Pumping Optimization Model for Pump and Treat Systems – 15091

Steve Baker *, Marinko Karanovic **, Kris Ivarson ***, Charles Miller ***, Matthew Tonkin ****
* Umtanum Enterprises
** S.S. Papadopulos & Associates, Inc.
*** CH2M HILL PRC
**** S.S. Papadopulos & Associates, Inc.

ABSTRACT

Pump and Treat systems are being utilized to remediate contaminated groundwater in the Hanford 100 Areas adjacent to the Columbia River in Eastern Washington. Design of the systems was supported by a three-dimensional (3D) fate and transport model. This model provided sophisticated simulation capabilities but requires many hours to calculate results for each simulation considered. Many simulations are required to optimize system performance, so a two-dimensional (2D) model was created to reduce run time. The 2D model was developed as a equivalent-property version of the 3D model that derives boundary conditions and aquifer properties from the 3D model. It produces predictions that are very close to the 3D model predictions, allowing it to be used for comparative remedy analyses. Any potential system modifications identified by using the 2D version are verified for use by running the 3D model to confirm performance.

The 2D model was incorporated into a comprehensive analysis system (the Pumping Optimization Model, POM) to simplify analysis of multiple simulations. It allows rapid turnaround by utilizing a graphical user interface that:

1. allows operators to create hypothetical scenarios for system operation,
2. feeds the input to the 2D fate and transport model, and
3. displays the scenario results to evaluate performance improvement.

All of the above is accomplished within the user interface. Complex analyses can be completed within a few hours and multiple simulations can be compared side-by-side. The POM utilizes standard office computing equipment and established groundwater modeling software.

INTRODUCTION

The Hanford site is located along the Columbia River in eastern Washington State. Nuclear production reactor operations there resulted in significant groundwater contamination from hexavalent chromium as well as other contaminants.

Groundwater pump-and-treat (P&T) was determined to be the proper technology for remediation of groundwater contamination along the river at the 100-HR-3 and 100-KR-4 groundwater operable units. P&T systems were designed with knowledge from sites worldwide that show that poorly managed P&T systems can be costly failures. Accordingly, a three-dimensional (3D) groundwater flow and contaminant transport (F&T) was developed to support design of the P&T facilities. The F&T model was constructed
using MODFLOW and MT3D customized to meet site-specific needs. The underlying MODFLOW code implements dynamic balancing of system influent-effluent rates, enabling seasonal (river-stage-dependent) P&T operations to be evaluated. This model offers sophisticated simulation capabilities to support system design.

The need for the P&T systems to be efficient was also considered in their design. Reasonable estimates of the time required to remediate Hanford groundwater via P&T vary widely, but can extend to several tens of years. Reductions in aquifer restoration time would result in large cost savings, and could also enhance the credibility of P&T as a remedy technology. The 3D model is an effective design tool, but it has a computational cost that can inhibit the iterative analyses required for remedy optimization.

In recognition of this, a P&T remedy analysis system referred to as the Pumping Optimization Model (POM) was created to enable project scientists to adjust the location and time-varying rates of extraction and injection – including the addition and abandonment of wells over time – to optimize the life cycle of the P&T remedies. The POM was developed as a 2D equivalent-property version of the fully 3D model, incorporating boundary conditions and aquifer properties derived from the 3D model that give sufficiently similar results to be relied upon for comparative remedy analyses.

This paper deals only with operating a fate and transport model to display predicted contaminant plumes under various remediation scenarios. Separate papers (Innovative Use of Cr(VI) Plume Depictions And Pump-and-Treat Capture Analysis to Estimate Risks of Contaminant Discharge To Surface Water at Hanford Reactor Areas - 15315 and Development of a Groundwater Transport Simulation Tool for Remedial Process Optimization – 15316) provide the geologic and hydrologic setting of the site, contamination history, and engineering information about the pump and treat systems.

**PUMPING OPTIMIZATION MODEL FUNCTIONALITY**

The POM is structured with two major components:

1. a graphical user interface, and
2. several F&T applications and utilities.

