

GMS 10.5 Tutorial mod-PATH3DU Transient

Particle tracking with a transient MODFLOW-USG model



Objectives

This tutorial demonstrates more about GMS's mod-PATH3DU interface and how transient simulations are done.

mod-PATH3DU

Prerequisite Tutorials Required Components

- MODFLOW-USG
- MP3DU

Time • 15–30 minutes



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1 Introduction

The particle path and time tracking simulation program mod-PATH3DU was written by Chris Muffles at S.S. Papadopulos & Associates for use with structured and unstructured grids. It is similar to MODPATH and works with unstructured grids and MODFLOW-USG.

This tutorial starts by opening a transient MODFLOW-USG model. A native text copy of the model is saved and MODFLOW runs on the native text. A new backward-tracking mod-PATH3DU model with points at the wells is then created. The mod-PATH3DU Model Checker is run and the errors that it identifies are fixed.

The model is then launched, the solution is imported, the wells are renamed in order to alter the capture zones, and a shapefile containing the pathline points is exported.

1.1 Getting Started

Do the following to get started:

- 1. If necessary, launch GMS.
- 2. If GMS is already running, select *File* / **New** to ensure that the program settings are restored to their default state.

2 Opening an Existing Model

To open a two-layer transient MODFLOW-USG model:

- 1. Click **Open** \overrightarrow{D} to bring up the *Open* dialog.
- 2. Select "Project Files (*.gpr)" from the *Files of type* drop-down.

- 3. Browse to the *Transient**Transient*\ directory and select "Transient.gpr".
- 4. Click **Open** to import the project and exit the *Open* dialog.

The project should appear similar to Figure 1.



Figure 1 Starting MODFLOW-USG model.

Flow is from left to right with the cells on the right side set as constant head cells with values of "139.0" to "119.0". There are several wells in the project that extract water from the model. There are five stress periods and the end time of the model is at 1,000,970.1 days. Linear contours showing head are turned on.

Before proceeding, it is recommended to save the project under a new name.

- 5. Select *File* | **Save As...** to open the *Save As* dialog.
- 6. Select "Project Files (*.gpr)" from the Save as type drop-down.
- 7. Enter "TransientMp3du.gpr" as the *File name*.
- 8. Click **Save** to create a new project file and close the *Save As* dialog.

3 Saving a Text Copy

MODFLOW files are read by mod-PATH3DU using its internal version of MODFLOW. Because of this, mod-PATH3DU cannot read the GMS-formatted MODFLOW files that use HDF5 to store array data. The next step is to save a native text copy of the MODFLOW simulation for mod-PATH3DU to use.

- 1. In the Project Explorer, double-click on "B Global" to bring up the *MODFLOW Global/Basic Package* dialog.
- 2. In the *MODFLOW version* section, turn on *Save native text copy*.
- 3. Click **OK** to close the *MODFLOW Global/Basic Package* dialog.
- 4. Select *File* | **Save** to save a text copy of MODFLOW to the project directory.

4 Running MODFLOW

To generate a solution for the native text copy version of the model, MODFLOW needs to be run. The typical way to run MODFLOW uses the GMS formatted copy of the model, so MODFLOW needs to run in a different way.

- 1. Select *MODFLOW* / *Advanced* | **Run MODFLOW Dialog...** to bring up the *Run MODFLOW* dialog.
- 2. In the *MODFLOW version* section, select USG.
- 3. Click **Name file** it bring up an *Open* dialog.
- 4. Navigate up one directory and open the *TransientMp3du_MODFLOW-ugrid_text* folder.
- 5. Select "TransientMp3du.mfn" and click **Open** to exit the *Open* dialog.
- 6. Click **OK** to close the *Run MODFLOW* dialog and bring up a command prompt window where MODFLOW will run.
- 7. When MODFLOW finishes running, close the command prompt window by pressing any key.

5 Creating a Backward Tracking mod-PATH3DU Model

The next step is to create the mod-PATH3DU model.

1. In the Project Explorer, right-click on "S" ugrid" and select New mod-PATH3DU menu item.

This adds "*multiplication*", a new mod-PATH3DU model, to the Project Explorer.

- 2. Right-click on " ugrid" and select **Rename**.
- 3. Enter "backward" and press *Enter* to set the new name.

5.1 Adding Starting Locations

- 1. Right-click on " backward" and select **Create Particles at Wells** to bring up the *Generate Particles at Wells* dialog.
- 2. Click **OK** to accept the defaults and close the *Generate Particles at Wells* dialog.

Notice the ring of starting locations created around the wells (Figure 2).

