

## ModelMate tutorial

For this tutorial, we will be using the “tc1” MODFLOW-2005 (Harbaugh, 2005) model in the Example directory of the ModelMate distribution. Sensitivity analysis and calibration of this example model is discussed in detail in Hill and Tiedeman (2007).

ModelMate stores all information it needs for a project in a single ModelMate project file, identified by the extension "mtc". Start ModelMate. On starting ModelMate, the user is prompted to open an existing file or provide a directory and name for a new project file. In the “Select ModelMate Project” window, click the file-open icon and browse to the Example directory. Enter "tc1\_test" in the File name field of the Browse window and click Open. ModelMate will add the extension "mtc" and return to the introductory window. Click OK to create the project file and open the main ModelMate window.

The main ModelMate window has two panels. The left panel is labeled "Model Analysis Application", and the right panel is labeled "Application/Model Connection".

The controls in the Model Analysis Application (left) panel are used to select a model-analysis application and specify settings for that application. In the current version of ModelMate, the only model-analysis application that is supported is UCODE\_2005 (Poeter and others, 2005), but support for additional applications may be added in the future.

The controls in the Application/Model Connection (right) panel are used to define parameters, observations, and predictions, which may be used by the selected model-analysis application (only UCODE\_2005 currently is supported).

ModelMate can import observation information included in a MODFLOW-2005 data set. If the MODFLOW name file lists a PVAL file, ModelMate can read the PVAL file to define parameters. In the Example directory, the tc1 data set includes a PVAL file named tc1.pval, which will be rewritten as needed by UCODE\_2005. Another copy of this file named tc1\_start.pval can be copied to recreate the tc1.pval file with the original parameter values (listed in table A1 on page 110 of USGS Open-File Report 00-184), if desired. Do not edit tc1\_start.pval.

### ***Import parameters from MODFLOW-2005***

To import parameters from the tc1 data set, on the menu bar of the main ModelMate window, select **File|Import|Parameters from MODFLOW-2005**. Select and open tc1.nam in the Example directory. The Parameters table in the right panel will be populated with parameter information read from tc1.pval. This step also creates a JUPITER template file named tc1\_pval.jtf, which is needed by UCODE\_2005 to generate new versions of the PVAL file. Using the menu bar, go to **Model|Model Input and Template Files** to see where these file names are stored in the ModelMate GUI. To see the template file that ModelMate created, open tc1\_pval.jtf with a text editor. Do not edit this file.

## ***Import observations from MODFLOW-2005***


To import observations from the tc1 data set, select **File|Import|Observations from MODFLOW-2005**. Again, select and open tc1.nam in the Example directory. A new window labeled Observations and populated with observation information read from the tc1 data set will open. The MODFLOW-2005 data set does not specify Statistic or StatFlag for observations, so the user needs to assign appropriate values for Statistic and StatFlag before closing the Observations window. Do that now. For the “Heads” observation group, specify Statistic as 1.0025 and StatFlag as Var. For the “Head\_Changes” group, specify Statistic as 0.0025 and StatFlag as Var. If you have flow observations, assign suitable values to Statistic and StatFlag, e.g. Statistic=0.1 and StatFlag=CV. Click OK to save the values you entered and close the Observations window. This step also creates a JUPITER extraction-instruction file named tc1.\_os.jif, which is required by UCODE\_2005 to extract model-calculated equivalents to the observations from the observations model-output file. Using the menu bar, go to **Model|Model Output and Instruction Files** to see where these file names are stored in the ModelMate GUI. Dismiss the “Model Output and Instruction Files” window. In the main window, click on the Observations tab and note that the number of observations, number of observation groups, and the name and number of observations in each group are displayed. If you want to open the Observations window again, click on “Open Observations Window....”

Alternatively, parameters and observations can be imported in one step by selecting **Import|Parameters and Observations from MODFLOW-2005**, but there is no need to repeat the import procedure if you have imported parameters and observations as described above.

