

CHAPTER III

METHODOLOGY

3.1 MODFLOW program

MODFLOW program that use in the thesis is Visual MODFLOW 3.0. Visual MODFLOW is a trademark, owned by Waterloo Hydrogeologic Inc. Visual MODFLOW is the most complete and easy-to-use modeling environment for practical applications in three-dimensional groundwater flow and contaminant transport simulations. This fully-integrated package combines MODFLOW, MODPATH, ZoneBudget, MT3Dxx/RT3D and WinPEST with the most intuitive and powerful graphical interface available. The logical menu structure and easy-to-use graphical tools allow the user to:

- Easily dimension the model domain and select units
- Conveniently assign model properties and boundary conditions
- Run the model simulations (MODFLOW, MODPATH, ZoneBudget, MT3Dxx/RT3D and WinPEST are seamless integrated)
- Calibrate the model using manual or automated techniques
- Visualize the results using 2D or 3D graphics

The model input parameters and results can be visualized in 2D (cross-section and plan view) or 3D at any time during the development of the model or the displaying of the results.

3.1.1 Hardware Requirement

The minimum system configuration for run Visual MODFLOW 3.0 are follow;

- Pentium II, 300 MHz (or equivalent)
- 64 MB of RAM (128 Mb recommend)
- CD ROM drive
- 100 Mbytes free disk space
- Windows 95/98/2000/NT 4.0 (Service Pack 3)

3.1.2 Visual MODFLOW 3.0 Interface

The Visual MODFLOW interface has been specifically designed to increase modeling productivity and decrease the complexities typically associated with building three-dimensional groundwater flow and contaminant transport models. In order to simplify the graphical interface, Visual MODFLOW is divided into three separate modules;

- a) The **Input** section
- b) The **Run** section
- c) The **Output** section

Each of these modules is accessed from the **Main Menu** when a Visual MODFLOW project is started or an existing project is opened. The **Main Menu** serves as a link to seamlessly switch between each of these modules to define or modify the model input parameters, run the simulations, calibrate the model and display results.

a) The **Input** section allows the user to graphically assign all of the necessary input parameters for building a three-dimensional groundwater flow and contaminant transport model. The input menus represent the basic “model building blocks” for assembling a data set for MODFLOW, MODPATH, ZoneBudget and MT3D/RT3D. These menus are displayed in the logical order to guide the modeler through the steps necessary to design a groundwater flow and transport model.

b) The **Run** section allows the user to modify the various MODFLOW, MODPATH, MT3D/RT3D and WinPEST parameters and options which are run-specific. These include selecting initial estimates, setting solver parameters, activating the rewetting packages, specifying the output controls, etc. Each of these menu selections has default settings, which are capable of running most simulations.

c) The **Output** section allows the user to display all of the modeling and calibration results for MODFLOW, MODPATH, ZoneBudget and MT3D/RT3D. The output menus allow you to select, customize and overlay the various display options for presenting the modeling results.

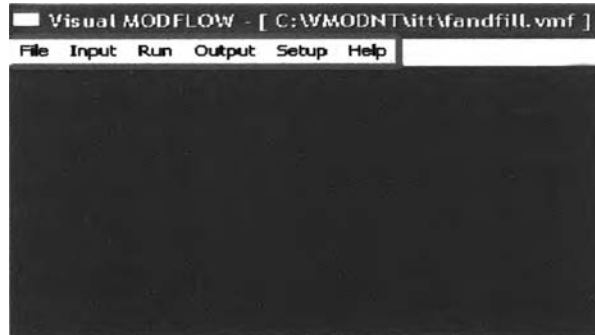


Figure 3.1 The Main Menu of Visual MODFLOW 3.0

The **Main Menu** screen contains the following options;

- **File** Select a file utility or exit Visual MODFLOW
- **Input** Design, modify and visualize the model grid and input parameters
- **Run** Enter or modify the model run settings and run the numerical simulations in either project mode or batch mode
- **Output** Visualize the model output (simulation results) using contour maps, color maps, velocity vectors, time-series graph, etc.
- **Setup** Select the “numerical engine” for both the flow and transport simulations
- **Help** get general information on how to use Visual MODFLOW

The **File** menu options are described below;

- **Open** Open an existing Visual MODFLOW data set
- **New** Creates a new Visual MODFLOW data set
- **Save as** Saves the current model to a different filename
- **Close** Closes the current model
- **Import MODFLOW** Imports an existing set of MODFLOW data files (*.BAS)
- **Export** Exports the model image to a graphics file (AutoCAD .DXF) or (*.DXF) or an Enhanced Windows Metafile (*.EMF)
- **Change Unit** Changes units in the current model (but does NOT convert the existing data values)
- **Print** Prints the model display area to the selected printer (with or without a description of the image)
- **Exit** Closes the project and shut down Visual MODFLOW

Screen Layout

After opening the Visual MODFLOW project and selecting the Input module, a screen layout similar to the figure below will appear.