- 3. **Zoom** \bigcirc in to see the particles around the wells.
- 4. When finished, select the **Frame** Q macro to view the entire grid.



Figure 2 Ring of particle starting locations around wells

5.2 Direction and Release Time

With starting locations at the wells, it is now possible to create a backward tracking simulation.

- 1. Right-click on " backward" and select **Options...** to bring up the *mod*-*PATH3DU Options* dialog (Figure 3).
- 2. Select "Options" from the list on the left.
- 3. Select "Backward" from the *Direction* drop-down.

ptions	DIRECTION	Backward 🔻
IFACE	Auto compute release time	True 🔻
	Release time	0.0
	TRACK_TO_TERMINATION	On 👻
	SIMULATION_END_TIME	1000000000.0
	CAPTURE_RADIUS	10.0
	DISPERSION	Off 👻
	INITIAL_STEPSIZE	1.0
	STAGNATION_DT	1.0e-015
	EULER_DT	0.0001
	ADAPTIVE_STEP_ERROR	1.0e-006
	MAX_DT	100000.0
	THREAD_COUNT	1
	REPEAT_DT	1.0
	REPEAT	1

Figure 3 mod-PATH3DU Options dialog.

Notice that *Release Time* is set to "0.0". Because the MODFLOW model is transient and the mod-PATH3DU *Direction* is set to "Backward", the *Release Time* should not be "0.0". It would typically be the end time of the MODFLOW model. In this model, that time happens to be "1000970.1".

However, notice that *Auto Compute Release Time* is set to "True". When GMS saves the mod-PATH3DU input files, it automatically sets the *Release Time* to either the MODFLOW end time (if doing backward tracking), or to "0.0" (if doing forward tracking). Therefore, *Release Time* does not need to be changed in this case.



The *Auto Compute Release Time* option will cause the *Release Time* to be set at "0.0" or the MODFLOW end time based on the *Direction*.

5.3 IFACE

IFACE is an input used by mod-PATH3DU to help track particles through cells containing a source or sink. The flow into or out of the cell due to the source or sink must be assigned to a cell face. For example, recharge would be assigned to the top cell face. IFACE values are integer values which vary from "0" to "6", with "0" indicating an internal source/sink (e.g. wells), "5" and "6" indicating the bottom and top faces, respectively, and values between "1" and "4" indicating side faces.

1. Select "IFACE" from the list on the left (Figure 4).

Historically, cells were always hexahedrons (six-faced) so this numbering scheme made sense. With unstructured grids, however, there can be any number of side faces on a cell. Therefore, with mod-PATH3DU, instead of specifying a value from "1" through "4" to indicate a side face, a value of "2" is used to indicate any side face, and mod-PATH3DU determines the specific side face internally.

IFACE input can be supplied to mod-PATH3DU in one of two ways: as cell-by-cell input via an auxiliary variable included in the MODFLOW boundary condition package files, or by specifying an IFACE value for each type of boundary condition in the *mod-PATH3DU Options* dialog. Both methods can be used together, with the IFACE values in the options dialog used only if the auxiliary variable method is not used.

mod-PATH3DU Options			23
Options	FTYPE IF	ACE	
IFACE	1 CHD 2		
	2 RCH 6		
Help	≞₄≞	OK Can	cel

Figure 4 IFACE values.

This table (Figure 4) is how IFACE values are specified. Notice there are two rows listed in the table, one for *CHD* and one for *RCH*. The names correspond to the names found in the cell to cell flow (CCF) file. GMS adds these two items automatically with all new mod-PATH3DU simulations. If these types of boundary conditions were not being used, mod-PATH3DU would ignore the IFACE values listed in the table, so it would not be necessary to delete them.



Two *IFACE* entries are created automatically by GMS and used by mod-PATH3DU, or ignored by it if they are not needed.

Wells are also included in this model, but IFACE is included by GMS as an auxiliary variable in the well package file so no IFACE value is needed in this table. The CHD package is being used for the constant head boundary condition and GMS does not automatically include IFACE as an auxiliary variable for this package, so the IFACE value listed in the table is necessary.

The value of "2" for *CHD* indicates that flow will be assigned to a side face for cells containing a constant head boundary condition. The value of "6" for *RCH* indicates that flow will be assigned to the top face for cells containing a recharge boundary condition.

The default IFACE values make sense for this model so no change is needed.

2. Click **OK** to exit the *mod-PATH3DU Options* dialog.

6 Running the Model Checker

GMS has a model checker for mod-PATH3DU that looks for obvious problems with the model setup and warns of potential errors or issues that may impact the model run.