The graphical user interface is a standard MS Windows application, written in MS Visual Studio. The F&T calculations are accomplished using standard MODFLOW/MT3D executables and utilities written in Fortran along with supporting batch files. The entire system can be operated entirely from within the user interface. To initiate an optimization scenario, analysts can:

1. specify extraction and injection well locations and time-varying pumping rates,
2. associate wells with specific treatment plants,
3. specify the number of stress periods to calculate, and
4. initiate a F&T calculation.
When the F&T calculation is complete, control returns to the user interface where analysts can see calculated contaminant plumes for the stress periods specified. Multiple scenarios can be viewed side-by-side to make comparison rapid and intuitive. Figure 1 shows an overview of the POM functional structure. It is initially configured with a “base” alternative that can be used to rapidly create a new alternative. If a new alternative is created, the base is copied to a new alternative (with a new name). The new alternative can then be edited allowing well locations and pumping rates to be adjusted. When the new alternative is ready, a F&T calculation driven by the assumptions specified can be run. Alternatively, an existing scenario can be edited and recalculated.

This “Optimization Loop” can be repeated many times, making adjustments during each iteration using the insight gained from previous iterations. This iterative process is not designed with an objective function and convergence criteria. Rather, it is intended to give the user an intuitive understanding of how the P&T system might be adjusted to achieve one of several objectives. For example, reduction of the maximum contaminant concentration might be important. Or, mass removal might be the objective. As applied to groundwater contaminant concentration near the Columbia River, the objective is to minimize the amount of contaminant that reaches the river.

After each optimization is completed, predicted contaminant plumes over time can be displayed and compared to other optimization scenarios.
Figure 2 is a screen shot showing the POM in use. Wells are represented by triangles; point up indicates an extraction well and point down an injection well. Plumes and well pumping rates shown are those at Stress Period 2/1/2024. Triangle size is proportional to the pumping rate for the well. The color of the triangle fill indicates which treatment plant the well is connected to. When the mouse hovers over a well, information about the well is displayed (199-H6-7 is displayed below). When the mouse hovers over a contour line, the head value is shown. When the mouse hovers over a plume, the concentration of hexavalent chrome at that location is shown in the title bar. The slider at the bottom controls which Stress Period is displayed. The toggle buttons at the top display the data as a video with frame interval in milliseconds taken from the text box labeled “Timer Interval”.

Figure 2: POM Operation
It was necessary to implement many innovative programming features in order to achieve the desired rapid analysis turnaround time. Innovations were required both for the MS Windows user interface and the F&T programs.

User Interface Design

The user interface was implemented as a single .NET Windows Presentation Foundation (WPF) application with one UserControl. All programming was accomplished in a RemObjects Oxygene add-in to MS Visual Studio.

The interface WPF Grid is implemented dynamically to allow display of single or multiple scenario results. An extension of the WPF Image class is constructed for each scenario and placed in an instance of the UserControl. The UserControl is then put into the appropriate Grid Column. Each Image extension contains two Image Classes and metadata properties that characterize the scenario. The first Image Instance contains the background bitmap, and the second contains a plume bitmap with appropriate transparencies assigned, well objects (again with some transparencies assigned) and partially transparent head contour Polylines.

Plumes are provided to the user interface from the F&T model calculations as text files, specifying a contaminant concentration for each cell in the model domain. The text files are a variant of standard “raster” files from MT3D, with structure modified so that they can be written and read using a buffer sized to maximize speed. The user interface creates a bitmap illustrating the plume for each Stress Period using the WriteableBitmap Class. The color of each pixel is determined by the contaminant concentration.

The WPF Shape Class is extended to create a “WellC” Class that contains:

$ a Shape Property,
$ a Property that can contain metadata for each treatment plant, and
$ metadata Properties and Fields that characterize each well.

Metadata is loaded from text files.

Head contours are simply Polylines read in from text files.

Plume bitmaps, WellC objects, and head contours are all oriented to the background bitmap using World Coordinates. They all are constructed for each Stress Period provided by the F&T model results.

The user interface includes standard Context Menu Items, TextBox objects for data entry, and a Slider to move among the Stress Periods. The Slider is the major control. Each time it changes all plume maps, WellC’s and Polylines are destroyed and then redrawn to display the new data.

Every aspect of the user interface must consider the tradeoff between:
constructing all objects to be used once when the application is loaded and storing them in Random Access Memory (RAM), and

constructing them only when needed.