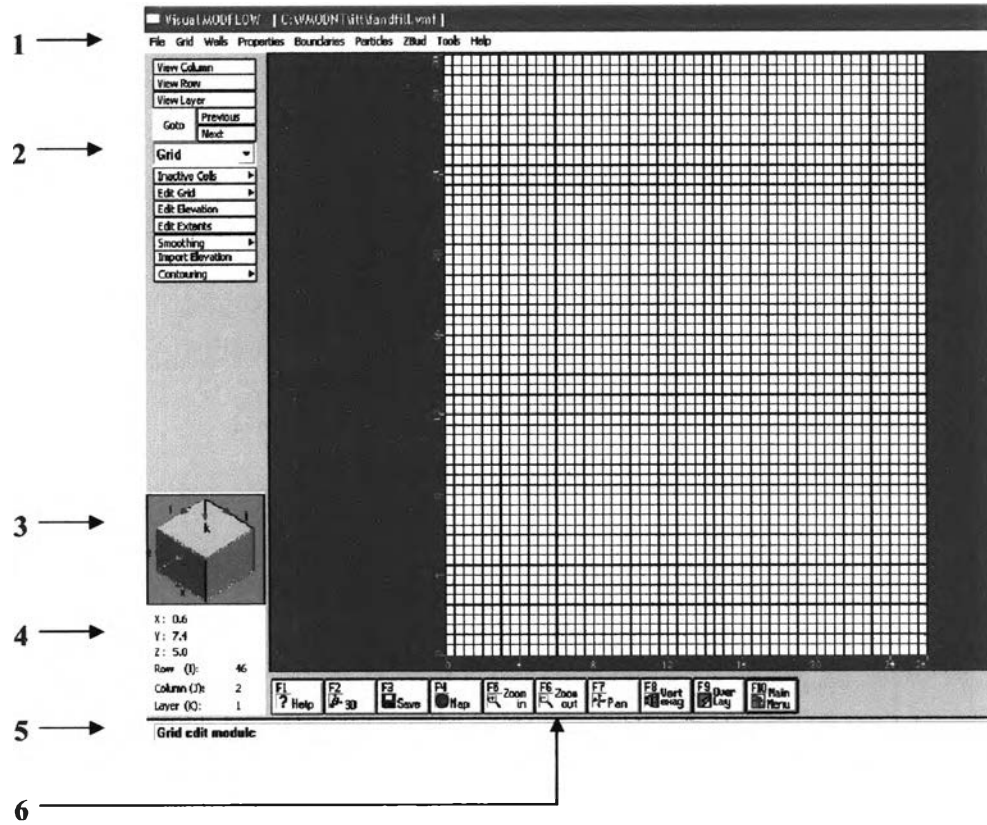


Figure 3.2 The Screen Layout of Visual MODFLOW

1. **Top Menu Bar:** Contains specific data category menus for each section of the interface (**Input, Output, and Run**)
2. **Side Menu Bar:** Contains the **View Control Buttons** plus tool buttons specific for each data category.

The view options are as follows;

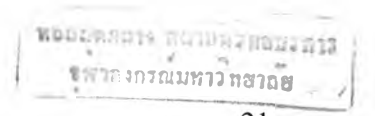
- **View Column** View a cross-section along a column
 - **View Row** View a cross-section along a row
 - **View Layer** Switch from cross-section to plan view
 - **Goto** View a specific column, row or layer
 - **Previous** View previous column, row or layer
 - **Next** View next column, row or layer
-
3. **Navigator Cube:** Provides a simplified 3D representation of the model domain highlighting the current layer, column, and row being viewed
 4. **Co-ordinates Area:** Shows the current location of the cursor in model co-ordinates, and shows the current cell indices on which the cursor is located
 5. **Status Line:** Describes the functionality and use of the feature currently highlighted by the cursor
 6. **Function Buttons:** Common functions to the **Input, Run and Output** screens can be selected by clicking on the button or by pressing the function key on your keyboard

The function buttons are as follows;

- **F1-Help** Opens the general help window
- **F2-3D** Opens the Visual MODFLOW 3D-Explorer
- **F3-Save** Saves the current data of the model
- **F4-Map** Import the display .DXF site map files

