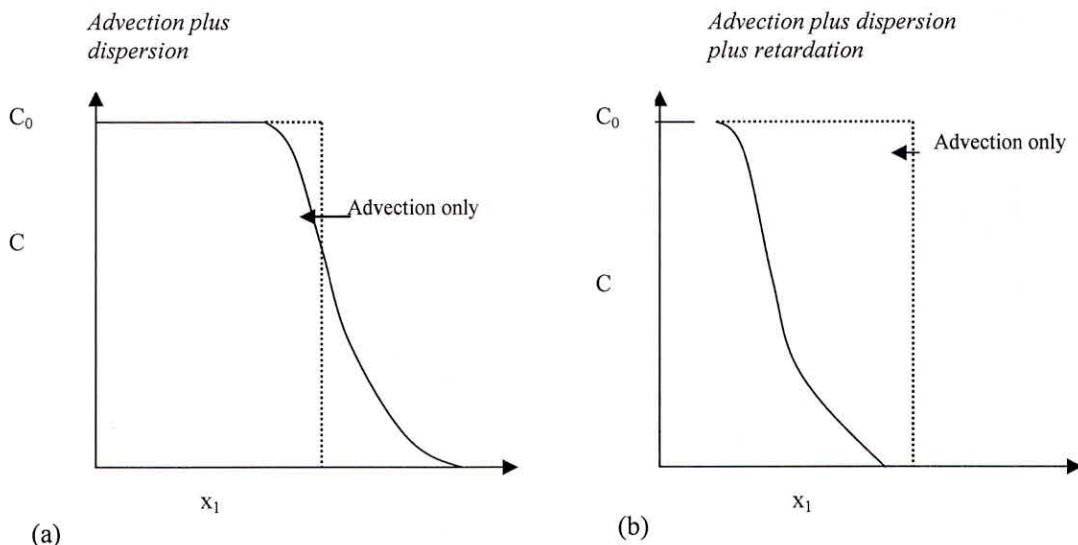


Fig. 7 Advection of fluid with concentration ; (a) with dispersion, (b) with dispersion and retardation due to adsorption.

DERIVATION OF TRANSPORT EQUATION

Advection Transport

Let us consider an elementary a control volume,  $\Delta V$ , having the shape of a rectangular parallel-piped box of dimensions  $\Delta x$ ,  $\Delta y$ ,  $\Delta z$  as shown in Fig. 5. We need to derive the transport equation in three dimensions for contaminant transport governed by advection only in terms of a Cartesian coordinate system,  $x$ ,  $y$ , and  $z$ . Let us introduce the concentrations of the mobile phase and the sorbed phase of the contaminant respectively. The concentration is expressed in terms of mass per unit volume of fluid as:  $C$  = mass of mobile phase per unit volume of fluid ( $ML^{-3}$ ),  $C_s$  = mass of sorbed phase per unit volume of fluid ( $ML^{-3}$ ).

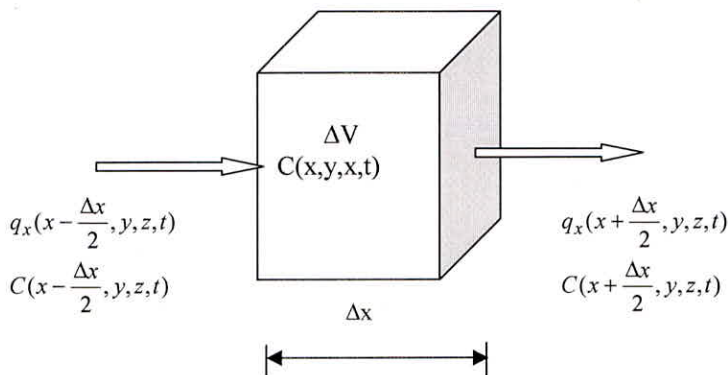


Fig. 8 Mass balance in a control volume

If the rate of decay is proportional to the total mass of solute present in  $\Delta V$  with proportionality constant  $\lambda$ , and if the porosity is  $n$ , then the mass balance for flow in the  $x$  direction may be written as:

Mass inflow due to advection – Mass outflow due to advection – decrease in mass due to decay = change of mass in the control volume. In mathematical expression,

$$\begin{aligned} & \left[ q_x \left( x - \frac{\Delta x}{2}, y, z, t \right) C \left( x - \frac{\Delta x}{2}, y, z, t \right) - q_x \left( x + \frac{\Delta x}{2}, y, z, t \right) C \left( x + \frac{\Delta x}{2}, y, z, t \right) \right] \Delta y \Delta z \Delta t \\ & - \left[ C(x, y, z, t) + C_s(x, y, z, t) \right] \lambda n \Delta x \Delta y \Delta z \Delta t \quad (3) \\ & = \left[ C \left( x, y, z, t + \frac{\Delta t}{2} \right) + C_s \left( x, y, z, t + \frac{\Delta t}{2} \right) - C \left( x, y, z, t - \frac{\Delta t}{2} \right) - C_s \left( x, y, z, t - \frac{\Delta t}{2} \right) \right] (n \Delta x \Delta y \Delta z) \end{aligned}$$

By dividing both sides of Eq. 3 by  $(\Delta x \Delta y \Delta z \Delta t)$ , and passing to the limit for  $\Delta x \rightarrow 0$ ,  $\Delta y \rightarrow 0$ ,  $\Delta z \rightarrow 0$ , and  $\Delta t \rightarrow 0$ , we obtain:

$$- \frac{\partial}{\partial x} (q_x C) - n \lambda (C + C_s) = n \frac{\partial}{\partial t} (C + C_s) \quad (4)$$

