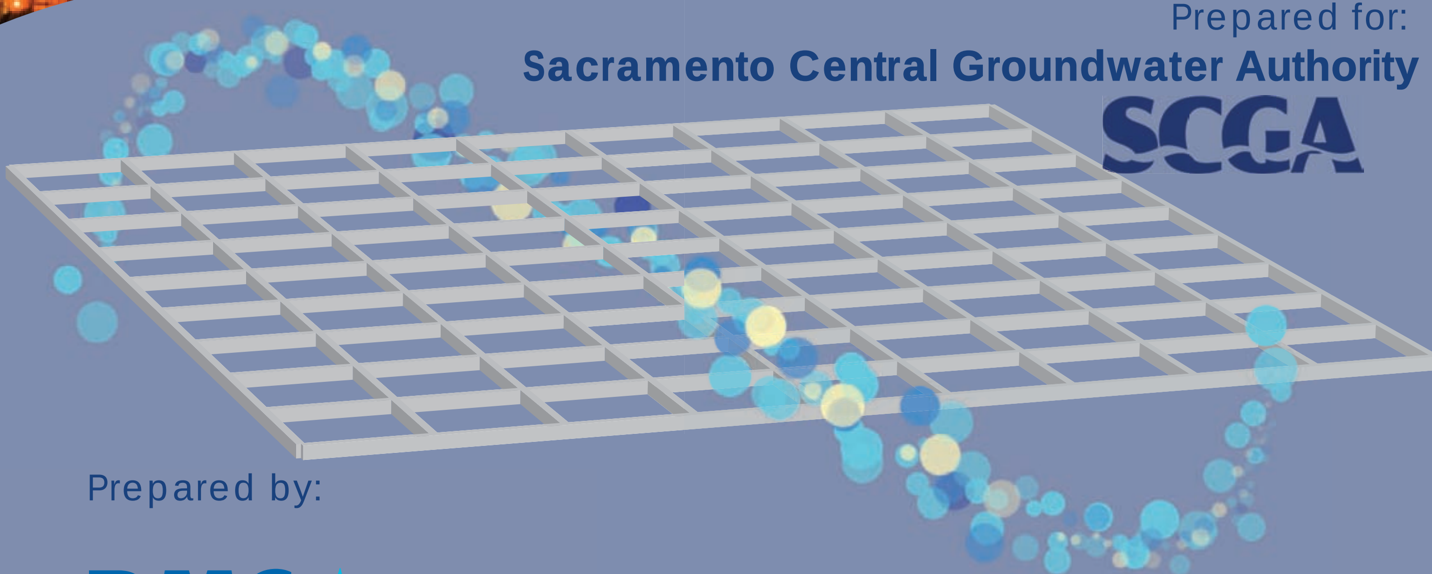
Groundwater Quality Sustainability

Integrated Hydrologic Modeling

Prepared for:

Sacramento Central Groundwater Authority

SCGA



Prepared by:

RMC Water and Environment

WRIME

October, 2011

BACKGROUND

In March 2010, the Sacramento Central Groundwater Authority (SCGA) Board of Directors passed a resolution to commission a study to assess the current conditions of the regional contamination plumes and to evaluate the potential future risks associated with the regional contamination sites to the groundwater supplies in the Central Sacramento County Groundwater Basin (Central Basin). This study was to be conducted in parallel to a similar study that the Sacramento Groundwater Authority (SGA) had initiated earlier for assessment of water quality risks in groundwater resources in the SGA area.

To conduct this study, the most comprehensive regional groundwater assessment modeling tool that is currently available for the county is used: the Sacramento Area Integrated Water Resources Model (SacIWRM) (RMC-WRIME, 2011). The extent of the regional contamination plumes used in this study was previously mapped by SGA. The hydrologic modeling assumptions for the Central Basin are primarily based on those used in the Zone 40 Water Supply Master Plan (WRIME, 2004).

The purpose of this memorandum is to describe the modeling process, and the results of the SacIWRM simulations in the SCGA area. For purposes of completeness, the memorandum presents the modeling assumptions and results in the SGA area as well.

