GMS 10.3 Tutorial
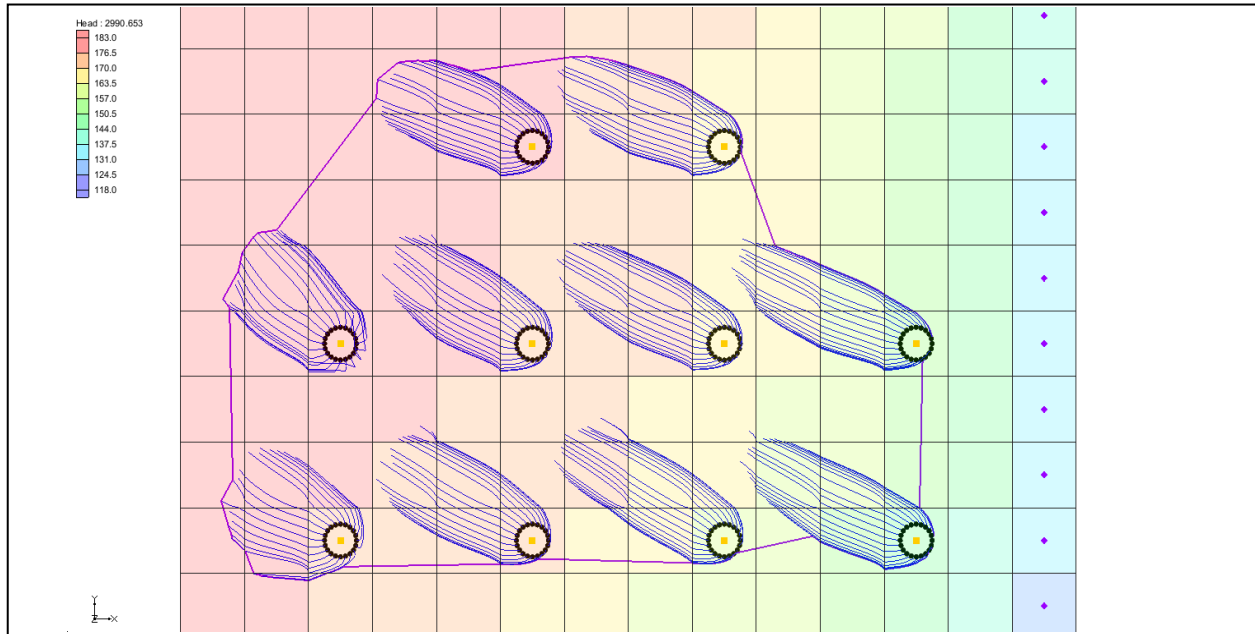
mod-PATH3DU Transient

Particle tracking with a transient MODFLOW-USG model

Objectives

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

Prerequisite Tutorials	Required Components	Time
• mod-PATH3DU	• MODFLOW-USG • MP3DU	• 15–30 minutes

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 run, 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

Begin by opening a two-layer transient MODFLOW-USG model.