If there are components of flow in all three directions, this becomes

$$- \left[ \frac{\partial}{\partial x} (q_x C) + \frac{\partial}{\partial y} (q_y C) + \frac{\partial}{\partial z} (q_z C) \right] - n \lambda (C + C_s) = n \frac{\partial}{\partial t} (C + C_s) \quad (5)$$

Adopting the assumption of linear sorption, which implies:

$$C = \frac{1}{R} (C + C_s) \quad (6)$$

where R is a dimensionless constant called the retardation factor. If R is independent of time, then

$$\frac{\partial}{\partial t} (C + C_s) = R \frac{\partial C}{\partial t} \quad (7)$$

Replacing Eqs.6 and 7 in Eq. 5, we get:

$$n R \frac{\partial C}{\partial t} + \left[ \frac{\partial}{\partial x} (q_x C) + \frac{\partial}{\partial y} (q_y C) + \frac{\partial}{\partial z} (q_z C) \right] = - n \lambda R C \quad (8)$$

Differentiating the terms in brackets and simplifying, we get:

$$\frac{\partial C}{\partial t} + \frac{1}{n R} \left[ q_x \frac{\partial C}{\partial x} + q_y \frac{\partial C}{\partial y} + q_z \frac{\partial C}{\partial z} + C \left( \frac{\partial q_x}{\partial x} + \frac{\partial q_y}{\partial y} + \frac{\partial q_z}{\partial z} \right) \right] = - \lambda C \quad (9)$$

Restricting to incompressible flow, the terms in parentheses vanish, and introducing velocity components, we get;

$$\frac{\partial C}{\partial t} + \frac{1}{R} \left[ v_x \frac{\partial C}{\partial x} + v_y \frac{\partial C}{\partial y} + v_z \frac{\partial C}{\partial z} \right] = - \lambda C \quad (10)$$

This equation is the *transport equation for solute transport with retardation and decay in an incompressible porous medium without the effect of hydrodynamic dispersion*. The transport equation is a first order partial differential equation, which can be integrated along its characteristics.

The retardation factor R is usually expressed in terms of another factor, called the distribution factor,  $K_d$ , defined by:

$$K_d = \frac{S}{C} \quad (11)$$



where  $S$  is defined as the ratio of the mass of sorbed material to the mass of solid material, both contained in some volume  $V$  of porous material. If  $\rho_b$  is the bulk density of solid material, then

$$S = \frac{C_s n V}{\rho_b V} = n \frac{C_s}{\rho_b} \quad (12)$$

$R$  is expressed in terms of  $K_d$  as:

$$R = 1 + \frac{C_s}{C} = 1 + \frac{\rho_b K_d}{n} \quad (13)$$

The units of the distribution factor are  $m^3/kg$ . The distribution factor is the quantity associated with retardation that is usually measured in the laboratory.

### Advection – Dispersion Transport

Applying the Ficks law of diffusion, which states that mass flux at any direction is proportional to the concentration gradient to that direction, to the advection component as shown in Fig. 4, one can derive the transport equation governed by the hydrodynamic dispersion. The flux of a single pollutant due to advection and dispersion can be expressed when the soil is completely saturated, as:

$$q_x C = n \left( V_x C - D_x \frac{\partial C}{\partial x} \right) \quad (14)$$

where  $V_x$  is the average seepage flow velocity of the pore fluid in the  $x$  direction,  $n$  is the porosity,  $D_x$  is the coefficient of dispersion along the flow direction,  $C$  is the concentration, and  $(q_x C)$  is the mass flux rate.

Considering mass flux rate in three Cartesian coordinate system,  $x$ ,  $y$ , and  $z$ , and putting the corresponding expression as Eq. 14 in Eq. 8, we get:

$$n R \frac{\partial C}{\partial t} + \left\{ \frac{\partial}{\partial x} \left[ n \left( V_x C - D_x \frac{\partial C}{\partial x} \right) \right] + \frac{\partial}{\partial y} \left[ n \left( V_y C - D_y \frac{\partial C}{\partial y} \right) \right] + \frac{\partial}{\partial z} \left[ n \left( V_z C - D_z \frac{\partial C}{\partial z} \right) \right] \right\} = -n \lambda R C \quad (15)$$

where  $V_x$ ,  $V_y$ , and  $V_z$ , and  $D_x$ ,  $D_y$ , and  $D_z$  are the average seepage flow velocities and the coefficients of dispersion in the  $x$ ,  $y$ , and  $z$  direction respectively. Differentiating the terms in the bracket of Eq.15, and assuming the flow is steady and soil is incompressible implying uniform flow velocity, porosity and coefficients of dispersion along the direction of flow; i.e.,  $\partial n / \partial x = 0$ ,  $\partial n / \partial y = 0$ ,  $\partial n / \partial z = 0$ , and  $\partial V_x / \partial x = 0$ ,  $\partial V_y / \partial y = 0$ ,  $\partial V_z / \partial z = 0$ , and also  $\partial D_x / \partial x = 0$ ,  $\partial D_y / \partial y = 0$ ,  $\partial D_z / \partial z = 0$ . Eq.15 reduces to:

$$n R \frac{\partial C}{\partial t} + n \left\{ \left[ V_x \frac{\partial C}{\partial x} - D_x \frac{\partial^2 C}{\partial x^2} \right] + \left[ V_y \frac{\partial C}{\partial y} - D_y \frac{\partial^2 C}{\partial y^2} \right] + \left[ V_z \frac{\partial C}{\partial z} - D_z \frac{\partial^2 C}{\partial z^2} \right] \right\} = -n \lambda R C \quad (16)$$