- **F5-Zoom In** Enlarge the display of a selected rectangular area
- **F6-Zoom Out** Resets the display area to show the entire model domain
- **F7-Pan** Drag the current view of the model in any direction to display a different model region
- **F8-Vert Exag** Set the vertical Exaggeration value for viewing cross-section along a row or column
- **F9-Overlay** Opens the **Overlay Control** window to make selected overlays visible and to customize the priority (order) in which they appear
- **F10-Main Menu** Returns to the **Main Menu** screen

The interface features described above are consistent for entire Visual MODFLOW interface. The tool buttons and options available on the Side Menu bar will change depending on the active data category in the **Input** and **Output** screen. For example, the tool buttons shown on the Side Menu bar in the figure 3.2 pertain to the **Grid** module, for designing and modifying the finite difference model grid. The tool buttons available for the **Properties** module are completely different.



3.1.3 Visual MODFLOW project files

Each Visual MODFLOW project consists of many different data files, each pertaining to a specific component of the model (e.g. model setup, grid data, flow boundary conditions, flow properties, particle locations, etc.) whereby each data file is distinguished by the file extension. For example;

- Projectname.VMF general model information
- Projectname.VMG model grid information
- Projectname.VMP flow model properties information
- Projectname.VMB flow model boundary condition information
- Projectname.VMW flow model pumping/injection well information
- Projectname.VMO flow model observation well information
- Projectname.VMA flow model particle locations (for MODPATH)

Although the data files associated with each Visual MODFLOW project are easily distinguished by the project name prefix, it is strongly recommended to create a separate folder for each modeling project to make it more practical to manage any map files or external data files associated with the project.

Although most of the data files associated with a Visual MODFLOW project are stored in ASCII format, it is not recommended to manually modify or manipulate the data in these files. Visual MODFLOW will not be able to successfully open a project if it encounters any unexpected or incorrect file formats in any of the data files related to the project.

The reason for these files are stored in ASCII format, and the reason the data structures are explained in Appendix is so advanced user would be able to generate their own Visual MODFLOW data sets using their own specialized programs and utilities. If this is attempted, it is strongly recommended to backup the original data files generated by Visual MODFLOW before replacing or manually modifying them.

3.2 Validation procedure

To validate the MODFLOW program two sets of studies are conducted. The first is to prove that MODFLOW program can be used to support the centrifuge scaling laws derived for centrifuge model tests. The second is to compare MODFLOW predictions with experimental results.

3.2.1 Use the MODFLOW program to prove the scaling law

This study is conducted to prove the scaling law with centrifuge model cases. The results of these studies are presented in the next Chapter.

3.2.1.1 Silica Flour test

Four Silica Flour models varying in heights of 0.210, 0.157, 0.140 and 0.105 meters are tested in 25, 33.3, 37.5 and 50g centrifugal accelerations, respectively. The conductivity constant (K) and dispersion must be calibrated first before simulate the model by run the model with K value with dispersion equal to 0. Then, try to adjust the dispersion slightly until get the appropriate value. The values of parameters that use in these tests are shown in Table 3.1.

Table 3.1 The values of parameters use in Silica Flour test

g	25 g	33.3 g	37.5 g	50 g	100 g
Parameters					
K (Conductivity constant, cm/sec)	3.05×10^{-3}	3.05×10^{-3}	3.05×10^{-3}	3.05×10^{-3}	3.05×10^{-3}
D* (Dispersion coefficient, m ² /sec)	1.6×10^{-8}	1.6×10^{-8}	1.6×10^{-8}	1.6×10^{-8}	1.6×10^{-8}
L.Dispersivity (m)	0.0005	0.0005	0.0005	0.0005	0.0005
X (Columns, m)	0.210	0.157	0.140	0.105	0.0525
Y (Rows, m)	0.210	0.157	0.140	0.105	0.0525
Z (Layers, m)	0.500	0.500	0.500	0.500	0.500
t (Time, second)	1000	564	445	250	62.5
n (Porosity)	0.344	0.344	0.344	0.344	0.344
S _s (Specific storage, l/m)	0.0001	0.0001	0.0001	0.0001	0.0001
S _y (Specific yield)	0.344	0.344	0.344	0.344	0.344
C _o (Initial concentration, mg/L)	100	100	100	100	100

3.2.1.2 Clays test

Two centrifuge tests are carried out on 100% Snowcal 50 models of height 0.102m and 0.051m subjected to centrifugal accelerations of 50g and 100g, respectively. The values of parameters that use in these tests are shown in Table 3.2.