- 1. Save 🖬 the project.
- 2. Right-click " backward" and select **Check Simulation...** to bring up the *Model Checker* dialog.
- 3. Click **Run Check** to begin the check.

Notice the errors about unit numbers (Figure 5). For some reason, mod-PATH3DU can only handle unit numbers that are 199 or less. These errors will be fixed in the next section.

4. Click **Done** to close the *Model Checker* dialog.

mod-PATH3DU requires that MODFLOW unit numbers be 199 or less.

Model Checker		×	
Run Check - Click on an error to select the objects in the display window Shift-click to select all objects with the same error.			
Errors found in model inputs	Fix Layer E	mors	
mod-PATH3DU MODEL:	Save Mess	ages	
Error: The unit number 211 for the DRN package must be 199 or less as require	_ Listing and	liana	
Error: The unit number 212 for the CHD package must be 199 or less as required	Listing options		
Error: The unit number 213 for the SMS package must be 199 or less as required	Suppress warnings		
No warnings detected in model.	Display	all errors	
	Oisplay specified max.		
	Max:	5	
Help		Done	

Figure 5 Model Checker dialog showing errors

6.1 Fixing Unit Numbers

To fix the unit numbers, do the following:

1. Select *MODFLOW* / Name File... to bring up the *MODFLOW* Name File dialog.

ll be included wi ing the Remove	hen running e button.	MODFL	OW. Unsupported files	can be removed from	m the model
= type	Package	Unit #	File Name	Edit Unsupported	
IST		11	TransientMp3du.out		
DATA(BINARY)	OC	12	TransientMp3du.hed		
DATA(BINARY)	OC	41	TransientMp3du.ccf		
DISU		13	TransientMp3du.disu		
BAS6		14	TransientMp3du.ba6		
BCF6		15	TransientMp3du.bc6		
DC		16	TransientMp3du.oc		
RCH		17	TransientMp3du.rch		
WEL		18	TransientMp3du.wel		
DRN		211	TransientMp3du.drn		
CHD		212	TransientMp3du.chd		
SMS		213	TransientMp3du.sms		

2. Scroll down so that unit numbers greater than "199" are visible (Figure 6).

Figure 6 MODFLOW Name File dialog.

- 3. Enter "19", "20", and "21" on the *DRN*, *CHD*, and *SMS* rows (respectively) in the *Unit* # column.
- 4. Click **OK** to exit the *MODFLOW Name File* dialog.



The MODFLOW Name File dialog can be used to change unit numbers.

6.2 Running the Model Checker

Now to rerun the *Model Checker* to make sure there are no more errors:

- 1. Right-click " backward" and select **Check Simulation...** to bring up the *Model Checker* dialog.
- 2. Click **Run Check** to begin the check.

No errors or warnings should be listed (Figure 7).

3. Click **Done** to close the *Model Checker* dialog.

Run Check	Click on an error to select the objects in the display window Shift-click to select all objects with the same error.	
No Errors or Warn	ings found in model inputs	Fix Layer Errors
mod-PATH3DU MO[No warnings detecte	DEL: d in model.	Save Messages
	inout.	Suppress warnings Display all errors Display specified max. Max: 5
Help		Done

Figure 7 Model Checker dialog with no errors or warnings.



The *Model Checker* looks for obvious problems in the model setup.

7 Saving and Running mod-PATH3DU

Before running mod-PATH3DU, it is advised to save the project.

1. Save 🖬 the project.

This saves the project again, this time including the mod-PATH3DU input files.

2. Right-click " backward" and select **Run mod-PATH3DU** to bring up the *MP3DU* model wrapper dialog

The *MP3DU* model wrapper dialog displays the output from the mod-PATH3DU run, and should finish within less than a minute. If the mod-PATH3DU run finishes successfully, the dialog displays "Normal termination of mod-PATH3DU." near the bottom of the dialog (Figure 8).

S MP3DU	X
c:\program files\gms 10.4 64-bit\models\mod-pat\mp3du.exe backward_mp3du.p3p	
Working on PATHLINE backward_mp3du Backward tracking 4th-order Runge-Kutta Step-doubling Scheme backward_mp3du.shp 260 particles	*
1 threads initialized [] 0 %	r l
Done	
Finished: Wed Aug 22 13:03:24 2018	
Elapsed time (seconds) : 12.846	
Elapsed time (minutes) : 0.2	=
Normal termination of mod-PATH3DU.	
MP3DU finished	*
Help Read solution on exit	Close

Figure 8 mod-PATH3DU model wrapper dialog

- 3. When mod-PATH3DU finishes, turn on *Read solution on exit* and click **Close** to exit the *MP3DU* model wrapper dialog.
- 4. Click **Redraw Display (**

This causes GMS to refresh the display after reading the pathline file. The project should appear similar to Figure 9.