Multiplying both sides of Eq.16 by  $\{n R\}$  and rearranging, we get:



$$\frac{\partial C}{\partial t} + \frac{1}{R} \left\{ V_x \frac{\partial C}{\partial x} + V_y \frac{\partial C}{\partial y} + V_z \frac{\partial C}{\partial z} - D_x \frac{\partial^2 C}{\partial x^2} - D_y \frac{\partial^2 C}{\partial y^2} - D_z \frac{\partial^2 C}{\partial z^2} \right\} = -\lambda C \quad (17)$$

Eq.17 is the three dimensional advection-dispersion-adsorption-decay equations for solute transport in porous media. The dispersion terms in three-dimensional flow determines the nine components of dispersion coefficient tensor, in such case, the generalized advection-dispersion-retardation-decay equation is given by:

$$\frac{\partial C}{\partial t} + \left\{ \frac{\partial}{\partial x_i} \left( \frac{V_i C}{R_d} \right) - \frac{\partial}{\partial x_i} \left( \frac{D_{ij}}{R_d} \frac{\partial C}{\partial x_j} \right) \right\} = -\lambda C \quad (18)$$

where  $V_i$  (  $i = 1,2, 3$ ) are the three components of mean flow velocity, and  $D_{ij}$ , are the nine components of dispersion tensor, which can be described as:

$$D_{ij} = \begin{bmatrix} D_{11} & D_{12} & D_{13} \\ D_{21} & D_{22} & D_{23} \\ D_{31} & D_{32} & D_{33} \end{bmatrix} \quad (19)$$

Eq.18 with an implicit source term is termed as generalized form of advection-dispersion-retardation-decay-source equation for solute transport in porous media. The solutions to Eq.18 for different complex boundary conditions give the spatial and temporal variation of concentration in a flowing medium. However, the analytical solutions for complex boundary conditions as evident in real life problems are not available. Analytical solution is available for simple boundary conditions and for the simplified situations in one-dimension. However, the analytical approach is the mathematically ideal way to solve these equations.

In simple one-dimensional case, i.e., the mean velocities of flow along y and z directions are zero so are the corresponding dispersion coefficients tensor. Assuming the flow to be one-dimensional i.e., along x-direction and the corresponding dispersion coefficient is longitudinal dispersion,  $D_L$ , Eq. 18 reduces to:

$$\frac{\partial C}{\partial t} + \frac{V_x}{R_d} \frac{\partial C}{\partial x} - \frac{D_L}{R_d} \frac{\partial^2 C}{\partial x^2} = -\lambda C \quad (20)$$

For  $R_d = 1$  and  $\lambda = 0$ , Eq. 20 reduces to simple advection-dispersion equation. There are two unknown parameters  $V_x$ , and  $D_L$  in the one-dimensional advection-dispersion equation. These parameters are to be known *a priori* to compute the concentration distribution over time and space. Knowing  $V_x$ , and  $D_L$ , concentration variation for a given perturbation can be obtained either by analytical method, or by semi-analytical method, or by numerical methods.

### PARAMETER ESTIMATION

To compute or forecast the threat of any injected solute in a flowing porous media of flow taking place in one-direction, two basic parameters,  $V$ , and  $D_L$  are required to be known *a priori*. These parameters are to be estimated from the field experiment or measurement. The pore water velocity can be estimated either by direct method (field measurement) or by indirect

method (flow modeling), while determination of dispersion coefficient is not a straightforward approach. However, researchers have suggested a number of methods for estimation of dispersion coefficient from the laboratory experiment data.

### Determination of Dispersivities

A vast number of experiments have been done to determine the relations between the dispersion coefficient and velocity distribution, as well as the molecular diffusion coefficient. Klotz et.al. (1980) Suggested the following form for the longitudinal dispersion coefficient:

$$D_L = \alpha_L V^m \quad (21)$$

where  $\alpha_L$  is the longitudinal dispersivity,  $V$  is the mean flow velocity, and  $m$  is the power of velocity. Experimental results show that  $\alpha_L$  is mainly dependent on the mean particle size and the uniformity coefficient,  $U = d_{60}/d_{10}$ . The range of 'm' varies between 1.07 to 1.1. Recommended values of longitudinal dispersivity in laboratory scale are given in Table 1.

**Table 1. Longitudinal dispersivity in laboratory scale.**

Range of Particle size (mm)	Exponential 'm'	Longitudinal dispersivity ' $\alpha_L$ '	Minimum flow velocity (m/s)
0.4 – 0.7	1.09	$3.96 \times 10^{-3}$	$1 \times 10^{-5}$
0.5 – 1.5	1.10	$5.78 \times 10^{-3}$	$8 \times 10^{-5}$
1.0 – 2.0	1.10	$8.80 \times 10^{-3}$	$1.5 \times 10^{-4}$
2.0 – 3.0	1.09	$1.30 \times 10^{-2}$	$2 \times 10^{-4}$
5.0 – 7.0	1.09	$1.67 \times 10^{-2}$	$3 \times 10^{-4}$
0.5 – 2.0	1.08	$3.11 \times 10^{-3}$	$5 \times 10^{-3}$
0.2 – 5.0	1.08	$8.30 \times 10^{-3}$	$5 \times 10^{-3}$
0.1 – 10	1.07	$1.63 \times 10^{-3}$	$5 \times 10^{-3}$
0.05- 20	1.07	$7.07 \times 10^{-3}$	$5 \times 10^{-3}$

For transverse dispersion coefficient,  $D_T$ , a similar expression can be used:

$$D_T = \alpha_T V^m \quad (22)$$

where  $\alpha_T$  is the transverse dispersivity, which is 6 to 20 times smaller than  $\alpha_L$ .

