Chapter 3
Theoretical development - groundwater flow and transport modeling and source identification

3.1 Introduction
Since groundwater moves at a very slow rate in aquifers, groundwater contamination and its source is normally detected much later (Freeze and Cherry, 1979). As a result, before a bore well shows deterioration in its water quality, it is likely that groundwater may have moved several kilometers from the source and a large aquifer area is already contaminated. A large number of surveillance bore wells will be required to properly track the movement of contaminants if the aquifer area involved is very large. It will be prohibitively costly to drill such a large network of bore wells. As is well known, remediation of contaminated groundwater is also a very costly affair. Therefore numerical modeling of groundwater flow and contamination plays a very important in the prediction of the movement of contaminants in an aquifer and also to optimize the remediation efforts.

Significant progress has been there in groundwater flow and contaminant transport modeling over the years. Many techniques have evolved and been applied in groundwater modeling such as finite difference, finite element, particle tracking methods, method of characteristics, modified method of characteristics, random transport models etc. Recently mesh free methods has also been applied to groundwater modeling. This section deals with the theoretical developments and application of mesh free methods to simulate groundwater flow and transport problems.

3.2 Sources of groundwater contamination
Groundwater can become contaminated in many ways. If rain water or surface water comes into contact with contaminated soil while seeping into the ground, it can become polluted and can carry the pollution from the soil to the groundwater. Groundwater can also become contaminated when liquid hazardous substances themselves soak down through the soil or rock into the groundwater. Some liquid hazardous substances do not mix with the groundwater but remain pooled within the soil or bedrock (Bear, 1979). These pooled substances can act as long-term sources of groundwater contamination as the groundwater flows through the soil or rock and comes into contact with them.

Aquifers are normally contaminated by agricultural activities, industrial waste and municipal sewage waste disposal practices. The major sources of groundwater pollution are Underground Storage Tanks (USTs), landfills, septic systems and hazardous waste sites (Freeze and Cherry, 1979). Other sources
include pesticides leaks or spills of industrial chemicals at manufacturing facilities, runoff of salt and other chemicals from roads and highways and fertilizer on agricultural land. Most of water contamination cases generally occur in highly developed areas, agricultural areas, and industrial zones.

Groundwater contaminants exist in many forms, and contaminant classification schemes can be based on any of several physicochemical characteristics. For example, contaminants may be classified based on their preference for association with the aqueous phase or with particles (Bear, 1979). Contaminant distinction based on phase preference is important as the phase(s) a contaminant associates with can affect its transport behavior and toxicology. Furthermore, the form taken by a contaminant can also affect the choice of treatment processes that may be implemented to remediate a contaminated area. In general, the physicochemical characteristics of groundwater contaminants and the surrounding aquifer will play critical roles in determining their fate, transport, and effects.

### 3.3 Mechanisms of Contaminant movement

The principal mechanisms of contaminant transport are advection, diffusion, dispersion, sorption, and decay (Bear, 1979). These processes are briefly discussed in this section in their simplest 1D form. Other processes such as hydrolysis, volatilization, and biotransformation may also play an important role depending on the type and nature of the contaminant and also the soil (Zheng and Bennet, 2002).

#### 3.3.1 Advection

The process by which solutes are transported by the bulk motion of the flowing groundwater is known as advection (Freeze and Cherry, 1979). Owing to advection, non-reactive solutes are carried at an average rate equal to the average linear velocity, $\bar{v}$, of the water. Here

$$\bar{v} = \frac{v}{n} = \frac{1}{n} (-K \nabla h)$$  \hspace{1cm} (3.1)

Here, $v$ is the specific discharge or Darcy flux and $n$ is the porosity. The advection process is also sometimes called convection. An estimation of the flow velocity is needed for an accurate estimation of the advective transport. In sand/gravel aquifers with significant groundwater, the plume movement is dominated by advection. Applying the conservation of mass principle to a control volume, it can be derived that the one dimensional advective transport equation in a homogeneous aquifer (Zheng and Bennet, 2002) as,

$$\frac{\partial C}{\partial t} = -v \frac{\partial C}{\partial x}$$  \hspace{1cm} (3.2)
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Here $C$ is the concentration of the solute. The main factors that control the advective transport are hydraulic conductivity or transmissivity, effective porosity of the porous material and the hydraulic gradient.

### 3.3.2 Diffusion

Diffusion is the flux of solute from a zone of higher concentration to one of lower concentration due to the Brownian motion of ionic and molecular species. Under steady-state condition, the diffusion flux $F$ is described by Fick’s first law (Bear, 1979),

$$ F = -D \nabla C $$ \hspace{1cm} (3.3)

where $D$ is the diffusion coefficient $[L^2 T^{-1}]$. For diffusion in porous media, Freeze and Cherry (1979) suggest taking an effective diffusion coefficient, $D^* = \omega D$ to account for the tortuosity of the flow paths with $\omega$ ranging from 0.5 to 0.01 for laboratory studies of non-adsorbed ions in porous geological materials. The change of concentration over time inside a control volume subject to diffusion flux is given by Fick’s second law,

$$ \frac{\partial C}{\partial t} = D^* \frac{\partial^2 C}{\partial x^2} $$ \hspace{1cm} (3.4)

The importance of diffusion increases as flow velocities decrease. Thus diffusion may be the governing transport mechanism in unfractured clays with low hydraulic conductivities. Diffusion can generally be neglected in gravel aquifers with high flow velocities. It can also be significant in fractured porous aquifers.