1. Click **Open** 📂 to bring up the *Open* dialog.

2. Select "Project Files (*.gpr)" from the *Files of type* drop-down.

3. Browse to the *Tutorials\MP3DU\Transient* directory and select "Transient.gpr".

4. Click **Open** to import the project and exit the *Open* dialog.

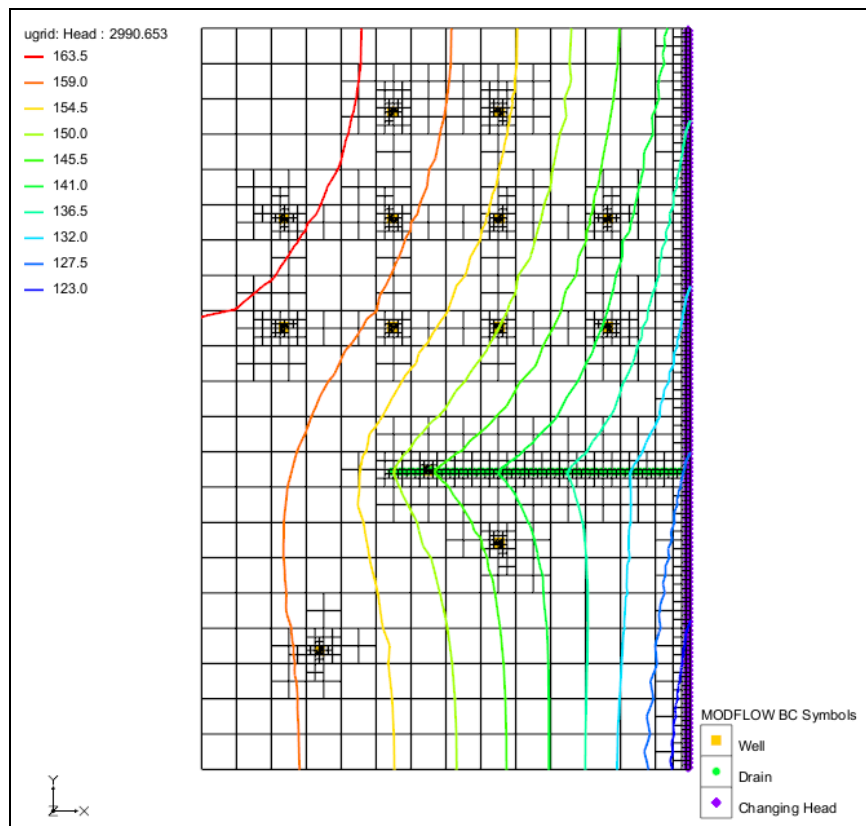The project should appear similar to Figure 1.

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, 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. For this tutorial, save a native text copy of the MODFLOW simulation for mod-PATH3DU to use.

1. In the Project Explorer, double-click on "🗔 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, run MODFLOW. 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** 📂 to 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.
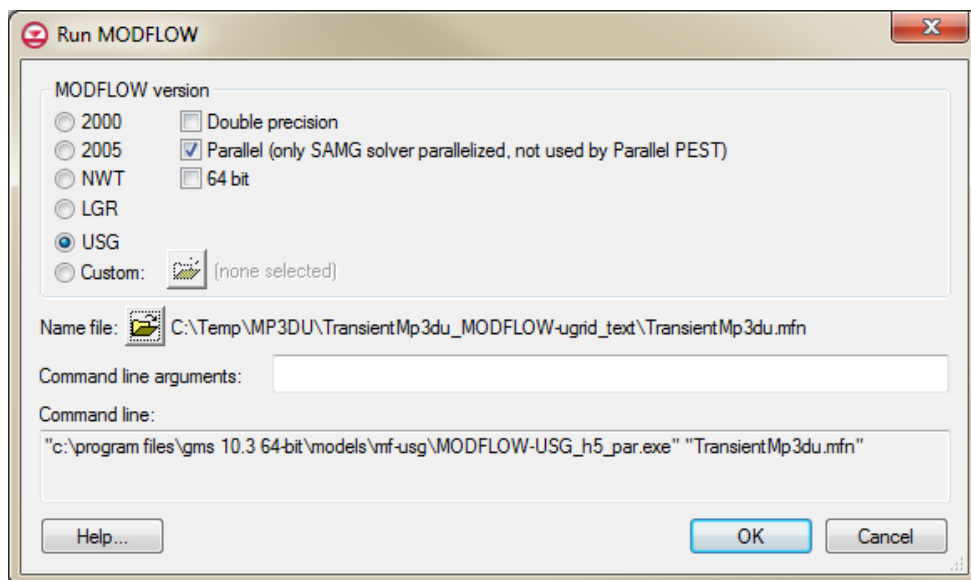

Figure 2   Run MODFLOW dialog.

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 "🔒 ugrid" and select **New mod-PATH3DU** menu item.

This adds "🎆 ugrid", 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 3).

3. **Zoom** 🔍 in to see the particles around the wells.

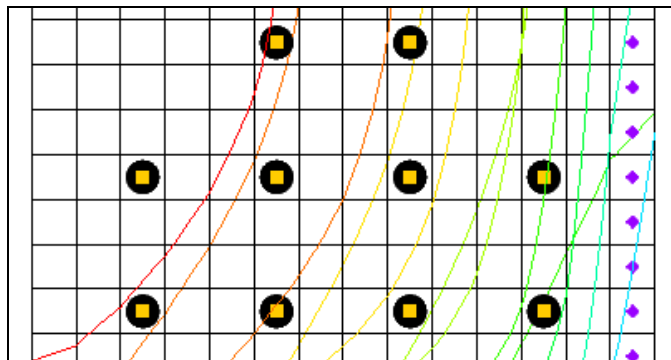4. When finished, select the **Frame** 🔍 macro to view the entire grid.