In laboratory scale, the longitudinal dispersion coefficient is determined from the column experiment. The water with tracer concentration  $C_0$  is continuously injected into a column containing sand or other materials of porous media from one end to displace the original water in the column without tracer. The concentration and volume of effluent water from other end of the column or at different depth of the column is measured. From the plot of the concentration versus depth as shown in Fig.9,  $D_L$  can be estimated using the following formula:

$$D_L = \frac{1}{8t} (x_{0.16} - x_{0.84})^2 \quad (23)$$

where  $x_{0.16}$  and  $x_{0.84}$  are the point, where relative concentration,  $C/C_0 = 0.16$  and  $0.84$  respectively. In time domain, Eq. 23 can be written as :

$$D_L = \frac{V^2}{8t_{0.5}} (t_{0.84} - t_{0.16})^2 \quad (24)$$



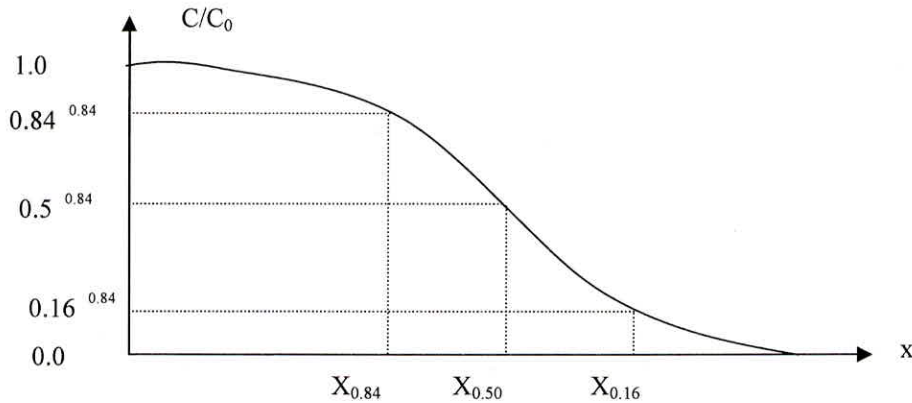


Fig. 9 The concentration distribution curve shown by error function

### Determination of mean flow velocity

The mean flow velocity can be determined by two ways: indirect *method and direct method*. The indirect determination involves the use of field data from pumping tests to calibrate the flow model and thus obtain the hydraulic conductivity,  $K$ , and effective porosity,  $n$ . Then  $K$  and  $n$  are substituted into Darcy's law to get the average velocity. As  $K$ ,  $n$  and the hydraulic gradient values may contain large errors, the velocities obtained by using this method may contain large errors, and hence not a reliable method all the time.

It is always better to take direct measurement of the flow velocity in the field because the transport model is very sensitive to errors in velocity. In the direct method, values of velocity are determined through measuring the movement of artificial tracers or environmental isotopes. The artificial tracers include salts, radioactive isotopes, coloring agents and so on.

### FORMULATION OF A GROUNDWATER QUALITY MODEL

From the above description, it could be noted that there are two kinds of distributed models in the simulation of groundwater quality: pure advection and advection-dispersion. The pure advection model is a simple one, in which the solute transport is assumed to be completely determined by groundwater flow. On the other hand, the advection-dispersion model is based on the theory of hydrodynamic dispersion in porous media. The constitution of the advection-dispersion model is, thus, shown in Fig.10.

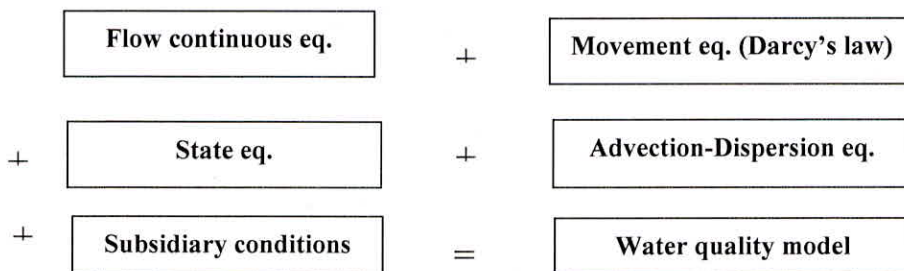


Fig. 10 The constitution of the water quality model on advection-dispersion.

In order to build a water quality model for an aquifer system, besides the selection of model structure, various hydrogeological parameters appearing in the governing equations and initial and boundary conditions must be determined. The input and output of a groundwater quality model is shown in Fig. 11.