### 3.3.3 Dispersion

Dispersion is the spreading of the plume that occurs along and across the main flow direction due to aquifer heterogeneities at both the small scale (pore scale) and at the macroscale (regional scale). Dispersion tends to increase the plume uniformity as it travels downstream. Factors that contribute to dispersion include faster flow at the center of the pores than at the edges, some pathways being longer than others, flow velocity larger in smaller pores than in larger ones. This is known as mechanical dispersion. The spreading due to both mechanical dispersion and molecular diffusion is known as hydrodynamic dispersion (Freeze and Cherry, 1979).

Dispersion equation in general is derived using Fick’s law, whereas, results from theoretical studies suggest that dispersion is non-Fickian near the source of contaminant and it generally becomes Fickian at larger times or travel distances where a constant dispersivity value is achieved (Anderson, 1984). A
phenomenological coefficient that combines the effects of diffusion and dispersion, known as dispersion coefficient is generally defined. As mechanical dispersion is more pronounced in the longitudinal direction than in the transverse direction, a longitudinal dispersion coefficient $D_L$ and a transverse dispersion coefficient $D_T$ are introduced. These coefficients are defined as,

$$
D_L = \alpha_L v + D^*
$$

$$
D_T = \alpha_T v + D^*
$$

where $\alpha_L$ is the longitudinal dispersivity [L], $\alpha_T$ is the transverse dispersivity [L], and $v$ is the pore velocity [LT$^{-1}$].

### 3.3.4 Retardation and Reactions

Sorption refers to the exchange of molecules and ions between the solid phase and the liquid phase. It includes adsorption and desorption. Adsorption is the attachment of molecules and ions from the solute to the rock material. Adsorption produces a decrease of the concentration of the solute or, equivalently, causes a retardation of the contaminant transport compared with water movement. Desorption is the release of molecules and ions from the solid phase to the solute (Zheng and Bennet, 2002).

The relationship between the solute concentration in the adsorbed phase and in the water phase is called a sorption isotherm. The simplest expression is the linear isotherm, called Henry’s equilibrium model,

$$
C_a = K_d C
$$

where $C_a$ is the sorbed concentration as mass of contaminant per mass of dry rock matrix dimensionless, $C$ is the dissolved concentration in mass of contaminant per volume of water [ML$^{-3}$], and $K_d$ is the distribution coefficient [L$^3$ M$^{-1}$]. This expression implies that there is equilibrium between the adsorbed concentration and the dissolved concentration. This can be assumed when the adsorption process is fast compared with advection of contaminant. Apart from the Henry’s model, many adsorption models are also used (Rastogi, 2007).

The adsorption causes retardation in the migration of contaminants compared with advection. The contaminant transport gets more retarded as the fraction adsorbed increases. This effect can be described by a retardation factor $R_a$, which for a linear isotherm, is

$$
R_a = 1 + \frac{(1 - n)\rho_s}{n} K_d
$$
where \( n \) is the porosity and \( \rho_x \) is the density of the solids. The retardation coefficient may take values from 1 to 10,000. The velocity of the solute front \( v_c \) (where the concentration is half that of the original concentration) is given by

\[
v_c = \frac{v}{R_a}
\]  

(3.8)

If sorption is taken into account, the 1D advection–dispersion equation then becomes,

\[
\frac{\partial C}{\partial t} = -\frac{v}{R_a} \frac{\partial C}{\partial x} + \frac{D_l}{R_a} \frac{\partial^2 C}{\partial x^2}
\]  

(3.9)

where the term on the left side represents the time rate of change in storage of contaminant in the control volume, the first term on the right-hand side represents the retarded advective inflow–outflow, and the last term represents the retarded diffusion and dispersion.

When there is chemical reaction (degradation) whereby the solute changes its form or if the solute undergoes radioactive decay, it decreases the concentration of the solute. The simplest model for decay of contaminants without transport is first order model,

\[
\frac{\partial C}{\partial t} = -\lambda C
\]  

(3.10)

where \( \lambda \) is the first order decay rate constant [T\(^{-1}\)]. This relation also applies to radioactive decay and degradation processes. Integration of equation (3.10) gives \( C = C_0 e^{-\lambda t} \) where \( C_0 \) is the concentration at time \( t = 0 \) and

\[
\lambda = \frac{\ln 2}{T_{1/2}}
\]  

(3.11)

\( T_{1/2} \) is the half-life of the radioactive isotope or of the degraded contaminant. The degradation causes a mass \( \lambda C \) to disappear per unit volume per unit of time. The transport equation including decay is then obtained by simply appending the quantity \(-\lambda C\) to the right-hand side of equation (3.9).