Figure 3   Ring of particle starting locations around wells

5.2   TrackingDirection and ReferenceTime

With starting locations at the wells, now create a backward tracking simulation.

1. Right-click on "🎆 backward" and select **Options…** to bring up the *mod-PATH3DU Options* dialog (Figure 4).

2. Select "Options" from the list on the left.

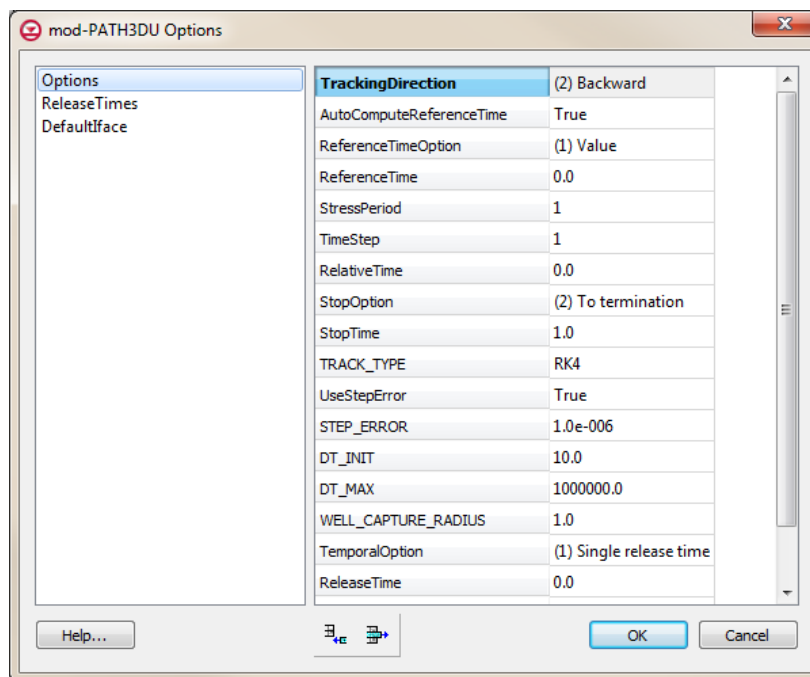3. Select "(2) Backward" from the *Tracking Direction* drop-down.

Figure 4   mod-PATH3DU Options dialog.

Notice that *ReferenceTime* is set to "0.0". Because the MODFLOW model is transient and the mod-PATH3DU *TrackingDirection* is set to "(2) Backward", the *ReferenceTime* 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 *AutoComputeReferenceTime* is set to "True". When GMS saves the mod-PATH3DU input files, it automatically sets the *ReferenceTime* to the either the MODFLOW end time (if doing backward tracking), or to "0.0" (if doing forward tracking). Therefore, *ReferenceTime* does not need to be changed in this case. Figure 5 illustrates this concept.
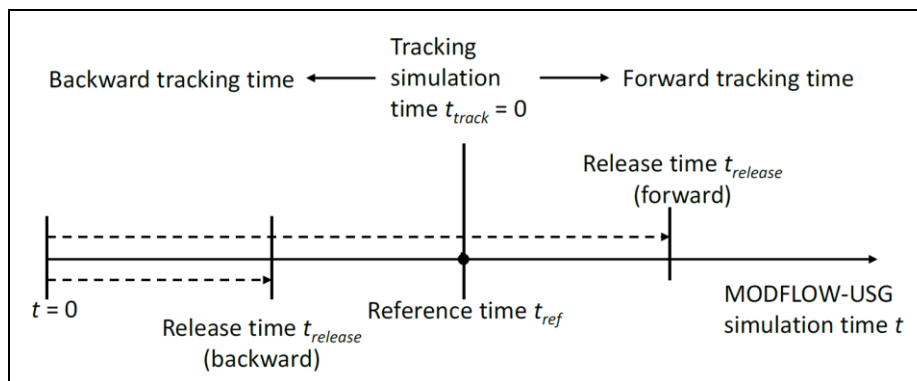

Figure 5   Illustration of time concepts in mod-PATH3DU[1]

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[1] Muffels, Christopher, et al (2016). *User's Guide for mod-PATH3DU: A groundwater path and travel-time simulator*, S.S. Papadopulos & Associates, Inc. and the University of Waterloo, p.16.