LIMITATIONS AND INTENT OF THE ANALYSIS

It is important to note that these simulations in no way attempt to characterize contaminant transport of the known plumes. The simulations are intended only to serve as a conservative estimate in characterizing flows of particles (i.e., water molecules) that are in the aquifer at any given time and to understand where those particles could move under the known and planned stresses (i.e., pumping) in the aquifer system over a long time interval (>100 years). The simulation relies solely of adjective flow characteristics of a particle in the aquifer and does not account for the effects of dilution, dispersion, sorption or any other characteristics of a compound necessary to characterize contaminant transport. These results are only intended to characterize potential pathways of these particles when taking into account the water supply and remediation extractions from the basin.

Our intent is to provide water suppliers with a tool to inform those agencies that could potentially be impacted of the types of future monitoring that they should consider. We also intend to provide the information from this regional model to the agencies responsible for remediation at the plumes characterized in this analysis. The results of the regional model could help improve boundary conditions and other assumptions for the more refined, local-scale models developed for these sites in order to better ensure effective capture of these contaminant plumes.

These results should not be interpreted as in any way as concluding that a contaminant associated with these known plumes will or will not be detected at any time in the future. Both water supply agencies and responsible parties for contamination should continue to practice due diligence in their monitoring programs to ensure a safe and sustainable public water supply in the basin.

SACRAMENTO AREA INTEGRATED WATER RESOURCES MODEL (SACIWRM)

Sacramento Area Integrated Water Resources Model (SacIWRM), formerly known as the Sacramento County Integrated Groundwater and Surface water Model (SacIGSM), is an analytical tool that has been used in the Sacramento region since 1992 for the purposes of evaluating land and water use planning, water supply conditions, conjunctive use options, water quality investigations, and other surface water and groundwater plans. The model was the primary analytical tool for analysis of the basin yield that became the cornerstone of the *Water Forum Agreement.* The SacIWRM (Figure 1) is a state-of-the-art water resources management model that integrates the surface water hydrologic system, the groundwater aquifer system, and land surface processes (precipitation and irrigation) into a single model. It allows water managers and decision makers to vary the agricultural and/or municipal and industrial water demands, land use, water use, groundwater pumping, surface water diversions, imported water, reservoir operations, aquifer parameters, and other water planning data, and view the effects and impacts of the changes on the groundwater and surface water systems, including stream-aquifer interactions. The model is currently the primary analytical tool for evaluation of the water management programs in the area, and is managed through an ArcView-based User Interface.

IWRM PARTICLE TRACKING MODEL

The IWRM Particle Tracking Model (IWRM_PTM) is a particle tracking post-processing package that was developed to compute two-dimensional flow paths using output from steady-state or transient (as small as daily simulation time-steps) groundwater flow simulations by IWRM. Once the groundwater head solutions from IWRM have been obtained at every node, the principal velocity components for each element are computed using the finite element shape functions and Darcy’s Law. In order to compute the path lines, IWRM_PTM uses a constant velocity throughout the element.

IWRM_PTM uses a technique (in-element particle tracking) that traces particles on an element-by-element basis. Given a velocity field, a particle is traced until either a boundary, an internal sink/source is encountered or the available time is completely consumed. IWRM_PTM can compute paths for simulated particles moving through the simulated groundwater system. In addition to computing particle paths, the model can keep track of the travel time for the particles. Data input for IWRM_PTM is a combination of data files. Detailed documentation of IWRM_PTM is provided in Appendix A.

METHODOLOGY

IWRM_PTM was utilized in order to track particles which represent contamination plumes in the SGA and SCGA areas. The movement of the particles was simulated over a 105-year hydrologic period for two different model scenarios, one with- and one without- conjunctive use.

Mapping Particles onto the Plumes

The IWRM_PTM simulated regional contamination plumes at Aerojet, Boeing, McClellan, Mather, and the downtown Sacramento Railyards. The location of these plumes, shown in Figure 2, was obtained from a shapefile provided by SGA. The initial particle locations were developed by overlaying a regular 250 meter grid on top of the plume shapefile as shown in Figure 3.

Model Updates

The SacIWRM Existing Conditions baseline model was recently updated, as summarized in a technical memorandum (WRIME, September 2007). As part of this work, the SacIWRM model was further updated to improve the accuracy of the work for this application.

Extended Hydrology

The previous baseline model used a 35-year hydrology from 1970 to 2004. The 35 year hydrology was repeated three times to develop a 105-year hydrology for this project. Figure 4 shows the American River Unimpaired Inflow to Folsom Reservoir (UIFR) index for the extended 35-year hydrology.