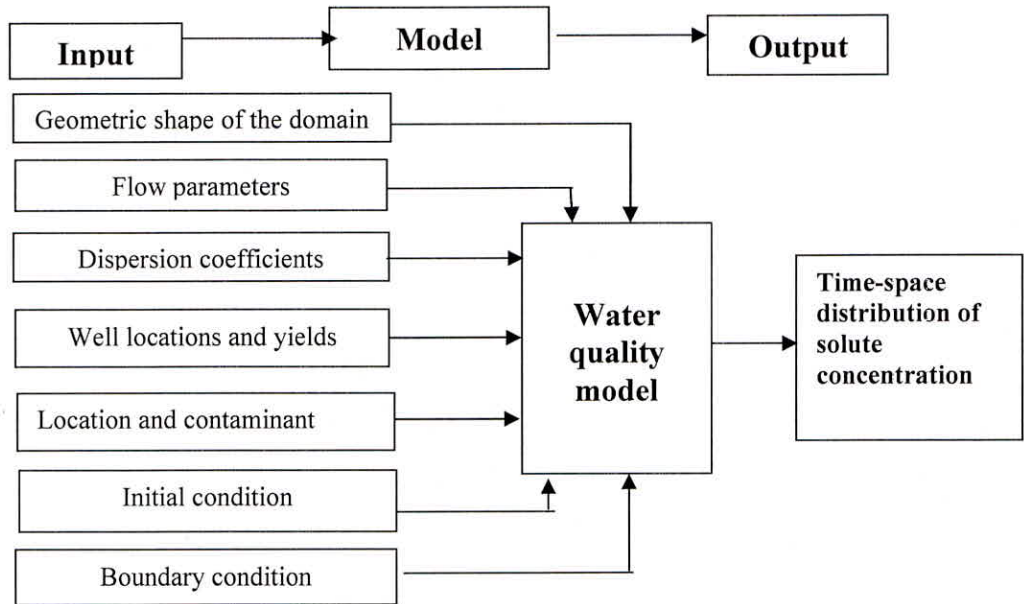


Fig. 11 Input and Output of the water quality model.

Advection-dispersion equation contains some parameters such as the dispersion coefficients; mean flow velocity, fluid density and source/sink terms. We should first determine their values, and then solve for the concentration distribution. Generally, the variation of solute concentration may affect the density and viscosity of the fluid, and conversely, the changes of fluid density and viscosity may cause the state of the flow field to change. In other words, the concentration distribution and the velocity distribution are interconnected. The concentration distribution is dependent on the velocity distribution, and vice versa. They are both unknown functions; therefore, a single equation of hydrodynamic dispersion is not enough to solve the transport problem. To solve the problem of groundwater quality in a saturated zone, we need the following system of non-linear partial differential equations:

the hydrodynamic dispersion equation,

$$\frac{\partial C}{\partial t} = \text{div} \left[ D \rho \text{grad} \left( \frac{C}{\rho} \right) \right] - \text{div}(CV) + I \quad (25)$$

the continuity equation,

$$\frac{\partial \rho}{\partial t} + \text{div}(\rho V) = 0 \quad (26)$$

the kinetic equation,

$$V_i = -\frac{k_{ij}}{\mu n} \left( \frac{\partial p}{\partial x_j} + \rho g \frac{\partial z}{\partial x_i} \right); (i, j = 1, 2, 3) \quad (27)$$

and the state equations,

$$\rho = \rho(C, p), \quad \mu = \mu(C, p) \quad (28)$$

where C denotes the solute concentration; p the pressure;  $\rho$  and  $\mu$  the density and viscosity of the fluid; D the hydrodynamic dispersion coefficient;  $k_{ij}$  the component of hydraulic conductive tensor; n the porosity;  $V_i$  the three component of mean velocity ; and I the source/sink term.

**Solution Technique**

First,  $\rho$  and  $\mu$  are to be determined by the state equations. Einstein’s summation convention can be used for finding  $\rho$  and  $\mu$ . Since mean velocity distribution changes the concentration distribution, the equations of the hydrodynamic dispersion system must be solved simultaneously. The iteration method for this case is described as follows: assume that solution at time t has been obtained, and we want to find solution at the next time,  $t + \Delta t$ . Estimate the concentration distribution by extrapolation method at  $t + \Delta t$  and use the state equations to calculate the relevant values of  $\rho$  and  $\mu$ . These values of  $\rho$  and  $\mu$  are then used into the continuity and kinetic equations to obtain the velocity V. Next, we calculate the coefficient of the advection-dispersion equation using V and solve advection-dispersion equation to update the concentration distribution at  $t + \Delta t$ . Using new concentration distribution, we can modify the values of  $\rho$  and  $\mu$ . This process is repeated until the concentration distribution does not change within certain accuracy. The solution process is shown by the flow chart in Fig. 12.

**Coupled Equations of Groundwater Flow and Mass Transport**

The advection-dispersion equation is coupled with the flow equation through continuity and kinetic equations. Let us consider some specific forms of these equations, which are often encountered in groundwater pollution problems.

For groundwater flow in saturated zone, we always use the water head,  $h = z + p/\rho g$ , as a dependent variable. For an isotropic porous medium, the kinetic equation, i.e., Darcy’s law can be expressed as:

$$V_i = - \frac{K}{n} \frac{\partial h}{\partial x_i}, \quad (i = 1,2,3) \tag{29}$$

where  $K = k \rho g/\mu$  is the hydraulic conductive of the isotropic porous medium, which depends on the density and viscosity of the fluid, as well as, permeability, k. For a homogeneous fluid, the partial differential equation of groundwater flow can be obtained by combining Darcy’s law and continuity equation:

$$S_s \frac{\partial h}{\partial t} = \text{div}(K \text{ grad } h) + W \tag{30}$$

where  $S_s$  is the specific storativity, and W is the source/sink term.