### 3.4 Governing equations and Boundary conditions

#### 3.4.1 Groundwater Flow

The governing equation describing the groundwater flow in a two dimensional inhomogeneous confined aquifer is given as (Bear, 1979)
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\[
\frac{\partial}{\partial x} \left[ T_x \frac{\partial h}{\partial x} \right] + \frac{\partial}{\partial y} \left[ T_y \frac{\partial h}{\partial y} \right] = S \frac{\partial h}{\partial t} + Q_w \delta(x - x_i)(y - y_i) - q \tag{3.12}
\]

Following initial conditions are used for transient analysis,

\[
h(x, y, 0) = h_0(x, y) \quad x, y \in \Omega \tag{3.13}
\]

Generally, the boundary conditions can be of two types, the prescribed head or flux. It can be written as:

\[
h(x, y, t) = h_1(x, y, t) \quad x, y \in \partial \Omega_1 \tag{3.14}
\]

\[
T \frac{\partial h}{\partial n} = q_1(x, y, t) \quad x, y \in \partial \Omega_2 \tag{3.15}
\]

For an unconfined aquifer, the governing equation is given as (Bear, 1979),

\[
\frac{\partial}{\partial x} \left[ K_x h \frac{\partial h}{\partial x} \right] + \frac{\partial}{\partial y} \left[ K_y h \frac{\partial h}{\partial y} \right] = S_y \frac{\partial h}{\partial t} + Q_w \delta(x - x_i)(y - y_i) - q \tag{3.16}
\]

For unconfined aquifer problems, the boundary conditions are:

\[
h(x, y, t) = h_1(x, y, t) \quad x, y \in \partial \Omega_1 \tag{3.17}
\]

\[
K h \frac{\partial h}{\partial n} = q_2(x, y, t) \quad x, y \in \partial \Omega_2 \tag{3.18}
\]

where \( h(x, y, t) \) is the Piezometric head (m) which is the state variable, \( K_x, K_y \) are the hydraulic conductivities in \( x \) and \( y \) directions, \( T_x, T_y \) are the transmissivities (m\(^2\)/d) in \( x \) and \( y \) directions, \( S \) is the storage coefficient, \( S_y \) is the specific yield, \( Q_w \) is the source or sink term (m\(^3\)/d/m\(^2\)). The flow region is represented by \( \Omega \) while the boundary is denoted by \( \partial \Omega \). \( \frac{\partial}{\partial n} \) denotes the normal derivative to the boundary. \( h_0(x, y) \) is the initial head in the flow domain (m), \( h_1(x, y, t) \) is the known head value of the boundary head (m) and \( q(x, y, t) \) is the known inflow rate (m\(^3\)/d/m).

### 3.4.2 Groundwater Solute Transport

The governing equation for contaminant transport of a single chemical constituent in groundwater is given by (Freeze and Cherry, 1979; Wang and Anderson, 1982; Desai et al., 2011 etc.)

\[
R \frac{\partial C}{\partial t} = \frac{\partial}{\partial x} \left( D_{xx} \frac{\partial C}{\partial x} \right) + \frac{\partial}{\partial y} \left( D_{yy} \frac{\partial C}{\partial y} \right) - \frac{\partial}{\partial x} \left( V_x C \right) - \frac{\partial}{\partial y} \left( V_y C \right) - \frac{c'w}{nb} - R\lambda C + \frac{q_w C}{n} \tag{3.19}
\]

where,

\( V_x, V_y \) ≡ Seepage velocity in \( x \) and \( y \) direction [LT\(^{-1}\)]

\( D_{xx}, D_{yy} \) ≡ components of dispersion coefficient tensor in \( x \) and \( y \) direction [L\(^2\)T]
C is the concentration of the dissolved species \([\text{ML}^{-3}]\); \(\lambda\) is the reaction rate constant \([\text{T}^{-1}]\); 
\(w\) = elemental recharge rate with solute concentration \(c^\prime\); \(n\) = porosity; \(b\) = aquifer thickness; 
\(R = \text{Retardation factor} = 1 + \rho_b K_d/n\), in which \(\rho_b\) is the media bulk density, \(K_d\) is the sorption coefficient and \(q_w\) = volumetric pumping rate from a source.

The initial condition is,

\[
C(x, y, 0) = f(x, y, 0) \quad (x, y) \equiv \Omega \tag{3.20}
\]

And the boundary conditions are of the form,

Dirichlet boundary condition:

\[
C(x, y, t) = g_1(x, y, t) \quad (x, y) \equiv \partial \Omega_1; \tag{3.21}
\]

Neumann boundary condition:

\[
(D_x \frac{\partial C}{\partial x}) n_x + (D_y \frac{\partial C}{\partial y}) n_y = g_2(x, y, t) \in \partial \Omega_2 \tag{3.22}
\]

Where \(\Omega\) is the flow domain, \(\Omega = \) boundary region \((\partial \Omega_1 \cup \partial \Omega_2 = \partial \Omega)\); \(f\) is a given function in \(\Omega\); \(g_1, g_2\) are functions along boundaries; and \(n_x, n_y\) are the components of the unit outer normal vector to the given boundary.