Remediation Operations

SacIWRM was updated using data on near-term planned remediation operations for Aerojet, Boeing, and Mather. McClellan operations were updated as part of the 2007 work, and no changes to McClellan operations are assumed in the near-term. No near-term groundwater remediation operations are planned at the Sacramento Railyards site. Table 1 shows the updated remediation operations as simulated in the SacIWRM.

These updates were incorporated to improve the simulation of planned remediation operations that are likely to influence the movement of the contamination plumes.

Municipal Pumping Distribution

SacIWRM was updated using the latest available (2009) production data from municipal operations that are near the existing contamination plumes: Carmichael Water District (CWD) and Sacramento Suburban Water District (SSWD). Figure 5 shows the updated pumping distribution for CWD and SSWD wells in the model.

Initial Groundwater Level Conditions

SacIWRM was updated using the latest available (2009) groundwater level data. Data was obtained and utilized from CWD and SSWD, Aerojet, and the California Department of Water Resources Water Data Library. Figure 6 shows the updated initial groundwater levels and the locations of all wells that were utilized for generating the groundwater level contours.

DEVELOPMENT OF MODEL SCENARIOS

In order to assess the effects of the regional conjunctive use in the SGA and SCGA areas on the potential movement of the regional contamination plumes, two model scenarios, one with- and one without- conjunctive use, were developed for the project.

- **Scenario 1:** The Baseline (Conjunctive Use) Scenario simulates planned operations of the basin with conjunctive use operations in place.
- **Scenario 2:** The Pumping Scenario simulates conditions when additional surface water sources are not available for conjunctive use operations.

The groundwater conditions and operations in the SCGA area, under both scenarios were assumed to be those under the Zone 40 Water Supply Master Plan (WRIME, 2005).

Table 2 summarizes the groundwater production for the City of Sacramento, Sacramento Suburban Water District, and the San Juan Family for each hydrologic year type (using the American River UIFR index) under each scenario. Table 3 shows the annual average groundwater and surface water supply mix for the three water purveyors under each scenario.

RESULTS

The movement of the particles for Aerojet, Mather, Boeing, Sacramento Railyard, and McClellan Plumes were examined for the Baseline Scenario. The SacIWRM results were processed using various ESRI ArcMap tools to assist in visualization and examination. Table 4 summarizes the simulated percent of particles that could potentially arrive at municipal production wells in the SGA Area. Figures 7, 8, 9, 10, 11, 12, and 13 show the location of the contamination plume particles after 5, 10, 15, 20, 25, 50, and 100 years from the beginning of the simulation respectively.

If the particles within the Aerojet Plume escape to the north of American River, it was assumed that they were not captured. Table 4 shows that 100% of the Aerojet Core Plume (defined as perchlorate above 4 ppb) was captured for the whole simulation period. However, 4% of the particles for the Aerojet Detect Level Plume (above the detection level) escaped to the north of American River within 5 years. Most of these particles that escaped were at the leading edge of the plume and were already at the north of the American River. The percent of particles escaped increases to 5% after 50 years and stays the same for the rest of the simulation.

The contamination plume boundaries for the Mather and Boeing Plumes from 2007 data were used as a criterion to estimate if the particles were captured for the Mather and Boeing plumes. Five percent of the particles from the Mather Plume escaped the plume boundary after 5 years. This percent increased gradually during the simulation period and stabilized at 20% after 100 years. None of the particles from the Boeing Plume escaped the plume boundary for the first 10-15 years of the simulation. Seven percent of the particles escaped the boundary after 15 years; this value remained constant for the remainder of the simulation. Discussions were held to share the results with those overseeing remediation operations at Mather, including a meeting on June 30, 2011. These discussions recognized the extensive monitoring performed at Mather and the ability of the remediation operations to be altered should the monitoring indicate that contaminants are escaping off-side. The discussion also highlighted possibilities of utilizing data from the regional groundwater model to improve the accuracy of more detailed site models and the need for coordination between Sacramento County and Mather with regards to development that could result in new production or the loss of monitoring facilities.