A model may be constructed by coupling the advection-dispersion equation with the flow equation by the aid of Darcy’s law, rather than using the general system of hydrodynamic dispersion equations. For a three-dimensional dispersion in three-dimensional flow fields, the model is:

The flow equation:

$$S_s \frac{\partial h}{\partial t} = \frac{\partial}{\partial x} \left( K \frac{\partial h}{\partial x} \right) + \frac{\partial}{\partial y} \left( K \frac{\partial h}{\partial y} \right) + \frac{\partial}{\partial z} \left( K \frac{\partial h}{\partial z} \right) + W \tag{31}$$

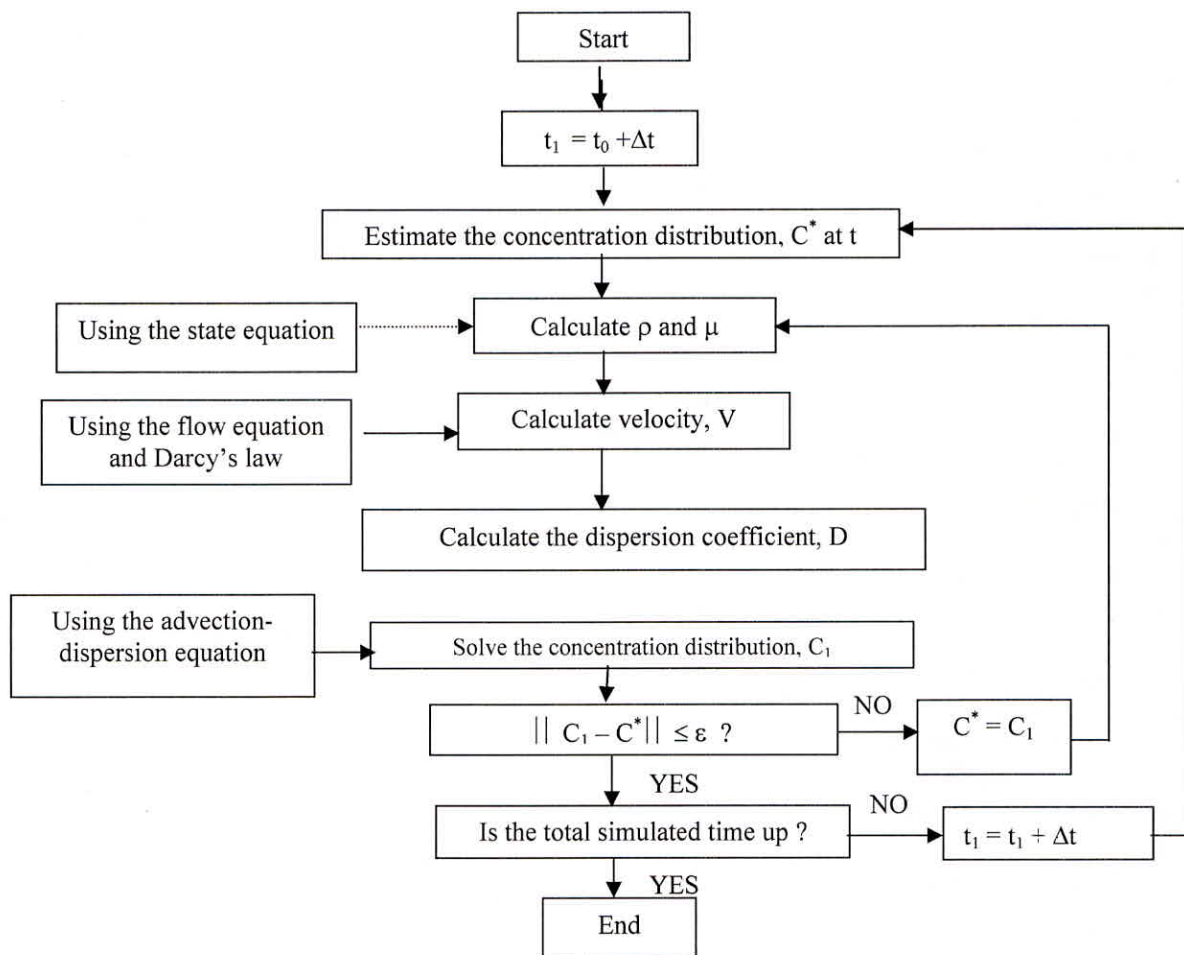


Fig. 12 Flow chart for solving advection-dispersion model in general case.

the dispersion equation:

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial x} \left( D_{xx} \frac{\partial C}{\partial x} + D_{xy} \frac{\partial C}{\partial y} + D_{xz} \frac{\partial C}{\partial z} - CV_x \right) + \frac{\partial}{\partial y} \left( D_{xy} \frac{\partial C}{\partial x} + D_{yy} \frac{\partial C}{\partial y} + D_{yz} \frac{\partial C}{\partial z} - CV_y \right) + \frac{\partial}{\partial z} \left( D_{xz} \frac{\partial C}{\partial x} + D_{yz} \frac{\partial C}{\partial y} + D_{zz} \frac{\partial C}{\partial z} - CV_z \right) + I \quad (32)$$

Eq. (31) is first solved to compute head,  $h$ . Next using the computed head in Darcy's law (Eq.30), the mean flow velocity is estimated. The estimated mean velocity is used in Eq. (32), computation of the concentration distribution.

### Complete Statement of Pollution Model

In earlier sections, we have derived the transport equations and discussed about how to formulate of a groundwater quality model. Now, let us work out as to how a real life pollution problem can be defined. The complete model of pollution consists of the following items:

- (i) Specification of the geometrical configuration of the closed surface that bounds the problem area, with possible segments at infinity,



- (ii) Specification of the dependent variable(s) of the pollution problem, i.e., the concentration  $C(x,t)$  of the specific constituent or constituents under consideration,
- (iii) Statement of a partial differential equations for every relevant species. Balance equations in terms of the various state variables of the problem,
- (iv) Specification of the numerical values of the transport and storage coefficients. Specific interest would be dispersivity and coefficient of molecular diffusion in porous medium under consideration,
- (v) Statement of the numerical values of the various source and sink terms,
- (vi) Statement of initial and boundary conditions that the state variables have to satisfy within the domain  $t = 0$  and on its boundaries at  $t > 0$ , respectively.