The seepage velocities \(V_x, V_y\) are evaluated from the flow equations by the following relations,

\[
V_x = -\frac{K_x}{n} \frac{\partial h}{\partial x}; \quad V_y = -\frac{K_y}{n} \frac{\partial h}{\partial y} \tag{3.23}
\]

where \(n\) is the porosity of the medium. The elements of the dispersion coefficient tensor are evaluated from the longitudinal dispersivity \((\alpha_L)\) and transverse dispersivity \((\alpha_T)\) from the relations (Bear, 1979):

\[
D_{xx} = \frac{\alpha_L V_x^2 + \alpha_T V_y^2}{V^2}; \quad D_{yy} = \frac{\alpha_T V_x^2 + \alpha_T V_y^2}{V^2}; \quad D_{xy} = D_{yx} = \frac{(\alpha_L - \alpha_T)V_xV_y}{V^2} \tag{3.24}
\]

where, \(V^2 = V_x^2 + V_y^2\). Equations (3.23) and (3.24) together provide the linkage or coupling between the groundwater flow and transport equations. The velocities computed from the flow equation are used as input to the transport equation.

### 3.5 Groundwater flow and transport modeling - numerical methods

Every groundwater model design consists of the following steps (Anderson and Woessner, 2002):

1. Establish the purpose of the model. It will determine the governing equations and code to be selected
2. Develop a conceptual model of the system
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3. Select the mathematical model (governing equation and computer code)
4. Model design
5. Calibration
6. Calibration sensitivity analysis
7. Model verification
8. Prediction
9. Presentation of results
10. Post audit

Figure 3.1 shows a flow chart of the groundwater modeling process (Anderson and Woessner, 2002).

The laws which govern the groundwater flow and solute transport are usually expressed in terms of partial differential equations (PDEs). For the vast majority of geometries and problems, these PDEs cannot be solved with analytical methods. Instead, an approximation of the equations can be constructed, based upon different types of discretization. These discretization methods approximate the governing PDEs with numerical model equations, which can be solved using numerical methods. The solution to the numerical model equations are, in turn, an approximation of the real solution to the PDEs. There are various discretization schemes for solving PDEs. The most widely used methods are the finite difference method (FDM) and finite element method (FEM). Both methods require the construction of a grid or mesh of the solution domain which can be computationally very costly. Meshfree method which does not require the construction of a mesh is gaining popularity in recent days. Brief descriptions of these methods are provided in this section.
3.5.1 Finite Difference Method

Finite difference methods (FDM) are numerical methods for solving differential equations by approximating them with difference equations, in which the derivatives are approximated by finite differences. The difference approximations of the derivatives of a function \( f(x) \) can be obtained from a Taylor series expansion (Wang and Anderson, 1982):

\[
f(x_0 + \Delta x) = f(x_0) + \frac{f'(x_0)}{1!} \Delta x + \frac{f''(x_0)}{2!} \Delta x^2 + \cdots + \frac{f^{(n)}(x_0)}{n!} \Delta x^n + R_n(x)
\]  

(3.25)
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The first derivative of the function can be obtained by truncating the series as,

\[ f(x_0 + \Delta x) = f(x_0) + f'(x_0)\Delta x + O(\Delta x^2) \]

or,

\[ f'(x_0) = \frac{f(x_0 + \Delta x) - f(x_0)}{\Delta x} + O(\Delta x) \tag{3.26} \]

This is known as the forward difference approximation of the first derivative. The backward difference approximation can be obtained by using Taylor series expansion for \( f(x_0 - \Delta x) \). Centered difference approximations can be obtained by combining the Taylor series expansions of \( f(x_0 + \Delta x) \) and \( f(x_0 - \Delta x) \). The centered difference approximation for the second derivative is obtained as (Wang and Anderson, 1982),

\[ f''(x_0) = \frac{f(x_0 + \Delta x) - 2f(x_0) + f(x_0 - \Delta x)}{\Delta x^2} + O(\Delta x^2) \tag{3.27} \]

To use finite difference method, the domain over which the differential equation is to be solved for is divided into a grid of discrete points (nodes). The differential equation is then written (discretized) on each node using the finite difference approximations of the derivatives i.e. FDM is a point wise approximation of the differential equation on each node. Appropriate boundary conditions are applied at the domain boundaries. The resulting system of equations is then solved using a numerical technique such as Gauss elimination or iterative method to get the nodal solutions.

Finite difference methods are one of the most popular methods for solving partial differential equations due to its simplicity. The MODFLOW codes (Harbaugh and McDonald, 1996) used for groundwater flow modeling and MT3DMS (Zheng and Wang, 1998) for solute transport modeling are both FDM codes. However, FDM has its own limitations. Its main drawback is that it cannot properly represent complex domains accurately and efficiently. It also has difficulty in implementing dissimilar or variable material properties.