## ***Assign model command line***

UCODE\_2005 requires a model-command line, which it uses to invoke model runs. First, use the menu item **Project|Program Locations** to open the Program Locations window and ensure that paths to the UCODE\_2005 and MODFLOW-2005 executable files are correct. If any path listed on the Program Locations window is invalid, its edit box will be red. If either the UCODE\_2005 or MODFLOW-2005 box is red, use the file-open icon button to browse and select the location on your system of the UCODE\_2005 and MODFLOW-2005 executables. For convenience, executable files for MODFLOW-2005 (mf2005.exe) and UCODE\_2005 (ucode\_2005.exe) are provided in the Bin directory of the ModelMate distribution. For now, it's acceptable if the GW\_Chart box is red. ModelMate now has the information needed to generate a model command for invoking MODFLOW-2005 to run the tc1 model. Use menu item **Model|Commands to Invoke Model** to open the Model Commands window. Click "Generate Command for Forward Primary MODFLOW Run" to have ModelMate generate the model-command line. Alternatively, if you use a batch or script file to start a model, you can browse and select that file; ensure that the file does not contain pause commands or other requirements for user response. Click OK to save the command line and close the Model Commands window.

## ***Save project file***

To save the project file, use the menu item **File|Save Project**. Alternatively, you can use the Save File () button on the tool bar located below the menu bar. Save the project file now and whenever additional changes are made to project entries. When the main window is active, the key combination <Ctrl>-S also may be used to save the project file.

## ***Define UCODE\_2005 input and output files***

At this point, the project contains the information needed to generate a UCODE\_2005 main input file and make a UCODE\_2005 run. However, before doing that, it would be better to define meaningful names for UCODE\_2005 input and output files rather than use the default names. Choose menu item **UCODE|File Names**. For now, just edit the file names for the Primary Model (in the upper box on the “UCODE\_2005 Input and Output File Names” window). Change Default\_Ucode\_main.in to tc1\_main.in and change Default\_Ucode\_main\_out to tc1\_main\_out. Click OK to save the new names and close the “UCODE\_2005 Input and Output File Names” window.

## ***Forward mode***


In the left panel of the main ModelMate window, ensure that Mode is set to Forward, and click Create UCODE\_2005 Input Files. Before the input file is created, the project will be saved. ModelMate will create a UCODE\_2005 input file with the name you specified in the “UCODE\_2005 Input and Output File Names” window. A small window will appear to notify you that the file was created successfully. If the file was not created for any reason or if information needed to create the file was lacking, you will be notified at this time. You can view the UCODE\_2005 input file by using menu item **View|UCODE Main Input File**. A file viewer will appear showing the contents of the UCODE\_2005 input file. You can leave the file viewer open or dismiss it. Clicking the “Create UCODE Input Files” button also creates a batch file named RunUcode\_tc1\_test.bat, which can be run outside of ModelMate to invoke UCODE\_2005 using the UCODE\_2005 input file created at the same time.

Make a UCODE\_2005 run by clicking the "Run UCODE" button in the left panel. This button saves the project and creates (or recreates) the UCODE\_2005 input file and RunUcode\_tutorial.bat file before invoking UCODE\_2005, so the previous step, where you clicked "Create UCODE\_2005 Input Files" to create the UCODE\_2005 input file, actually was unnecessary. However, there likely will be situations in which you want to create the UCODE\_2005 input file without invoking UCODE\_2005. When the "Run UCODE" button is clicked (and after the project is saved and the UCODE\_2005 input file is created), an MS-DOS command window is opened, where UCODE\_2005 is invoked. You can view UCODE\_2005 screen output in the DOS window. Dismiss the DOS window by clicking the X or by pressing any key when the DOS window is active.


## ***File viewer***

View UCODE\_2005 output by using menu item **View|UCODE Main Output File**. Toolbar buttons, from left to right, allow the user to open a file, reload a file, exit the viewer, go to the top of the file, go to the bottom of the file, search for text, or toggle

word wrapping. The menus contain options for doing the same things. You can leave the file viewer open or dismiss it.

In the current version of ModelMate, there are two copies of the file viewer: one for viewing the UCODE\_2005 input file and one for viewing the UCODE\_2005 output file. When these files are changed (e.g. by rerunning UCODE\_2005), you can reload the revised input or output file by using the **File|Reload Current File** menu item in the file viewer, or by clicking the Reload  button.