All of the particles from the Sacramento Railyard Plume remained south of the American River for the first 20-25 years of the simulation. Four percent (1 particle) of the particles escaped to the north of American River after 25 years. The percent of escaping particles increased to 12% (3 particles) after 50 years and remained constant after that. The particles for the McClellan Plume stayed within the McClellan plume boundary for most of the simulation. One particle (1%) escaped the boundary after 50 years. The number of particles that escaped increased to 3 (3%) after 100 years.

Figure 14 presents a comparison of the path of three selected particles at the leading edge of the Aerojet plume for both the Baseline Scenario and the Pumping Scenario. Because the regional groundwater gradient dominates the groundwater flow fields, conjunctive use does not significantly change the movement of the particles representing the Aerojet plume. In the short term, conjunctive use may potentially delay the particle movement by a few years.

REFRENCES

RMC-WRIME. (October 2011). *Sacramento County Integrated Water Resources Model (SacIWRM) – Model Documentation. Prepared for SGA, SCGA, and SSCAWA*

WRIME. (December 2004*). Hydrologic and Modeling Analysis forZone 40 Water Supply Master Plan – Prepared for Sacramento County DERA*

WRIME. (July 2005). *Sacramento County Integrated Groundwater and Surface water Model (SacIGSM)- Refinement and Update, Prepared for the Sacramento County DERA*

WRIME. (September 2007). *Sacramento County Integrated Groundwater and Surface water Model - Model Refinement – Prepared for SGA*