### 3.5.2 Finite Element method

In contrast to the FDM, the finite element method (FEM) divides the solution domain into simply shaped regions or elements (Desai et al., 2011). An approximate solution is then developed for each of these elements. The total solution is then generated by coupling together (assembling) the individual solutions over each element taking care to ensure continuity at the inter-element boundaries. FEM thus uses continuous, piecewise smooth functions to approximate the unknown quantity. FEM is characterized by the following three basic features (Desai et al., 2011),
1. The domain of the problem is represented by a collection of simple sub-domains, called finite elements. The collection of finite elements is called the finite element mesh.

2. Over each finite element, the physical process is approximated by functions of desired type (polynomials or otherwise), and algebraic equations relating physical quantities at selective points, called nodes, of the elements are developed.

3. The element equations are assembled using continuity and/or “balance” of physical quantities.

The use of elements, rather than a rectangular grid, allows a much accurate representation of complex and irregularly shaped domains. Further, the values of the unknown variable can be generated continuously across the entire domain rather than at isolated grid points.

The main steps involved in a FEM solution of a PDE are (Desai et al., 2011; Segerlind, 1984):

1. Discretization of the domain into finite elements.

2. Development of element equations: develop element equations to approximate the solution for each element. This consists of two steps:
   (i) Choose an appropriate function (called trial function) to approximate the solution. The trial function has parameters which have to be determined so that it satisfies the differential eqn. as closely as possible. Usually the approximation function is a linear combination of basis functions:
   \[ u(x) = \sum_{i=0}^{n} \phi_i(x) u_i \]  
   (3.28)
   where \( \phi_i(x) \) ’s are known as basis functions or shape functions and \( u_i \) are the nodal values of the unknown function \( u(x) \).
   (ii) Since it is not an exact solution, substitution of the trial function into the differential equation will produce an error (called residual), \( R(x) \). The coefficients of the trial functions are evaluated such that it approximates the solution in an optimal way i.e. the residual (or error) is made as small as possible (minimized) or forced to be zero. The residual is usually multiplied with a weight function, \( w_i(x) \) before minimization i.e.
   \[ \min \int_{\Omega} w_i(x) R(x) dx \]  
   (3.29)

3. Assembly of element equations taking care of continuity and/or balance of physical quantities.
4. Application of boundary conditions
5. Solving the system of equations
6. Post-processing of the solution

It may be noted that finite element method approximates a solution by minimizing the associated error function (residual). The minimizing process automatically finds the linear combination of basis functions which is closest to the solution (Zienkiewicz and Taylor, 2000).

In FDM the differential operators are approximated from Taylor’s series expansions while in FEM the unknown variable itself is approximated with a shape function of one’s choice. This provides enormous flexibility with FEM in approximating the unknown function. The shape of the elements can also be chosen by the modeler according to the requirements of the problem domain. These flexibilities, together with the ability to represent any complex geometry makes FEM one of the most widely used approach for solving PDEs. Several commercial softwares based on FEM are available for performing simulations in various areas of engineering and scientific endeavors (Pepper and Heinrich, 1992).

However, creating a grid or mesh for FEM can be computationally very costly. Consequently FEM is not suitable for those applications which require frequent meshing such as adaptive analysis, simulation of large deformation, crack propagation, breakage of materials etc.

### 3.5.3 Meshfree Methods

Meshfree methods provide an alternative to the mesh based methods and seeks to address the inherent shortcomings of numerical methods that rely on meshes. A truly meshfree method requires only a set of scattered nodes within and on the boundary to represent the modeling domain and no information is required on the connectivity of the nodes throughout the process of solving the problem (Liu and Gu, 2005). However, for most of the methods classified as meshfree methods, the connectivity of the nodes is determined at the run time. In conventional numerical methods (FDM, FEM etc.), the definition of the connectivity of the nodes needs to be determined \textit{a priori}.

The minimum requirement for a meshless method is that a predefined mesh is not necessary at least in field variable interpolation. Unlike FEM where shape functions are determined for each element, meshless methods compute the shape functions using a support domain. A support domain of a point is a collection of nodes used to approximate the function value at that point (Liu and Gu, 2005). The equations of a mesh free method can be formulated using the shape functions and a strong or weak form system equation. The procedures of forming system equations are slightly different for different meshfree methods. Several variants of meshfree methods have been proposed in the last three decades. These methods have been discussed in Liu and Gu (2005), Nguyen et al. (2008), Belytschko et al.(1996) etc.
### 3.5.4 Comparison of FEM and Meshfree model

The solution procedures of FEM and meshfree methods are as shown in the Figure 3.2 (Liu and Gu, 2005). Both the methods follow similar procedures. The differences are at the 2\textsuperscript{nd} and 3\textsuperscript{rd} stages viz., mesh generation and shape function construction. FEM requires a mesh but meshfree methods require only the nodal coordinates.