## **WATER QUALITY STANDARDS**

The Bureau of Indian Standards (BIS) earlier known as Indian Standards Institution (ISI) has laid down the standard specifications for drinking water (BIS, 1991). In order to enable the users, exercise their discretion towards water quality criteria, the maximum permissible limit has been prescribed especially where no alternate source is available. The national water quality standards describe essential and desirable characteristics required to be evaluated to assess suitability of water for drinking purpose (BIS, 1991). Drinking Water Specifications as prescribed by Bureau of Indian standards are given in Table 2.

## **WATER QUALITY ASSESSMENT FOR IRRIGATION PURPOSE**

Irrigation water quality refers to its suitability for agricultural use. The concentration and composition of dissolved constituents in water determine its quality for irrigation use. Quality of water is an important consideration in any appraisal of salinity or alkali conditions in an irrigated area. A good quality water has the potential to cause maximum yield under good soil and water management practices. However, the quality of irrigation water depends primarily on its silt and salt content. Water used for irrigation always contains measurable quantities of dissolved substances, which, as a general collective term, are called salts. They include relatively small but important amounts of dissolved solids originating from dissolution or weathering of the rocks and soils and dissolving of lime, gypsum and other salt sources as water passes over or percolates through them. Whatever may be the source of irrigation water, viz., river, canal, tank, open well or tube well, some soluble salts are always dissolved in it. The nature and quality of dissolved salts depends upon the source of water and its course before use and determine the quality of irrigation water.

With good quality water there should be very infrequent or no problems affecting productivity. However, with poor quality water, various soil and cropping problems can be expected to develop. Special management practices may then be required to maintain full crop productivity. Of the several factors influencing irrigation water quality, the generally accepted criteria for judging the quality are:

- Salinity
- Relative Proportion of Sodium to other Cations (SAR)
- Residual Sodium Carbonate (RSC)
- Boron

**Table 2. Drinking Water Specifications (IS: 10500:1991)**

S.No.	Characteristics	Desirable limit	Permissible limit
<i>Essential Characteristics</i>			
1.	Colour, Hazen units, Max	5	25
2.	Odour	Unobjectionable	-
3.	Taste	Agreeable	-
4.	Turbidity, NTU, Max	5	10
5.	pH value	6.5 to 8.5	-
6.	Total hardness (as CaCO <sub>3</sub> ), mg/L, Max	300	600
7.	Iron (as Fe), mg/L, Max	0.3	1.0
8.	Chlorides (as Cl), mg/L, Max	250	1000
9.	Residual free chlorine, mg/L, Max	0.2	-
<i>Desirable Characteristics</i>			
10.	Dissolved solids, mg/L, Max	500	2000
11.	Calcium (as Ca), mg/L, Max	75	200
12.	Magnesium (as Mg), mg/L, Max	30	75
13.	Copper (as Cu), mg/L, Max	0.05	1.5
14.	Manganese (as Mn), mg/L, Max	0.1	0.3
15.	Sulphate (as SO <sub>4</sub> ), mg/L, Max	200	400
16.	Nitrate (as NO <sub>3</sub> ), mg/L, Max	45	100
17.	Fluoride (as F), mg/L, Max	1.0	1.5
18.	Phenolic compounds (as C <sub>6</sub> H <sub>5</sub> OH), mg/L, Max	0.001	0.002
19.	Mercury (as Hg), mg/L, Max	0.001	-
20.	Cadmium (as Cd), mg/L, Max	0.01	-
21.	Selenium (as Se), mg/L, Max	0.01	-
22.	Arsenic (as As), mg/L, Max	0.05	-
23.	Cyanide (as CN), mg/L, Max	0.05	-
24.	Lead (as Pb), mg/L, Max	0.05	-
25.	Anionic detergents (as MBAS), mg/L, Max	0.02	1.0
26.	Chromium (as Cr <sup>6+</sup> ), mg/L, Max	0.05	-
27.	PAH, mg/L, Max	-	-
28.	Mineral oil, mg/L, Max	0.01	0.03
29.	Pesticides, mg/L, Max	Absent	0.001
30.	Alkalinity, mg/L, Max	200	600
31.	Aluminium (as Al), mg/L, Max	0.03	0.2
32.	Boron, mg/L, Max	1	5

The safe limits of electrical conductivity for crops of different degrees of salt tolerances under varying soil textures and drainage conditions are given in Table 3. The quality of water is commonly expressed by classes of relative suitability for irrigation with reference to salinity levels. The recommended classification with respect to electrical conductivity, sodium content, Sodium Absorption Ratio (SAR) and Residual Sodium Carbonate (RSC) are given in Table 3.