> The *AutoComputeReferenceTime* option will cause the *ReferenceTime* to be set at "0.0" or the MODFLOW end time based on the *TrackingDirection*.

5.3   Default 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 "DefaultIface" from the list on the left (Figure 6).

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 a default IFACE value for each type of boundary condition. Both methods can be used together, with the default IFACE values used only if the auxiliary variable method is not used.
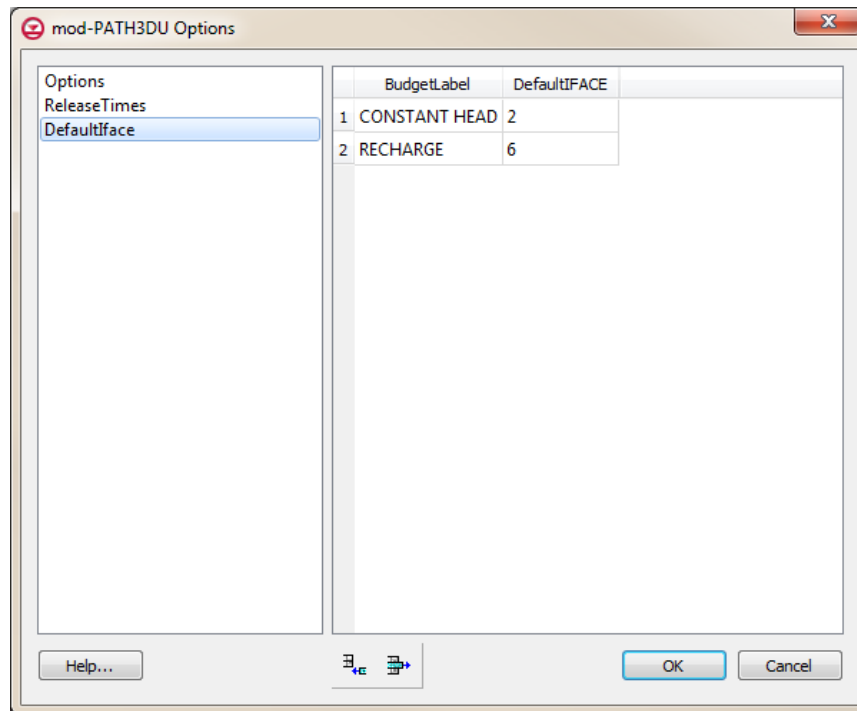

Figure 6   Default Iface values.

This table (Figure 6) is how default IFACE values are specified. Notice there are two rows listed in the table, one for *CONSTANT HEAD* and one for *RECHARGE*. 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 default IFACE values listed in the table, so it would not be necessary to delete them.

> Two *DefaultIface* 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 default 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 default IFACE value listed in the table is necessary.

The value of "2" for *CONSTANT HEAD* indicates that flow will be assigned to a side face for cells containing a constant head boundary condition. The value of "6" for *RECHARGE* 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. Right-click "⚝ backward" and select **Check Simulation…** to bring up the *Model Checker* dialog.

2. Click **Run Check** to begin the check.

Notice the errors about unit numbers (Figure 7). These errors will be fixed in the next section.

