CHAPTER II

LITERATURE REVIEW AND THEORETICAL BACKGROUND

2.1 MODFLOW development

2.1.1 MODFLOW introduction

The modular finite-difference groundwater flow model well known as MODFLOW, is a program for simulating confined or unconfined and saturated flow in one, two or three dimensions. It allows both steady-state and transient simulations. At least with the public domain packages, it does not simulate unsaturated flow or solute and heat transport. However, MT3D (Zheng, 1990) and MOC3D (Konikow et. al., 1996), both of which rely on MODFLOW, can simulate solute transport.

In comparatively recent survey (Geragthty and Miller Software Newsletter, 1992), MODFLOW is the most popular groundwater modeling program. Some reasons for this popularity may be;

1. The program is applicable to most types of groundwater modeling problems.
2. The original packages in the program are well structured and documented.
3. The source code is in the public domain and thus can be checked for errors and modified by anyone with the necessary mathematical and programming skills.
4. The program is accepted by regulatory agencies and in litigation.
5. Ongoing modifications of the program continue to increase its capabilities.

Public domain and proprietary packages have been written for MODFLOW both within the US Geological Survey (USGS) where it was originally created and outside the USGS. Since MODFLOW was written, a variety of public-domain and proprietary programs have built upon it either by using the output of MODFLOW as the input for additional modeling or by extending the capabilities of MODFLOW. The public-domain programs that build upon MODFLOW include MT3D (Zheng, 1990), MODFLOWP (Hill, 1992 and 1994) and MOC3D (Konikow et al., 1996).

Table 2.1 Public domain packages for MODFLOW not in original version of MODFLOW

Abbreviation	Package name	Purpose
PCG1	Preconditioned Conjugate-Gradient Package 1	Used to solve finite-difference equations
BCF2	Block-Centered Flow 2	Allow dry cells to become wet
RIV2	River Package 2	Used for routing river flow downstream from one river reach to another
STR1	Streamflow-Routing Package	Used to simulate streamflow routing
RINT1	River Interactions Package	Simulate streamflow routing and river interaction with alluvial deposits
PCG2	Preconditioned Conjugate-Gradient Package 2	Used to solve finite difference equations
IBS1	Interbed Storage Package 1	Allows simulation of water release be interbeds
CHD1	Time-Variant Specified-Head Package 1	Used for specified heads that vary with time
BCF3	Block-Centered Flow 3	Allows more accurate simulations
GFD1	Generalized Finite-Difference 1	Allows direct specification of all intercell conductances
LAK1	Lake Package 1	Used to simulate lakes
None	Modified Stream Package	Used to simulate streamflow routing including streams that flow into or out of lakes
HFB1	Horizontal-Flow Barrier Package 1	Simulates the effects of thin vertical barriers to horizontal flow such as intrusions or faults
SHY1	Hydrograph Package	Saves hydrograph data for specified cells
BAR and CUT	Flow-Barrier 1 and Canyon-Cutter Packages 1	These packages simulate pinchouts and the effects of thin vertical barriers to horizontal flow such as intrusions, faults or canyons
TLK1	Transient Leakage Package 1	Simulates leakage from confining layers in transient quasi-three-dimensional models
DE45	Direct-Solution Package 5	Used to solve finite difference equations
RES1	Reservoir Package 1	Used to simulate flow into and out of reservoirs
None	Spatial variable anisotropy package	Allows spatially variable anisotropy
FHB1	Flow and Head Boundary Package 1	Used for transient specified head and specified flux boundaries

Both MODFLOW itself and a variety of related programs are freely available on the internet. The most prominent source is the USGS itself. However, a variety of other sites exist that have either the source code or executable versions of MODFLOW (Table 2.1). In some instances, the non-USGS versions have extra capabilities that the USGS version lacks.

2.1.2 MODFLOW preprocessors

Although MODFLOW is a powerful program, it can be described as user-friendly. All input for the program is in the form of large text files that describe the grid structure, hydraulic properties, boundary conditions and transient data. These files must follow a strict format. If the format requirements are violated MODFLOW will either not be able to run or will produce incorrect results. To alleviate this problem, a large number of processors have been developed that provide a graphical user interface for MODFLOW. In some cases, the programs are either freeware or shareware.