**Finite Element Method**

- Creation of geometry
- Mesh generation
- Shape functions generated based on a pre-defined element
- Discretized system equations
- Solution of field variables
- Post-processing of solution

**Meshfree Method**

- Creation of geometry
- Node generation
- Shape functions generated based on nodes in a local support domain
- Discretized system equations
- Solution of field variables
- Post-processing of solution

*Figure 3.2: Comparison of solution procedures of FEM and Meshfree methods*

The construction of the shape functions in these two methods is also quite different. In the finite element method, the shape functions are constructed using predefined elements, and the shape functions are the same for the entire element. But in MFree methods, the shape functions constructed are usually only for a particular point of interest based on selected local nodes located within a small region called the support domain of the point of interest (Liu and Gu, 2005). As such the shape functions can change when the point of interest changes. Once the global discretized system equation is established, the two methods follow the same procedure. The main differences between FEM and meshfree methods are listed below (Liu and Gu, 2005):
1. FEM requires the creation of a mesh while meshfree methods require only the generation of nodes.
2. Shape function creation in FEM is based on pre-defined elements while in meshfree methods it is based on a local support domain.
3. Imposition of essential boundary condition is easy in FEM but the same will require special treatments in meshfree methods.
4. Computational speeds are in general slower in meshfree methods as compared to FEM.
5. Meshfree methods, in general, yields more accurate solutions as compared to FEM.
6. Due to the requirement of a mesh, carrying out adaptive analysis with FEM is difficult especially in 3D. The same can be done much easier in meshfree methods.
7. It may be mentioned that FEM is a well-developed method whereas meshfree methods are in developmental stages with many issues yet to be addressed. Consequently while there are several commercial software packages for FEM, only a few codes are available for meshfree methods.

Since the solution procedure is the same for FEM and meshfree methods after the global discretized system is obtained, many of the techniques developed for FEM can be applied to meshfree methods also.

### 3.6 Groundwater source identification

Contaminant transport in groundwater is governed by advection-dispersion equation (ADE). Contaminant source identification involves solving the advection-dispersion equation backward in time. The problem of contaminant source identification is illustrated with a one dimensional case here. For a non-reactive contaminant, the one-dimensional (1-D) heterogeneous transport in a semi-infinite domain, described by the ADE is (Atmadja and Bagtzoglou, 2001b):

\[
\frac{\partial C}{\partial t} = \frac{\partial}{\partial x} \left[ D(x) \frac{\partial C}{\partial x} \right] - \frac{\partial}{\partial x} [u(x)C] \tag{3.30}
\]

with initial and boundary conditions:

\[
C(x_1, t) = C_{in}(t) \quad 0 \leq t \leq T_{obs} \tag{3.31}
\]

\[
C(\infty, t) = 0 \quad 0 \leq t \leq T_{obs} \tag{3.32}
\]

\[
C(x, T_{obs}) = C_T(x) \quad 0 \leq x \leq \infty \tag{3.33}
\]

where \(u(x)\) is the transport velocity in the x-direction and \(x\) is distance. In the pollution source location identification, the source \((x_i)\) information is not known, but measurements of the spatial distribution of the plume are given at time, \(T_{obs}\). For the release history reconstruction, usually the source location is assumed to be known, but the contaminant source function, \(C_{in}(t)\) is unknown. Finding the source
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location and the time history of the solute in groundwater can be categorized as a problem of time inversion. This means solving the governing equations backward in time. Modeling contaminant transport using reverse time is an ill-posed problem since the process, being dispersive is irreversible. Because of this, the solutions have discontinuous dependence on data and are sensitive to errors in the data.

A problem is categorized as a well-posed problem if (1) the solution exists; (2) the solution is unique; and (3) the solution is stable (Ortega and Rheinboldt, 1970). Problems that do not satisfy these criteria are called ill-posed. For the groundwater contamination problem, the plume has to have originated from someplace, therefore, physically, the plume exists. However, in rigorous mathematical terms, the fact that there exists a present day plume concentration does not necessarily mean that we satisfy the existence criterion. The solution exists only when we have perfect and consistent model and data that satisfy extremely restrictive conditions. Satisfying the stability criterion is a difficult task to accomplish since numerical schemes, which are usually implemented as a marching procedure are unstable for negative time steps, and make it impossible to solve contaminant transport problems backward in time.

Regarding the non-uniqueness of the solution, there is no method that can bypass this inherent problem. In inverse problems, one of the common practices to overcome the stability and non-uniqueness criteria is to make assumptions about the nature of the unknown function so that the finite amount of data in observations is sufficient to determine that function (Ala and Domenico, 1992). This can be achieved by converting the ill-posed problem to a properly posed one by stabilization or regularization methods. In the case of groundwater pollution source identification, additional information such as potential release sites and chemical fingerprints of the plume are usually available to make this possible.

### 3.6.1 Source identification Methods

A number of source identification techniques have been proposed. An overview of the developed methodologies can be found in Atmadja and Bagtzoglou (2001b), Michalak and Kitanidis (2004) and Sun et al. (2006). These methods may broadly be subdivided into four major groups (Atmadja and Bagtzoglou, 2001b) namely: optimization methods, analytical solution and regression approaches, direct methods, probabilistic and geo-statistical approach. Each of the methods is subject to significant drawbacks and limitations. A broad classification of the proposed methods is discussed below.