FIGURES AND TABLES

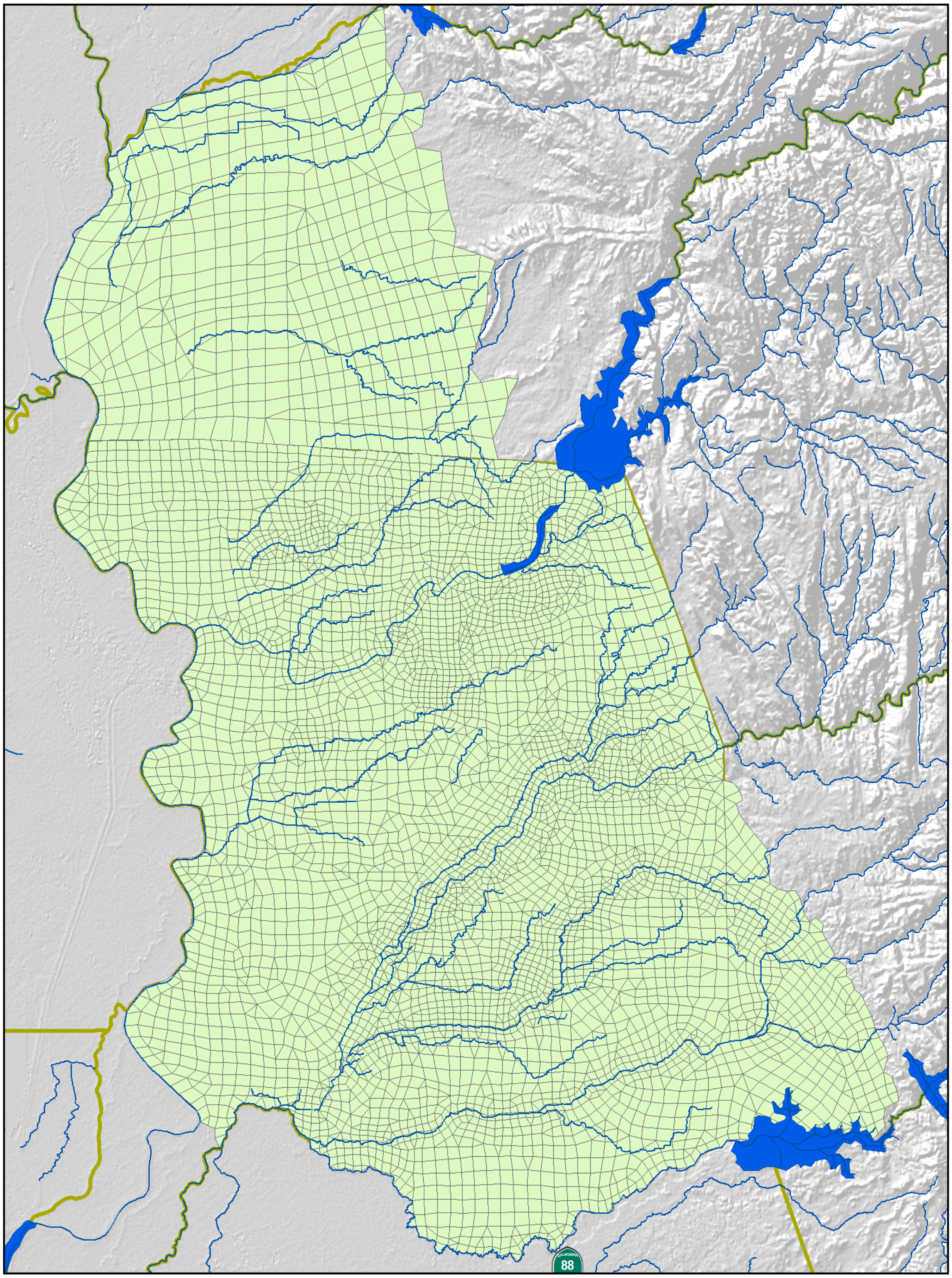


Figure 1: SacIWRM Model Area

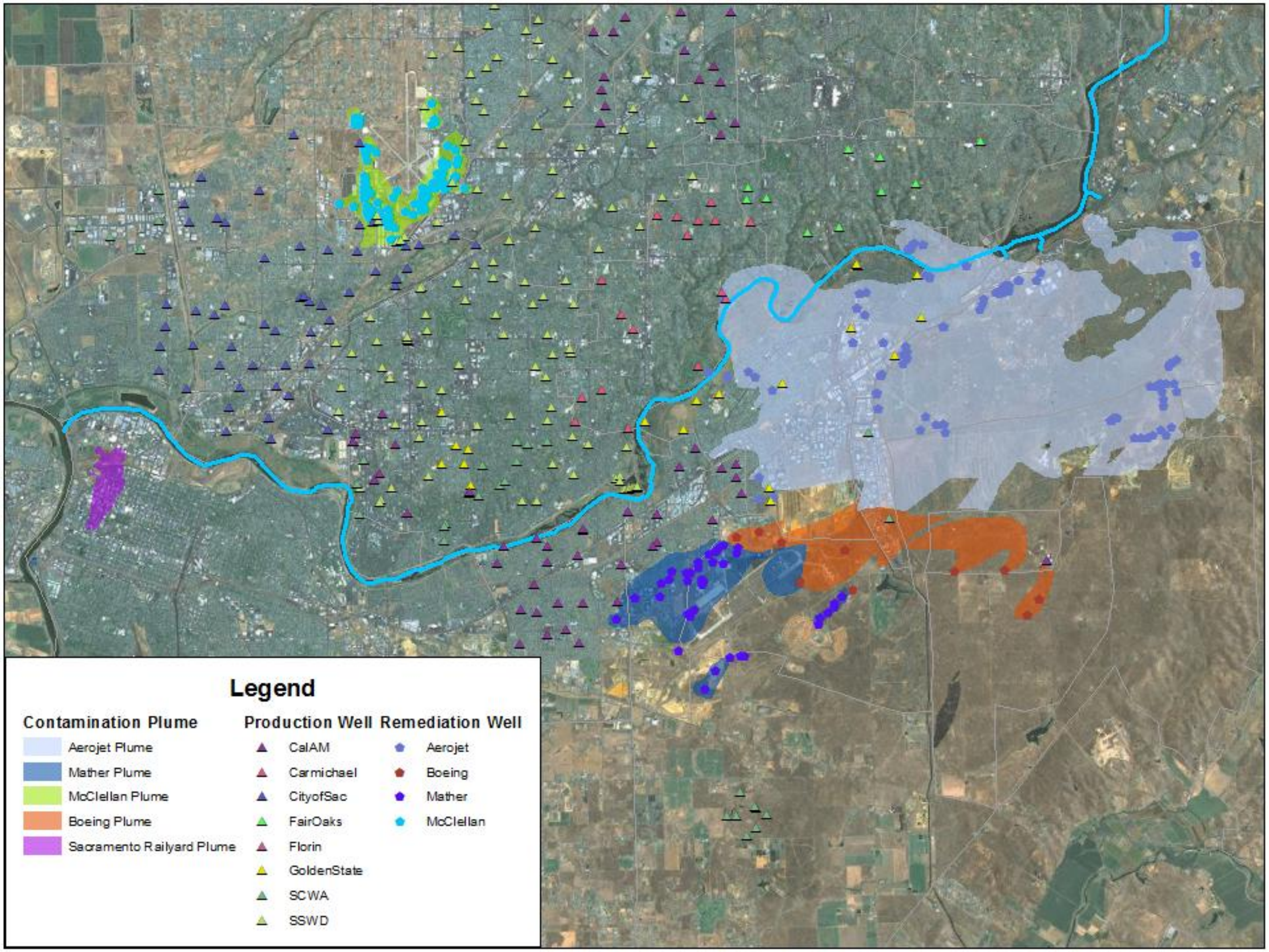


Figure 2: Regional Contamination Plumes (Based on 2007 Data) and Production/Remediation Wells