Some shareware processors interface for MODFLOW are;

1. **MODUSER** can be obtained from the Computer Oriented Geological Society ftp site among other places. It is a DOS program and has a US$ 10.00 registration fee. It supports the original MODFLOW-88 packages. It can be used to set up a grid and assign values to cells by clicking on the cells. In a brief test of MODUSER, it was not clear how to reenter data in order to correct mistakes.
2. **UNCERT** (Wingle et al., 1995 and Wingle, 1997) is a freeware MODFLOW preprocessor for Unix. It is reputed to do more than just act as a MODFLOW preprocessor.
3. **MFI** (Harbaugh, 1994) is freeware. It supports MODFLOW-96, the stream package and MOC-3D. To use the DOS version a spreadsheet program that can read and write Lotus 123.WK1 files is required, such as Microsoft Excel. MFI requires a bit more work to install properly than do most modern programs, the Config.sys file must be modified and a batch file run. Every time MFI is run, a batch file must be copied into the directory

where MFI is installed. This batch file controls the interaction between MFI and the spreadsheet program. MFI deletes this file when it exits, so it cannot be left in the directory with MFI. MFI appears to be an effective program for creating MODFLOW input files. It is much less user-friendly than commercial prepocessors.

The USGS also provides another free user interface for MODFLOW,

1. **MODFLOW-GUI** (Shapiro et. al., 1997) is a plug-in for Argus open numerical environments (Argus ONE). The MODFLOW-GUI is more sophisticated than MODUSER or MFI because the data defining the model are independent of the grid. Thus, the grid can be altered without requiring the user to reenter data. The MODFLOW-GUI also provides postprocessing of MODFLOW data.
2. **RADMOD** (Reilly and Harbaugh, 1993a and b) is a special purpose tool that can be used to prepare radially symmetrical models using the General-Finite Difference Package. It only prepares the input file for the General-Finite Difference Package and not the remaining MODFLOW packages.

2.1.3 MODFLOW postprocessors

The USGS provides several programs for processing and display of the data from MODFLOW and related programs. For examples,

1. **CONTOUR** (Harbaugh, 1990a) is a Unix program for creating contour maps from gridded data.
2. **MODPATH** (Pollock, 1994) is a particle tracking program for MODFLOW models. It have both version of Dos and Unix.
3. **ZONEBUDGET** (Harbaugh, 1990b) is used to create water budgets for particular zones in a MODFLOW model. Version for DOS and Unix are available from the USGS. It is easy to use and effective.

2.1.4 MODFLOW documentation

MODFLOW and related programs are exhaustively documented in USGS publications which may be purchased at nominal fees. Documentation for some of the newer packages can be downloading from the USGS MODFLOW page as Postscript or pdf files. These documents provide the theoretical basis for the programs, detailed explanations of the source code, input formats and example applications. This documentation is a critical reason for the success of MODFLOW. Because MODFLOW is detailed enough to allow users to add additional packages to the program: something which can be said of no other USGS groundwater modeling program. The documentation seems overwhelming for beginners. The original documentation (McDonald and Harbaugh, 1988) is 586 pages long and represents about one third of the total documentation now available.

A useful resource for beginners is the manual of MODFLOW instructional problems from the Environmental Protection Agency (Anderson, 1993). It gives 20 examples of simple MODFLOW models each designed to illustrate how to use specific aspects of MODFLOW. It is an excellent source of information on how best to use MODFLOW and to avoid common errors.

Environmental Simulation, Inc. has converted the MODFLOW documentation to a pair of Windows Help files. These files are not shareware because they cost US$ 25.00. These help files are included with their preprocessors Groundwater Vistas, but may be purchased separately.

2.2 Geotechnical Centrifuge

A geotechnical centrifuge is a powerful testing tool for modeling the transport of contaminants in soils. The simulation of identical effective stress states in scaled centrifuge model and equivalent prototype ensures the modeling of soil properties including hydraulic conductivity. Centrifuge modeling is particularly applicable in replicating the physical transport of dense pollutants due to gravitational gradients. The increased acceleration field is essential to correctly study such phenomena in reduced scale models.

Body force due to gravity plays an important role in geotechnical engineering problems. It is impossible to simulate body force in real structures through conventional scaled models in the 1g gravitational field. When the model linear dimensions are reduced by a factor N and centrifuge experiments conducted at an enhanced acceleration field of N g, stresses and strains at homologous points of model and the prototype would be identical. With appropriate choice of acceleration level and model size, it is possible to produce similarity conditions satisfactorily for most applications.