### ***View analysis results in GW\_Chart***

After a run of UCODE\_2005 has been made, GW\_Chart (Winston, 2000) may be used to visualize selected UCODE\_2005 results. If the user has installed GW\_Chart (version 1.20.0.1 or later), GW\_Chart may be invoked from ModelMate. First, however, the user must use menu item **Project|Program Locations** to define the path where the GW\_Chart executable resides. To invoke GW\_Chart, use menu item **Postprocessing|GW\_Chart**. GW\_Chart will be started using the \_os data-exchange file generated by the most recent UCODE\_2005 run for the selected UCODE\_2005 mode. Alternatively, GW\_Chart may be started by clicking on the GW\_Chart  button on the toolbar. Charts based on other data-exchange files may be generated in GW\_Chart after it starts.

### ***Sensitivity analysis mode***

In the right panel of the main ModelMate window, select the Parameters tab and define selected parameters as adjustable, as follows. You can add a new parameter group with the "Add Group" button. Add one group named "HydCond" and another named "Fixed". In the Parameter Groups Table in the right panel, define parameter group attributes as follows:

<b>Group name</b>	<b>Adjustable</b>	<b>Transform</b>
ParamDefault	Yes (box checked)	No (box unchecked)
HydCond	Yes	Yes
Fixed	No	No

In the Parameters Table, assign parameters HK\_1, VERT\_K\_CB, HK\_2, and RIVERS to group HydCond. Assign parameters VERT\_ANI\_1 and VERT\_ANI\_2 to group Fixed. To view all parameters and all groups, you may wish to enlarge the window or move the divider between the Parameters Table and the Parameter Groups Table. Leave other parameters assigned to group ParamDefault. Save the project.

In the left panel, under Mode, select Sensitivity Analysis. Click "Run UCODE\_2005". On the menu bar, click **View|UCODE Main Output File** to view the results of the UCODE\_2005 run. Sensitivity-analysis results reveal some large parameter correlations and small sensitivities. See Hill and Tiedeman (2007, p. 60-66) for detailed discussion of sensitivity-analysis results.

## ***Parameter estimation mode***

Before making a parameter estimation run, in the Parameter Groups Table in the right panel of the main ModelMate window, set Sensitivity Method to “2: Central Differences” for groups ParamDefault and HydCond. In the left panel under Mode, select Parameter Estimation. Use menu item **UCODE|Parameter Estimation Settings** to open the Parameter Estimation Settings window. At the top of this window, change MaxIter to 10; other settings can be left set to their default values. Click OK to save the revised MaxIter value and close the Parameter Estimation Settings window. Create the UCODE\_2005 input file and run UCODE\_2005. Click **View|UCODE Main Output File** to view the results of the UCODE\_2005 run. Parameter-estimation results are unsatisfactory (note the large confidence intervals on the parameter estimates in the Parameter Summary), likely due to large parameter correlations. See Hill and Tiedeman (2007, p. 87-89) for detailed discussion of parameter-estimation results.

## ***Prior information***

To define prior information, select menu item **UCODE|Prior Information**. This will open the Prior Information Control window. In the Prior Information Control window, ensure that the checkbox labeled "Use Prior Information" is checked to enable use of prior information equations. Click "Define Linear Prior Information". Add prior information as desired. The equation is the name of a parameter or an expression that is a linear combination of parameters. Pages 94-95 in Techniques and Methods 6-A11 explain input to define linear prior information for UCODE\_2005. For example, enter a prior information item with Name: Pri\_K1; Group: DefaultPrior; Equation: HK\_1; Prior Info Value: 0.0004; Statistic: 0.0001; StatFlag: SD. Click OK to save the prior information data and close the Linear Prior Information window. Close the Prior Information Control window. Save the project file and rerun UCODE\_2005 in Parameter Estimation mode and view the output. Addition of prior information has reduced the uncertainty (note smaller confidence intervals) associated with the estimated parameters. See Hill and Tiedeman (2007, p. 90-91) for detailed discussion of addition of prior information and its effect on the regression.

## ***Prediction mode***

A MODFLOW-2005 model with name file tc1pred.nam will be used as a predictive model. It uses heads generated by the tc1 model as starting heads and it has no steady-state stress periods. The WELLS\_TR parameter is defined in the Well Package input file but is not active for any stress period (other wells are defined). Otherwise, it is like the tc1 model. The observation process of MODFLOW-2005 is used in tc1pred to define predictions.