Tradeoff a) requires a longer startup time and a large amount of RAM. However it makes operation very fast when changing between Stress Periods. Tradeoff b) loads more rapidly and requires less RAM but response to user commands is slower. The user interface is written to allow the user to make some tradeoff choices to accommodate the user’s objectives and computer capabilities.

The most significant tradeoff involves creation of plume bitmaps from text files. Even of fast computers, it takes hundreds of milliseconds to create a bitmap. So the user interface allows three options: 1) creating each plume map when needed, 2) storing each plume map to RAM when it is first created, and 3) saving the plume map as a file when it is first created.

When the cursor hovers over a model domain cell, the user interface displays the predicted contaminant concentration at the cell. If the array of concentrations is calculated each time that the slider changes, it takes about as long to build the array as it does to create the bitmap. An option is provided to save the concentration arrays to RAM when they are first calculated.

Save to RAM decisions must be made carefully. On computers with less than 16 GB of RAM, save to ram can easily exhaust the computer’s capacity. What happens then depends on how paged memory is set up. Overloading RAM can either slow the computer down significantly or cause it to crash.
Flow and Transport Model Design

A directory structure designed to perform the two dimensional groundwater flow and transport calculations is provided for each alternative considered. Figure 3 shows the structure under “Alt1”, the base case alternative.

Figure 3: Flow and Transport Calculation Structure

When a user initiates a new flow and transport calculation, the user interface calls a batch file in MODFLOW-MT3D which performs the following tasks:

- Convert the desired number of Stress Periods to a MODFLOW input format,
- Convert well data created in the user interface to a MODFLOW input format,
- Convert well pumping rates specified in the user interface to a MODFLOW input format,
- Run MODFLOW,
- Run MT3D,
- Calculate plumes from the .UCN file and put them in the Layer01 directory as text files, and
- Calculate head contours from the .HDS file and put them in Layer01 as text files.

All calculations called by the main batch file are performed by batch files in subdirectories, utilities written in Fortran, or MODFLOW-related flow and transport executables.

While the time required to complete these calculations is small compared to normal flow and transport calculations, it does take some time. It takes about three hours to calculate plumes and contours for the Hanford River Corridor model with 174 wells and 289 Stress Periods.

The user interface provides a capability to change the head contour interval and line thickness. Changing the line thickness is done entirely within the user interface, so it is accomplished essentially instantly. Changing the interval requires reading the .HDS file, so it takes some time for the Fortran utility to run and return control to the user interface. But this is much faster than making a complete recalculation because it does not require rerunning either MODFLOW or MT3D.
CONCLUSIONS

In the short time that the POM has been employed by the remedy scientists, it has provided significant insight. For example, POM analyses have shown that significant reduction in the time required for cleanup can be realized by adjusting pumping rates to accommodate seasonal variations in river stage. Figure 4 illustrates how the POM was used to improve projected plume concentrations near the K reactors at Stress Period 2/1/2024. The plumes on the left were calculated adjusting pumping rates to respond to anticipated river stage. Pumping rates were held constant when calculating the plumes on the right. This subtle change predicts a significant improvement after years of pumping.

The scenario displayed in the title bar is the one under the mouse. In this figure the mouse is over the right image where the “x” is. The scenario is “04 Actual Pumping Rates Projected” and the plume concentration under the mouse is 30 micrograms per liter. The maximum calculated concentration for this Stress Period and scenario is 3458 micrograms per liter.

Figure 4: Optimization by Changing Pumping Rates to Accommodate River Stage
Figure 5 illustrates a different use for the POM. Two wells (H1-5 and H4-81) were changed from extraction to injection for the prediction on the left. Two extraction wells were added to the prediction on the right to compare relative effectiveness in slowing plume migration to the North.

Figure 5: Optimization by Adding Wells and Changing Pumping Rates

A simplified optimization process that provides insight into groundwater flow response to pumping would be a valuable asset to many pump-and-treat systems, both existing systems and future ones. Of course, groundwater fate and transport will be different for each system, requiring site-specific models. Except for the site-specific model the POM process is generic; that is, the process of developing a 2D equivalent-property model and incorporating it into the POM user interface could be implemented at any site.