#### 3.6.1.1 Direct inversion of advection-diffusion equation

This class of approaches uses deterministic direct methods to solve the governing equations backward in time to reconstruct the release history of the contaminant plumes. The inversion is achieved by using appropriate integral equations or other transformations to represent the contaminant transport. Methods falling into this class of approaches are the Tikhonov regularization approach (Skaggs and Kabala, 1994),
method of quasi-reversibility (Skaggs and Kabala, 1995), the minimum relative entropy (MRE) inversion method (Woodbury et al., 1998), Fourier series based inversion technique (Birchwood, 1999), the marching-jury backward beam equation (MJBEE) method (Atmadja and Bagtzoglou, 2001a) etc. These methods have been applied to reconstruct the spatial and temporal plume release history in homogeneous and heterogeneous media. However, such methods are very sensitive to noise or errors in the concentration data and in some cases can only recover the plume history partially.

3.6.1.2 Analytical solution and regression

Analytical methods are an inverse method based on analytical solution of the contaminant transport problems and parameter estimation using linear or non-linear regression. Sidauruk et al., (1998) presented an inverse method based on the analytical solution that provides a complete estimate of the dispersion coefficients, flow velocity, amount of pollutant, its initial location and time of origin. Ala and Domenico (1992) developed an inverse analytical technique that can determine the source strength, the advective position of the contaminant front for the instantaneous contaminant plumes at air force base. Other analytical solutions methods were proposed by Butcher and Gauthier (1994), Alapati and Kabala (2000) etc. The analytical solution and regression techniques have been applied only to very simple geometries and flow conditions. They are also very sensitive to noise in the input data. Consequently their utility is very limited.

3.6.1.3 Probabilistic and geo-statistical method

Probabilistic and geo-statistical approaches employ probabilistic techniques such as geo-statistics to deduce the probability of the location of the sources. These techniques are among the first which attempts to solve the ADE backward in time without relying on optimization approaches. Methods belonging to this class are the random walk particle method (Bagtzoglou et al., 1992), backward in time solution of stochastic differential equations (Wilson and Liu, 1994), adjoint method (Neupauer and Wilson, 1999), probabilistic approach combining Bayesian theory and geo-statistical techniques (Snodgrass and Kitanidis, 1997) etc. The probabilistic and geo-statistical techniques have been used to assess the relative importance of each potential source and produce the maps of time and location probability. These techniques have limitations in application to complex geometries. Some of the methods require that potential sources be known a priori and that the release incidents are assumed to be instantaneous and occurring simultaneously.

3.6.1.4 Simulation-Optimization (SO) approach

These approaches were among the first to be proposed for groundwater source identification. In these methods, a forward simulation is run with different possible sets of sources and the predicted solution is
compared to the measured spatial and temporal concentration data. Since an infinite number of plausible combinations of sources are there, an optimization model is required. The optimization model searches for the particular combination of sources which leads to minimum differences with the observed data. Simulation-optimization approaches were first proposed by Gorelick et al., 1983) using linear programming and regression as the optimizer. Since then several such approaches have been proposed using various optimization methods, some of which also includes simultaneous parameter estimation. Wagner, (1992) used non-linear maximum likelihood for simultaneous source identification and parameter estimation. Other optimization technique proposed include non-linear optimization model (Mahar and Datta, 2000), artificial neural network (ANN) (Singh and Datta, 2004), genetic algorithm (GA) (Singh and Datta, 2006) etc. SO approaches have been applied to both steady state and transient source identification problems, hydro-geologic and source parameters identification and groundwater quality monitoring. It has the potential to be applicable in field scale problems with complex geometries. However, non-uniqueness of groundwater source identification and sensitivity to noise in input data pose a challenge for these methods.

### 3.7 Stability criterion

There are certain stability issues associated with the numerical modeling of groundwater flow and solute transport. These issues arise from the approximations used in spatial and temporal discretization. In this section, some of the issues which can drastically affect the outcome of the numerical model of the groundwater flow and solute transport are discussed (Bear, 1979; Zheng and Bennet, 2002).

**Stability in time integration:** Of the different time-stepping techniques, the explicit method is the most simple. However it is only conditionally stable. When the size of the time step, $\Delta t$ exceeds a certain limit, the numerical errors incurred by the solution will be amplified as the time marches forward leading to a situation where the solution is dominated by the errors and becomes an invalid or unstable solution. Consider the one-dimensional groundwater flow in a confined equation,

$$ T \frac{\partial^2 h}{\partial x^2} = S \frac{\partial h}{\partial t} \tag{3.34} $$

The explicit method is stable only when the following relation holds between the spatial grid size ($\Delta x$) and the time step size ($\Delta t$) (Wang and Anderson, 1982):

$$ \frac{T \Delta t}{S (\Delta x)^2} \leq \frac{1}{2} \tag{3.35} $$

Thus the nodal spacing and time step size cannot be independently chosen when using the explicit method. For the two dimensional problem, the stability condition is,
Similarly, for the one-dimensional advection-dispersion equation (Zheng and Bennet, 2002),

\[ \frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial t^2} - v \frac{\partial C}{\partial x} \] (3.37)

the explicit method is stable only when,

\[ \frac{D \Delta t}{(\Delta x)^2} \leq \frac{1}{2} \Rightarrow \Delta t \leq \frac{(\Delta x)^2}{2D} \] (3.38)

The explicit method is a special case of the general $\theta$- method of time integration (Richtmyer and Morton, 1967). In this technique, the time derivative is replaced by a simple forward difference while the solution is replaced by a weighted value of the previous time-step solution and current solution e.g. for the groundwater flow problem, \( h = \theta h^{t+\Delta t} + (1 - \theta) h^t \), \( \theta \in [0,1] \). When \( \theta = 0 \), it reduces to the explicit method. The $\theta$-method is unconditionally stable only when \( \theta \geq 1/2 \), otherwise it is only conditionally stable.