Since we aren't importing parameters defined for the predictive model (which would replace the parameters you imported from the main model), you need to manually create a JUPITER template file for the PVAL file of the predictive model. One way to do this is to use Windows Explorer to make a copy of the template file generated for the tc1 model (file tc1\_pval.jtf) and name the copy tc1pred\_pval.jtf. Do that now.

Import the tc1pred "observations" as predictions. To do this, use menu item **File|Import|MODFLOW-2005 Observations as Predictions**. Select and open


tc1pred.nam in the Example directory. The Predictions window will open. For prediction group “Heads”, define MeasStatistic as 1.0025 and MeasStatFlag as VAR. For group “Head\_Changes”, define MeasStatistic as 0.0025 and MeasStatFlag as VAR. Click OK. When observations are imported as predictions, extraction-instruction files are created.

The model-input and corresponding template files for the predictive model need to be defined. Select menu item **Model|Predictive Model Input and Template Files**. Define one row in the table shown in the "Predictive Model Input and Template Files" window. For the Model Input File, browse to select tc1pred.pval in the Example directory. For the Template File, select tc1pred\_pval.jtf, which you created above. Click OK.

A command line for the predictive model needs to be defined. To do this, use menu item **Model|Commands to Invoke Model**. In the Model Commands window, click "Generate Command for Forward Predictive MODFLOW Run". Click OK.

Select **UCODE|File Names** to open the “UCODE\_2005 Input and Output File Names” window. In the Predictive Model box, change Default\_Ucode\_pred.in to tc1\_pred.in and change Default\_Ucode\_pred\_out to tc1\_pred\_out. Click OK and save the project file.

To make a forward predictive model run, in the left panel under Mode, select Prediction. Then select **UCODE|Settings**. In the UCODE\_2005 Settings window, ensure that the "Calculate Prediction Sensitivities" box is not checked. Dismiss the UCODE\_2005 Settings window. Make a UCODE\_2005 run and view the output. In the current version of ModelMate, if \_dm, \_pc, \_mv, and \_paopt files (which are required by UCODE\_2005 when run in Prediction mode) with the file name base associated with the predictive model do not exist, the \_dm, \_pc, \_mv, and \_paopt files created when UCODE\_2005 was run in Parameter Estimation mode are copied to have the base name associated with the predictive model.

To make a prediction-sensitivity run, select **UCODE|Settings**. In the UCODE\_2005 Settings window, check the “Calculate Prediction Sensitivities” box and click OK to save the change and close the “UCODE\_2005 Settings” window. Make a UCODE\_2005 run. Graphical displays of the results can be viewed by invoking GW\_Chart from the **Post-processing** menu or by clicking the GW\_Chart  button on the toolbar.

## ***Derived Parameters***

ModelMate supports derived parameters. To use derived parameters, select **UCODE|Derived Parameters**. This will open the “UCODE Derived Parameters” window, where all parameters are listed. To convert a parameter to a derived parameter, check the box in the Derived column for each parameter that is to be derived from one or more other parameters, and provide an equation for that parameter. The equation must be constructed as described in Chapter 7 of Poeter and others (2005). For example, In the “UCODE Derived Parameters” window, check the Derived box for the parameter named VERT\_K\_CB. For the equation, type:

$$0.5\text{E-}3 * \text{HK}_1$$

This ensures that UCODE will maintain a ratio of VERT\_K\_CB to HK\_1 equal to  $0.5 \times 10^{-3}$ . Click OK to save the changes and dismiss the “Derived Parameters” window.

The Parameters table in the main ModelMate window can be configured to display the Derived attribute for each parameter. To display the Derived attribute on the Parameters table, click “Configure Tables,” then in the “Configure Parameter Tables” window, for the Derived attribute select “Show in Parameters Table”. The checkboxes in the Derived column can be used to toggle a parameter between being an ordinary parameter and being a derived parameter. The “Start Value” attribute of a parameter is unaffected by its “Derived” status and is saved. The Start Value of a derived parameter has no effect in UCODE\_2005; when a parameter is derived, its value is determined by its equation and the parameter(s) that appear in the equation.