Table 3.2 The values of parameters use in Snowcal 50 test

g	100 g (no adsorption)	100 g	50 g
Parameters			
K (Conductivity constant, m/sec)	5×10^{-9}	5×10^{-9}	5×10^{-9}
D* (Dispersion coefficient, m ² /sec)	2.2×10^{-11}	2.2×10^{-11}	2.2×10^{-11}
L. Dispersivity (m)	0.0002	0.0002	0.0002
X (Columns, m)	0.051	0.051	0.102
Y (Rows, m)	0.051	0.051	0.102
Z (Layers, m)	11	11	11
t (Time, minute)	187.2	187.2	748.8
n (Porosity)	0.25	0.25	0.25
S _s (Specific storage, 1/m)	0.0001	0.0001	0.0001
S _y (Specific yield)	0.25	0.25	0.25
C _o (Initial concentration, mg/L)	100	100	100
SPI (Adsorption, 1/(mg/L))	-	5×10^{-8}	5×10^{-8}

3.2.1.3 Monterey 0/30 sand test

Part 1: These tests were conducted to study influence of velocity on hydrodynamic dispersion. Three sets of tests were performed on Monterey 0/30 sand with different average interstitial velocity at 25g acceleration. The values of parameters that use in these tests are shown in Table 3.3.

Table 3.3 The values of parameters use in Monterey 0/30 sand test part 1

Average interstitial velocity	0.137 cm/s	0.117 cm/s	0.104 cm/s
Parameters			
K (Conductivity constant, m/sec)	4×10^{-7}	4×10^{-7}	4×10^{-7}
D (Dispersion coefficient, m^2/sec)	1.5×10^{-9}	1.5×10^{-9}	1.5×10^{-9}
L. Dispersivity (m)	0.0005	0.0005	0.0005
X (Columns, m)	0.208	0.208	0.208
Y (Rows, m)	0.208	0.208	0.208
Z (Layers, m)	0.5	0.5	0.5
t (Time, second)	109.489	128.205	144.231
n (Porosity)	0.35	0.35	0.35
S _s (Specific storage, 1/m)	0.0001	0.0001	0.0001
S _y (Specific yield)	0.35	0.35	0.35
C ₀ (Initial concentration, mg/L)	100	100	100

Part 2: These tests were performed in 1g acceleration. Three samples of heights 0.102m, 0.203m and 0.406m were subjected to average interstitial velocities of 0.036 cm/s, 0.20 cm/s and 0.13 cm/s, respectively. The values of parameters that use in these tests are shown in Table 3.4.

Table 3.4 The values of parameters use in Monterey 0/30 sand test part 2

Average interstitial velocity Parameters	0.036 cm/s	0.020 cm/s	0.013 cm/s
K (Conductivity constant, m/sec)	3×10^{-5}	3×10^{-5}	3×10^{-5}
D^* (Dispersion coefficient, m^2/sec)	5×10^{-7}	4.8×10^{-8}	1.5×10^{-9}
L.Dispersivity (m)	1.3847×10^{-3}	2.08×10^{-4}	2.192×10^{-4}
X (Columns, m)	0.102	0.203	0.406
Y (Rows, m)	0.102	0.203	0.406
Z (Layers, m)	0.5	0.5	0.5
t (Time, second)	566.67	1624	3435.385
n (Porosity)	0.35	0.35	0.35
S_s (Specific storage, 1/m)	0.0001	0.0001	0.0001
S_y (Specific yield)	0.35	0.35	0.35
C_o (Initial concentration, mg/L)	100	100	100

3.2.2 Comparison to experimental results

A study of contaminant transport with appropriate properties is used to quantitatively validate MODFLOW program. The result of this study is presented in the next Chapter.

“A study of contaminant transport involving density driven flow and hydrodynamic clean up” (Hellowell and Savvidou, 1994)

This study showed the contaminant transport pattern by using a centrifuge to accelerate the experiments. This study presented the transport of a non-sorbing dense pollutant from a landfill into a homogenous saturated silt layer. The values of parameters that use in this test is shown in Table 3.5.

Table 3.5 The values of parameters use in experiment test

Parameter Description	Value
K (Conductivity constant, m/sec)	2.3×10^{-7}
D^* (Dispersion coefficient, m^2/sec)	7.3×10^{-10}
L.Dispersivity (m)	3.26×10^{-4}
X (Columns, m)	30
Y (Rows, m)	26
Z (Layers, m)	10
t (Time, hour)	26.5
n (Porosity)	0.45
S_s (Specific storage, l/m)	0.0001
S_y (Specific yield)	0.45
C_0 (Initial concentration, mg/L)	100