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

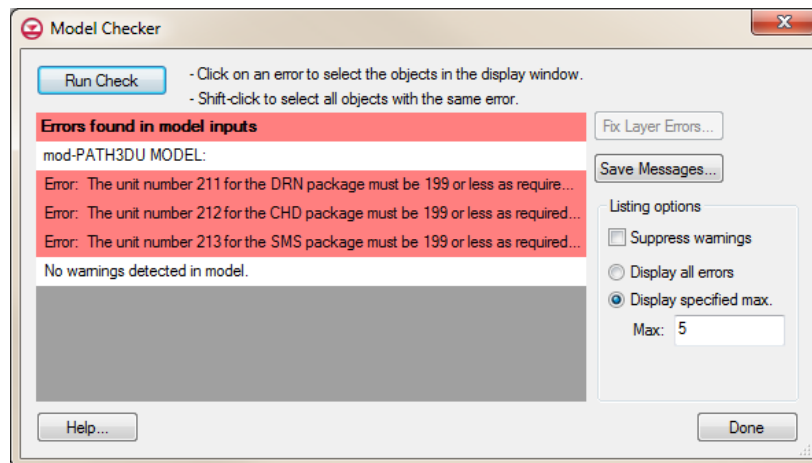> mod-PATH3DU requires that MODFLOW unit numbers be 199 or less.

Figure 7   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.

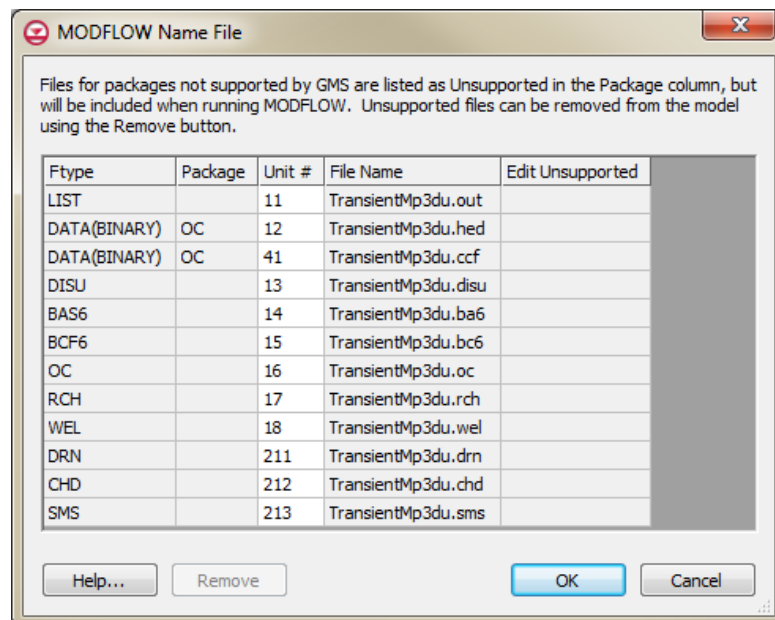2. Scroll down so that unit numbers greater than "199" are visible (Figure 8).

Figure 8   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 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 9).

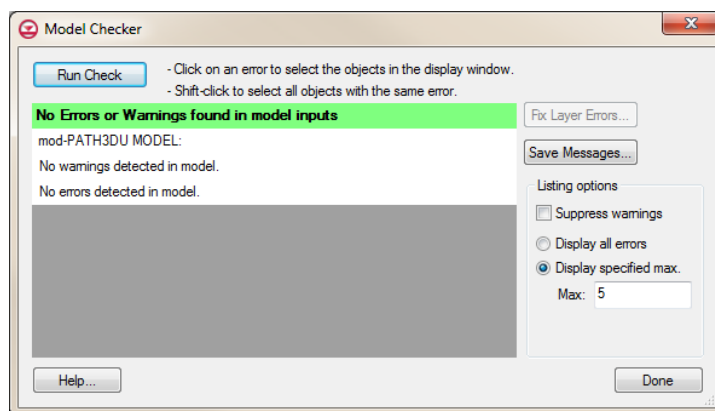3. Click **Done** to close the *Model Checker* dialog.