If you want to see that VERT\_K\_CB will be treated as a derived parameter, configure the Parameters Table to show the Derived column as described above. Ensure that the UCODE mode is set to Parameter Estimation and make a UCODE run.

### ***Configuring Tables***

Many of the windows in ModelMate contain two tables, which show members and groups for various types of items used in UCODE\_2005. For example, on the Parameters tab of the main window are a Parameters table and a Parameter Groups table. Many attributes can be controlled on a member-by-member basis, by group, or by default. To configure the parameter tables, on the Parameters tab click the “Configure Tables” button. Some attributes can only be placed on one of the two tables or assigned by default.

UCODE\_2005 input will be prepared according to the visible configuration. Consider, for example, the Parameters and Parameter Groups tables. Suppose that in an initial configuration the Transform attribute is visible in the Parameter Groups table and the Transform box is checked for one or more parameter groups. If the configuration is then changed so that for the Transform attribute the configuration selection is “No Table (use default)” then neither table will have a Transform column, and in UCODE\_2005 input, neither the Parameter\_Groups input block nor the Parameter\_Data input block will contain a Transform column. As a result no parameters will have Transform specified as true, because the default for Transform is “no”. The Observations, Prior Information, and Prediction windows also have tables that can be configured in this way. The one exception to the rule that UCODE input is prepared according to the visible configuration is the Derived column in the Parameters Table; derived-parameter definitions will be included in input used by UCODE\_2005 regardless of whether the Derived column is visible in the Parameters table or hidden. Each table-configuration setup is saved in the project file.

The “Configure Parameter Tables” window also contains a setting labeled “Freeze Parameter Names”. This setting is turned on (checked) by default. The setting affects the appearance and behavior of the Parameter Name column of the Parameters Table on the Parameters tab of the main window. The effect of this setting is as follows:

- Checked
  - The Parameter Name column has a gray background;

- When the Parameters Table is scrolled to the right, the Parameter Name column stays visible;
- Parameter names cannot be edited; and
- Parameter names cannot be selected for copying.
- Unchecked
  - The Parameter Name column has a white background;
  - When the Parameters Table is scrolled to the right, the Parameter Name column scrolls as well and may be hidden;
  - Parameter names can be edited; and
  - Parameter names can be selected for copying.

## ***Generic Models***

The current version of ModelMate provides minimal support for generic models. In ModelMate, a generic model is any model for which ModelMate does not provide model-specific support in preparation of template and instruction files. In the current version of ModelMate, any model other than a MODFLOW-2005 model is considered a generic model. When using a generic model, the user must prepare template and instruction files. To enable use of a generic model, select **Model|Model Settings** to open the Model Settings window. In the Model Settings window, select Generic and click OK.

## ***References***

Harbaugh, A.W., 2005, MODFLOW-2005, the U.S. Geological Survey modular ground-water model--the Ground-water Flow Process: U.S. Geological Survey Techniques and Methods, bk. 6, chap. A16, variously paginated, available at <http://pubs.er.usgs.gov/usgspubs/tm/tm6A16>. MODFLOW-2005 is available at <http://water.usgs.gov/nrp/gwsoftware/modflow2005/modflow2005.html>.

Hill, M.C. and Tiedeman, C.R., 2007, Effective groundwater model calibration: with analysis of data, sensitivities, predictions, and uncertainty: John Wiley & Sons, Hoboken, N.J., 455 p.

Poeter, E.P., Hill, M.C., Banta, E.R., Mehl, Steffen, and Christensen, Steen, 2005, UCODE\_2005 and six other computer codes for universal sensitivity analysis, calibration, and uncertainty evaluation constructed using the JUPITER API: U.S. Geological Survey Techniques and Methods, bk. 6, chap. A11, 283 p., available at <http://pubs.er.usgs.gov/usgspubs/tm/tm6A11>. UCODE\_2005 is available at <http://igwmc.mines.edu/freeware/ucode/>.

Winston, R.B., 2000, Graphical User Interface for MODFLOW, Version 4: U.S. Geological Survey Open-File Report 00-315, 27 p. GW\_Chart is available at [http://water.usgs.gov/nrp/gwsoftware/GW\\_Chart/GW\\_Chart.html](http://water.usgs.gov/nrp/gwsoftware/GW_Chart/GW_Chart.html).