Centrifuge modeling is now firmly established as a dependable research tool in geotechnical engineeringfor seeking solutions to problems relating to foundations, dams, tunnels, offshore structures, hazardous waste disposal, geo-environmental engineering and earthquake engineering. Some special features of this physical modeling technique are;

- Scalability of model physical parameters to prototype without recourse to complex soil constitutive relations
- Simulation of earthquake effects
- Accelerated study of time-dependent diffusion phenomena

The geotechnical centrifuge, first proposed 75 years ago in the United States and the USSR, has become highly developed internationally within geotechnical engineering over the last 30 years. The opportunities are enormous when using these physical models. For example,

- The effects on natural or engineered structures of an explosion can be safely and correctly simulated.
- The movement of a contaminant spilled when the soil is undergoing freezing or thawing can be modelled correctly.
- Ground remediation techniques can be modeled controlling prior conditions and dissecting models after to assess the effectiveness of the technique.
- Sinkholes can be created.
- Testing a host of variations in site conditions.
- The response of a reinforced soil system can be monitored at conditions including failure.

2.3 Basic concept of Centrifuge Scaling Law

The correct scaling of physical parameters relating to contaminant transport is essential for similitude of these processes in the centrifuge model and prototype. Dimensional analysis (Laut 1975, Arulanandan et al., 1988) and inspectoral techniques (Bachmat 1967, Hensley, 1988) have been used to derive the general scaling laws for centrifuge modeling of contaminant migration. The relevant laws are

$$t_p = n^2 t_m$$

$$u_p = \frac{1}{n} u_m$$

$$c_p = c_m$$

$$l_p = n l_m$$

Where; n = the scaling factor
u = the pore fluid velocity (L/T)
t = the time factor (T)
c = the concentration of pollutant
l = the length of the scale (L)
p-m symbolize the prototype and model respectively

These laws assume that the dispersive process are identical in model and prototype, and the adsorption of contaminant obeys a rapid linear equilibrium model. These assumptions are applicable to this study where dispersion does not dominate and non-sorbing contaminant is used.

2.4 Physical properties and principles

2.4.1 Darcy's law

The birth of groundwater hydrology as a quantitative science can be traced to the year 1856. It was in that year that a French hydraulic engineer named Henry Darcy published his report on the water supply of the city of Dijon, France. In the report Darcy described a laboratory experiment that he had carried out to analyze the flow of the water through sands. The results of his experiment can be generalized into the empirical law that now bears his name. Darcy's law can be written as;

$$v = -K\frac{dh}{dl}$$

Where; v = the Darcy's velocity (L/T)

K = the hydraulic conductivity constant (L/T)

h = the hydraulic head (L)

$\frac{dh}{dl}$ = the hydraulic gradient

2.4.2 Porosity and void ratio

If the total unit volume V_T of soil or rock is divided into the volume of the soil portion V_s and the volume of the soils V_v, the porosity n is defined as;

$$n = V_v / V_T$$

It is usually reported as a decimal fraction or a percent.

2.4.3 Steady-state flow and transient flow

Steady-state flow occurs when at any point in a flow field the magnitude and direction of the flow velocity are constant with time.

Transient flow (unsteady flow or nonsteady flow) occurs when at any point in a flow field the magnitude or direction of the flow velocity changes with time.

2.4.4 Hydrodynamic dispersion

The process by which solutes are transported be the bulk motion of the flowing groundwater is known as advection. Owing to advection, nonreactive solutes are carried at an average rate equal to the average linear velocity, $\bar{v}$, of the water. There is a trendency, however for the solute to spread out from the path that it would be expected to follow according to the advective hydraulics of the flow system. This spreading phenomenon is called hydrodynamic dispersion. It causes dilution of the solute. It occurs because of mechanical mixing during fluid advection and because of molecular diffusion due to the thermal-kinetic energy of the solute particles. Diffusion is a dispersion process of importance only at low velocities. The coefficient of hydrodynamic dispersion can be expressed in terms of two components;

$$D_l = \alpha_l \bar{v} + D^*$$

Where; D_l = the coefficient of hydrodynamic dispersion in the longitudinal direction

α_l = the characteristic property of the porous medium known as the dynamic dispersivity or simply as dispersivity (L)

D^* = the coefficient of molecular diffusion for the solute in the porous medium (L^2/T)

$\bar{v}$ = the Darcy's velocity