Figure 9   *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, 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 "End of mod-PATH3DU simulation. Normal termination." near the bottom of the dialog (Figure 10).
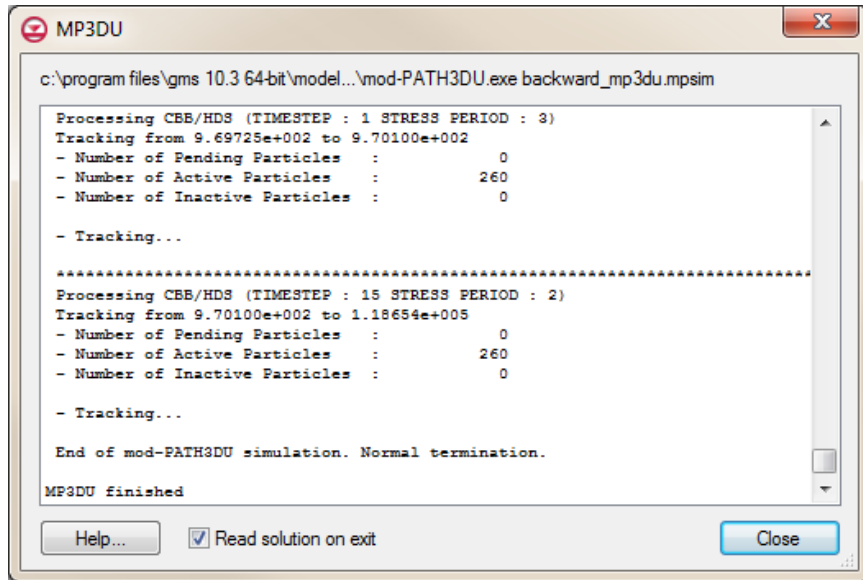
Figure 10   mod-PATH3DU model wrapper dialog

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 11.
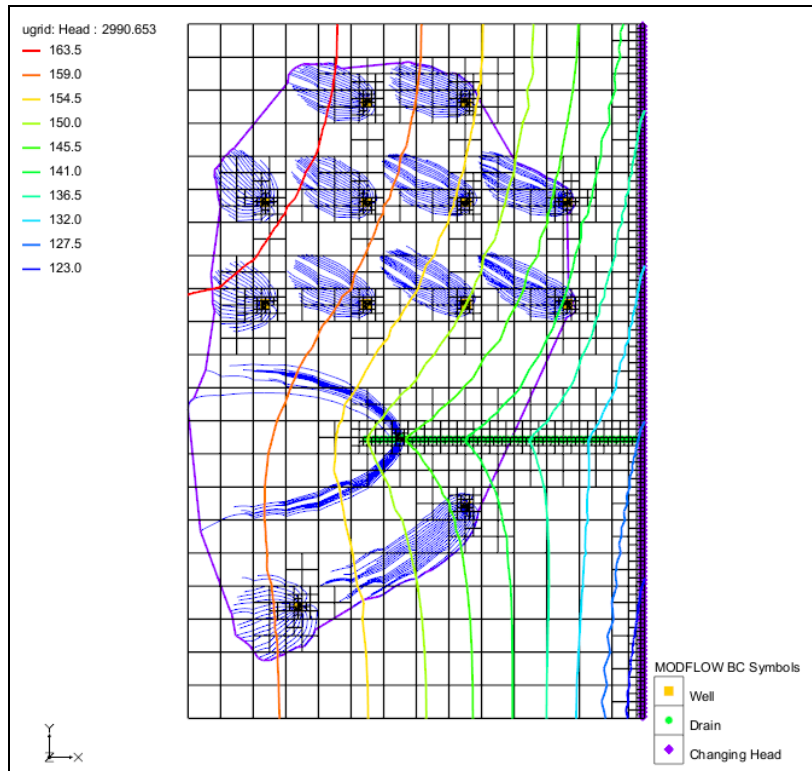

Figure 11   Pathline solution showing pathlines tracking backward from the well.

5. If desired, **Zoom** 🔍 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** 🖥 to bring up the *Display Options* dialog.