**Table 3. Safe Limits of Electrical Conductivity for Irrigation Water**

S.No.	Nature of soil	Crop growth	Upper permissible safe limit of EC in water, $\mu\text{S}/\text{cm}$
1.	Deep black soil and alluvial soils having clay content more than 30% soils that are fairly to moderately well drained	Semi-tolerant	1500
		Tolerant	2000
2.	Having textured soils having clay contents of 20-30% soils that are well drained internally and have good surface drainage system	Semi-tolerant	2000
		Tolerant	4000
3.	Medium textured soils having clay 10-20% internally very well drained and having good surface drainage system	Semi-tolerant	4000
		Tolerant	6000
4.	Light textured soils having clay less than 10% soil that have excellent internally and surface drainage system	Semi-tolerant	6000
		Tolerant	8000

**Table 4. Guidelines for Evaluation of Irrigation Water Quality**

Water class	Sodium (Na) %	Electrical conductivity, $\mu\text{S}/\text{cm}$	SAR	RSC meq/l
Excellent	< 20	< 250	< 10	< 1.25
Good	20-40	250-750	10-18	1.25-2.0
Medium	40-60	750-2250	18-26	2.0-2.5
Bad	60-80	2250-4000	> 26	2.5-3.0
Very bad	> 80	> 4000	> 26	> 3.0

**Salinity**

Salinity is broadly related to total dissolved solids (TDS) and electrical conductivity (EC). High concentration of TDS and electrical conductivity in irrigation water may increase the soil salinity, which affect the salt intake of the plant. The salts present in the water, besides affecting the growth of the plants directly, also affect the soil structure, permeability and aeration, which indirectly affect the plant growth. Soil water passes into the plant through the root zone due to osmotic pressure. As the dissolved solid content of the soil water in the root zone increases, it is difficult for the plant to overcome the osmotic pressure and the plants root membrane are able to assimilate water and nutrients. Thus, the dissolved solids content of the residual water in the root zone also has to be maintained within limits by proper leaching. These effects are visible in plants by stunted growth, low yield, discoloration and even leaf burns at margin or top.

**Sodium Adsorption Ratio (SAR)**

Any increase in the SAR of irrigation water increases the SAR of soil solution. This ultimately increases the exchangeable sodium of the soil. Generally, there is a linear relationship between SAR and exchangeable sodium percentage (ESP) of the soil upto moderately ESP levels, and at high ESP levels the relationship tends to be curvilinear.

A high salt concentration in water leads to formation of a saline soil and high sodium leads to development of an alkali soil. The sodium or alkali hazard in the use of water for irrigation is determined by the absolute and relative concentration of cations and is expressed in terms of Sodium Adsorption Ratio (SAR). If the proportion of sodium is high, the alkali hazard is high; and conversely, if calcium and magnesium predominate, the hazard is less. There is a



significant relationship between SAR values of irrigation water and the extent to which sodium is absorbed by the soil. If water used for irrigation is high in sodium and low in calcium, the cation-exchange complex may become saturated with sodium. This can destroy the soil structure owing to dispersion of the clay particles. A simple method of evaluating the danger of high-sodium water is the sodium-adsorption ratio, SAR (Richards, 1954):

$$SAR = \frac{Na^+}{\sqrt{(Ca^{2+} + Mg^{2+}) / 2}} \quad (33)$$

The sodium percentage is calculated as:

$$Na\% = \frac{Na^+ + K^+}{Ca^{2+} + Mg^{2+} + Na^+ + K^+} \times 100 \quad (34)$$

where all ionic concentrations are expressed in milliequivalent per liter. Calculation of SAR for given water provides a useful index of the sodium hazard of that water for soils and crops. A low SAR (2 to 10) indicates little danger from sodium; medium hazards are between 7 and 18, high hazards between 11 and 26, and very high hazards above that. The lower the ionic strength of the solution, the greater the sodium hazard for a given SAR.

## REFERENCES AND BIBLIOGRAPHY

- Bear, J. 1972. Dynamics of Fluids in Porous Media, Elsevier, New York.
- Bear, J. 1979. Hydraulics of Groundwater, McGraw-Hill, New York.
- Cherry, J.A., R.W. Gillham, and J.F. Pickens. 1975 Contaminant Hydrogeology, 1. Physical Process, Geosci. Can., vol.2.
- Dagan, G. 1989 Flow and Transport in porous Formations, Springer-Verlag, Berlin.
- Freeze, R.A., and J.A. Cherry. 1979. Groundwater, Prentice-Hall, Englewoods Cliffs, New Jersey.
- Fried, J.J. 1975. Ground Pollution, Elsevier Scientific, Amsterdam.
- Klotz, D., K.P., Seiler, H. Moser, and F. Neumaier. 1980. Dispersivity and velocity relationship from laboratory and field experiments, J. of Hydrol., 45(3/4), 169-184.
- Jain, C. K. 2006. Groundwater Contaminants and Assessment, in: Groundwater modeling and management, ( Eds. N.C. Ghosh, and K.D. Sharma). Capital Publishing Company, New Delhi., 594p.
- Ghosh, N. C. 2006. Contaminant Transport Modelling in Groundwater, in: Groundwater modeling and management (Eds. N.C. Ghosh, and K.D. Sharma). Capital Publishing Company, New Delhi., 594p.
- Lapidus, L., and G.F. Pinder. 1982. Numerical Solution of Partial Differential Equations in Science and Engineering, John Wiley & Sons Inc., New York.
- Peaceman, Donald, W. 1977. Fundamentals of Numerical Reservoir Simulation, Elsevier Scientific Publishing Company, New York.
- Strack, Otto, D.L. 1982. Groundwater Mechanics, Prentice Hall, New Jersey.
- Strecker, E.W., and W. Chu. 1986. Parameter identification of a groundwater contaminant transport model, Ground Water, 24(1), 56-62.
- Sunm N-Z. 1994. Inverse Problems in Groundwater Modeling, Kluwer Publishers, The Netherlands.
- Sun, Ne-Zheng. 1996. Mathematical Modeling of Groundwater Pollution, Springer-Verlag, New York Inc.