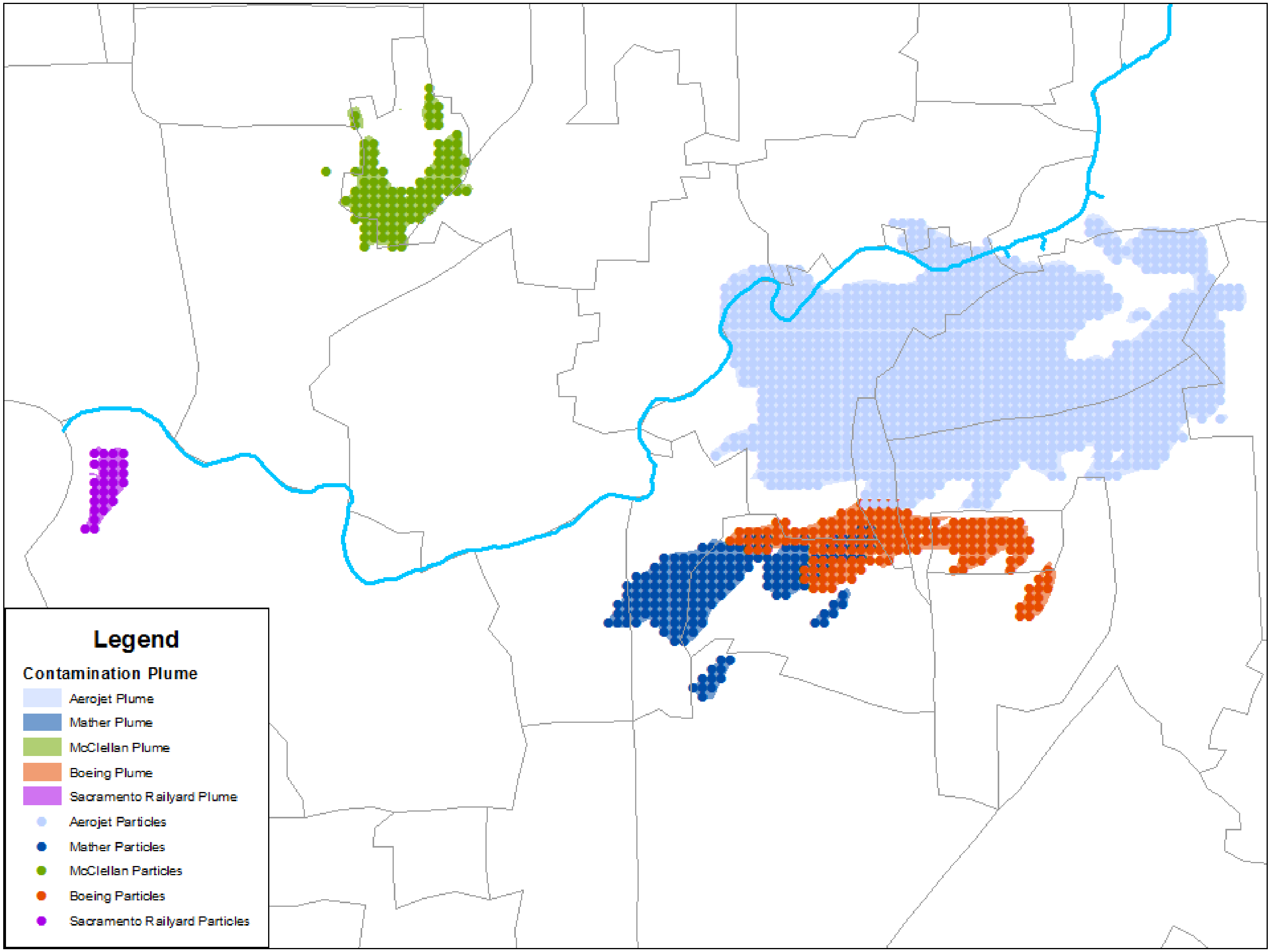


Figure 3: Contamination Plume Particles

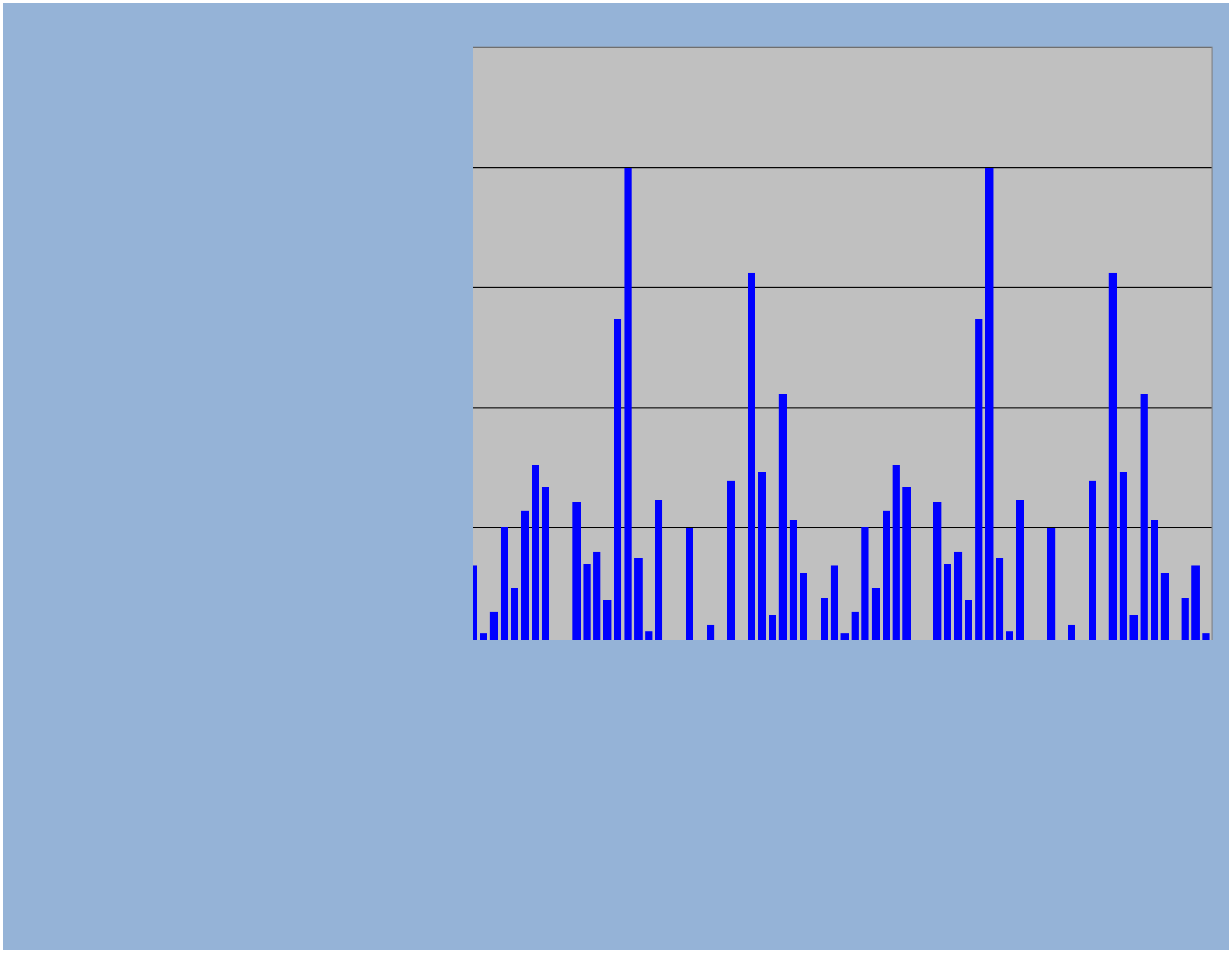


Figure 4: American River Unimpaired Inflow to Folsom Reservoir (UIFR)