2. Select "UGrid Data" 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 12). 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.
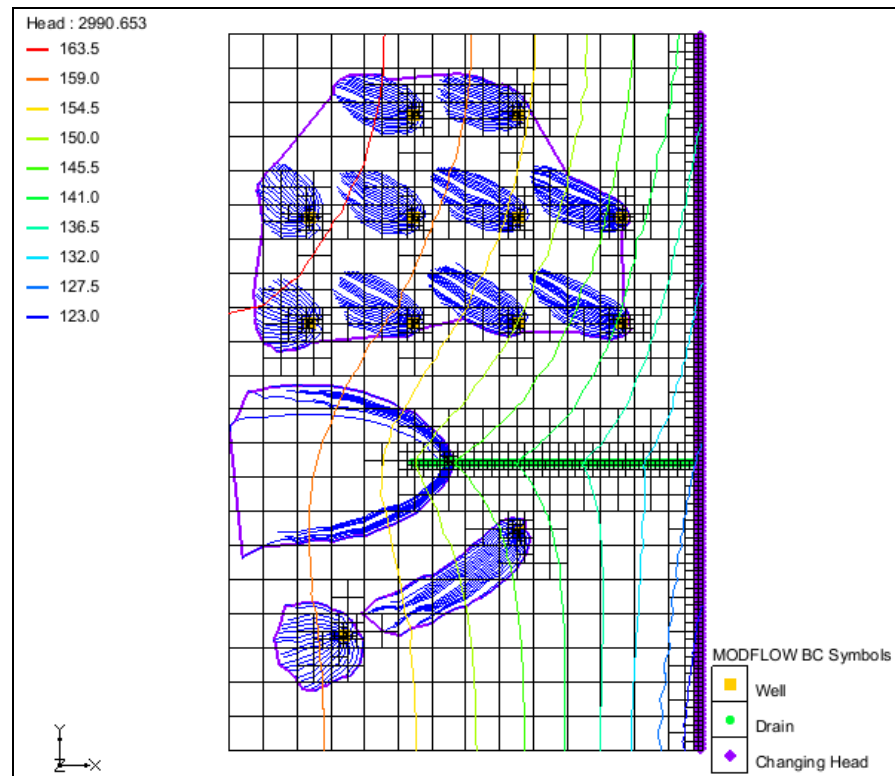
Figure 12   Capture zones for different well groups

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** 📂 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** 🖥 to bring up the *Display Options* dialog.

9. Select "UGrid Data" from the list on the left.

10. On the *UGrid* tab, turn off *Cell edges* and *Face contours*.

11. Turn on *UGrid shell*.

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** ◈.

The project should appear similar to Figure 13.

17. Using the **Rotate** ✣ 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.

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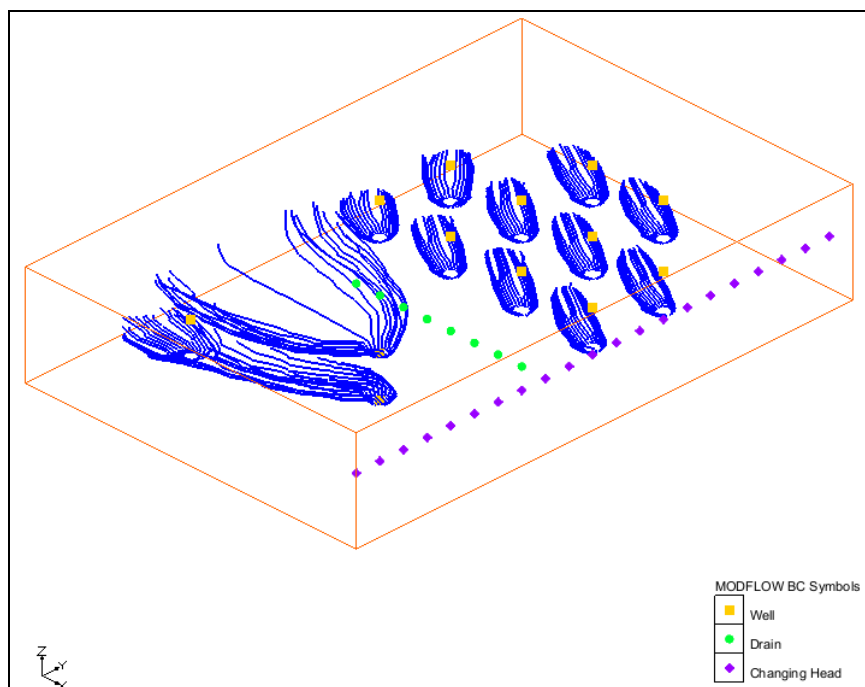

Figure 13   Pathline shapefile in 3D.

10   Conclusion

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

- The *AutoComputeReferenceTime* option will cause the *ReferenceTime* to be set at "0.0" or at the MODFLOW end time based on the *TrackingDirection*.

- Two *DefaultIface* 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.