**Artificial oscillation and Numerical dispersion:** Artificial oscillation and numerical dispersion are two issues encountered in numerical modeling of advectively dominated transport problems. The root cause of these instabilities is the truncation error incurred by the derivative terms. To illustrate the idea, let us consider the one dimensional transport problem (eqn. 3.37). From Taylor series expansion (Zheng and Bennet, 2002),

\[ C(x + \Delta x) = C(x) + \Delta x \cdot \frac{\partial C}{\partial x} + \frac{(\Delta x)^2}{2} \cdot \frac{\partial^2 C}{\partial x^2} + O(\Delta x^3) \]

Substituting this expression, eqn. (3.39) into the RHS of eqn. (3.37) and neglecting terms with \( O(\Delta x^2) \), we get,

\[ \frac{\partial C}{\partial t} \approx D \frac{\partial^2 C}{\partial t^2} - v \left( \frac{C(x + \Delta x) - C(x)}{\Delta x} - \frac{\Delta x}{2} \cdot \frac{\partial^2 C}{\partial x^2} \right) \] (3.40)

Re-arranging the terms,

\[ \frac{\partial C}{\partial t} = \left( D + v \frac{\Delta x}{2} \right) \frac{\partial^2 C}{\partial x^2} - v \left( \frac{C(x + \Delta x) - C(x)}{\Delta x} \right) \] (3.41)
It may be observed that an artificial dispersion term has been added with dispersion coefficient, $v \Delta x/2$ as a truncation error. If $D \leq v \Delta x/2$, then the artificial dispersion term starts dominating over the actual dispersion and the solution will be invalid.

**Artificial oscillation**: Oscillations are the overshoot or undershoot in the numerical solution. It arises when a sharp concentration front is present i.e. when the problem is advection-dominated. The degree to which the transport problem is dominated by advection is measured by a quantity called Peclet number ($Pe$) (Zheng and Bennet, 2002). For a one-dimensional uniform flow field, it is given by:

$$Pe = \frac{v \Delta x}{D}$$  \hspace{1cm} (3.42)

A smaller value of Peclet number is desirable to for an oscillation free numerical solution. It has been shown that when $Pe \leq 2$, numerical oscillations are removed (Huyakorn and Pinder, 1983). Larger the physical dispersion ($D$), smaller the Peclet number. The Peclet number is also dependent on the grid spacing used. Smaller grid spacing leads to smaller $Pe$. However to keep the Peclet number within a small value, the grid spacing $\Delta x$ may have to be so small as to be impractical. There are several ways to deal with high Peclet number flow problems such as upstream weighting, streamline upwind Petrov-Galerkin (SUPG) etc. (Onate, 1998)

**Courant number**: Another source of numerical dispersion lies in the approximation of the time derivative. A quantity used to estimate numerical dispersion while solving the advection-dispersion (AD) equation is the Courant number (Zheng and Bennet, 2002). The Courant number ($Cr$) reflects the number of cells (or the fraction of a cell) that a solute particle will traverse by advection in one time step. It is defined as,

$$Cr = \frac{v \Delta t}{\Delta x}$$  \hspace{1cm} (3.43)

The numerical dispersion is dependent on the Courant number and is used as the accuracy requirement for the solution of AD equation (Zheng and Bennet, 2002). When advection dominates dispersion, designing a model with a small ($<1$) Courant number will decrease oscillations, improve accuracy and decrease numerical dispersion. To obtain sufficiently accurate solutions, it is generally required that $Cr$ be less than or equal to one. The Courant number requirement nevertheless put a limit on the time-step size to be used in implicit or Cranck-Nicholson schemes, even though these schemes are unconditionally stable.

### 3.8 Closure

This chapter has discussed the various physical processes which are associated with groundwater flow and solute transport. The partial differential equations (PDE) that governs these processes have been
elaborated along with the available numerical methods for solving them such as FDM, FEM and the meshfree methods. Each of these methods has its own strengths and weaknesses. Over and above these, various numerical stability issues also arise during groundwater flow and solute transport modeling and they have been briefly discussed. The primary root cause of these stability problems is the truncation or approximation errors that are implicit in the numerical methods. This chapter also discussed the broad classifications of the methods used for groundwater source identification and the limitations of each of them. The next chapter proposes a meshfree method for modeling groundwater flow and solute transport. Meshfree methods can overcome some of the difficulties associated with mesh-based approaches.