Figure 9 Pathline solution showing pathlines tracking backward from the well.

- 5. If desired, **Zoom** \bigcirc^{t} in and examine the pathlines.
- 6. **Save** the project when done reviewing the pathlines as it now contains the solution.

8 Capture Zones and Well Groups

Notice the purple line surrounding all the pathlines. This line encloses a capture zone.

- 1. Click **Display Options** T to bring up the *Display Options* dialog.
- 2. Select "UGrid: ugrid [Active]" from the list on the left.
- 3. In the *Capture zones* section of the *Particles* tab, notice that *Delineate by well* is selected and *Boundary* is turned on.

Delineate by well groups wells together by name, and creates a capture zone using the pathlines for each well in the group. Turning on *Boundary* makes the capture zone boundary visible.

4. Click **Cancel** to close the *Display Options* dialog.

8.1 Creating Well Groups

To create different well groups, modify the well names.

- 1. Select *MODFLOW* | *Optional Packages* | **WEL Well...** to bring up the *MODFLOW Well Package* dialog.
- 2. Enter "D" in the *Name* column on row 1.
- 3. Enter "C" in the *Name* column on row 2.
- 4. Enter "B" in the *Name* column on row 3.
- 5. Enter "A" in the *Name* column on rows 4–13.
- 6. Click **OK** to exit the *MODFLOW Well Package* dialog.
- 7. Click **Redraw Display**
- 8. Save 🖬 the project.

Notice how the capture zone boundary lines have changed (Figure 10). The wells at the top of the model are grouped together in one capture zone, and the other wells each have individual capture zones.



Wells can be grouped together in the same capture zone by setting their names equal in the MODFLOW Well package.



Figure 10 Capture zones for different well groups

9 Exporting a Shapefile

The pathline solution can be exported to a shapefile for viewing in a GIS application. Three types of shapefiles can be exported: a point shapefile containing each pathline point, a line shapefile containing each pathline, and a polygon shapefile containing the capture zone polygons.

- 1. Right-click " backward" and select **Export...** to bring up the *Export mod-PATH3DU* dialog.
- 2. Select "Pathline Shapefile (*.shp)" from the Save as type drop-down.
- 3. Enter "backward.shp" as the *File name*.
- 4. Click **Save** to export the shapefile and close the *Export mod-PATH3DU* dialog.
- 5. Click **Open** if to bring up the *Open* dialog.
- 6. Select "Shapefiles (*.shp)" from the *Files of type* drop-down.
- 7. Select "backward.shp" and click **Open** to import the shapefile and exit the *Open* dialog.
- 8. Click **Display Options** T to bring up the *Display Options* dialog.
- 9. Select "UGrid: ugrid [Active]" from the list on the left.
- 10. On the UGrid tab, turn off Cell edges and Face contours.
- 11. Turn on UGrid boundary.
- 12. Select "GIS Data" from the list on the left.
- 13. Select "Blue" from the *Lines* drop-down.
- 14. Click **OK** to exit the *Display Options* dialog.
- 15. Turn off " backward" in the Project Explorer.
- 16. Switch to **Oblique View** \bigotimes .

The project should appear similar to Figure 11.

17. Using the **Rotate** \checkmark tool, examine the pathlines in 3D.

The lines in the shapefile are 3D lines, just as they are in GMS. The shapefile can be imported into another GIS application, if desired.



Shapefiles of pathlines, path points, or capture zone polygons can all be exported from GMS.



Figure 11 Pathline shapefile in 3D.

10 Conclusion

This concludes the "mod-PATH3DU Transient" tutorial. The following key concepts were discussed and demonstrated in this tutorial:

- The *Auto Compute Reference Time* option will cause the *Reference Time* to be set at "0.0" or at the MODFLOW end time based on the *Tracking Direction*.
- Two *IFACE* entries are created automatically by GMS and may be used by mod-PATH3DU if needed.
- mod-PATH3DU requires that MODFLOW unit numbers be 199 or less.
- Use the *MODFLOW Name File* dialog to change unit numbers.
- The mod-PATH3DU model checker looks for obvious problems in the model setup.
- Wells can be grouped in the same capture zone by setting their names to equal values in the *MODFLOW Well Package* dialog.
- GMS can export shapefiles of pathlines, path points, or capture zone polygons.