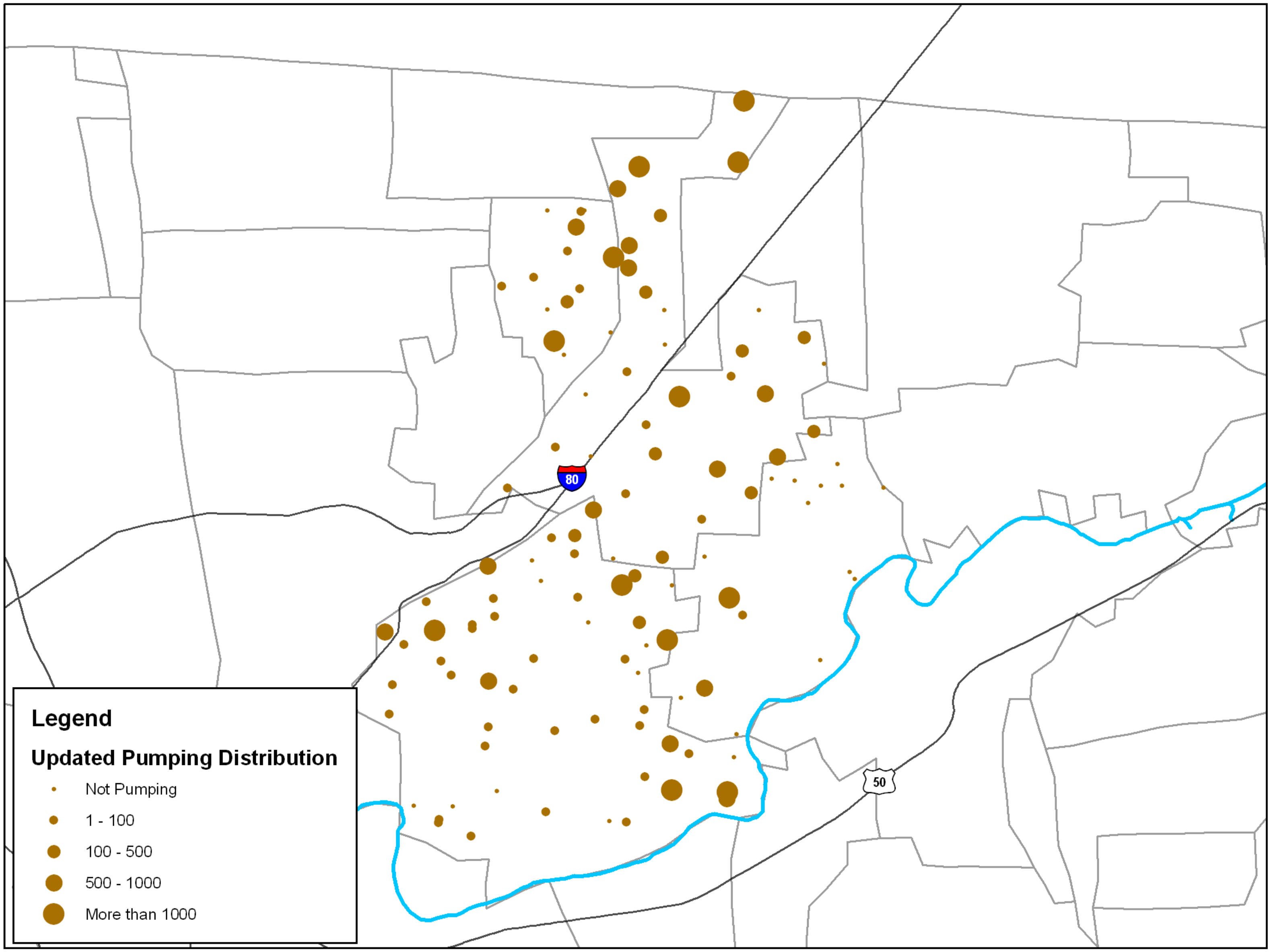


Figure 5: Updated Pumping Distribution for CWD and SSWD Wells in SacIWRM (AFY)

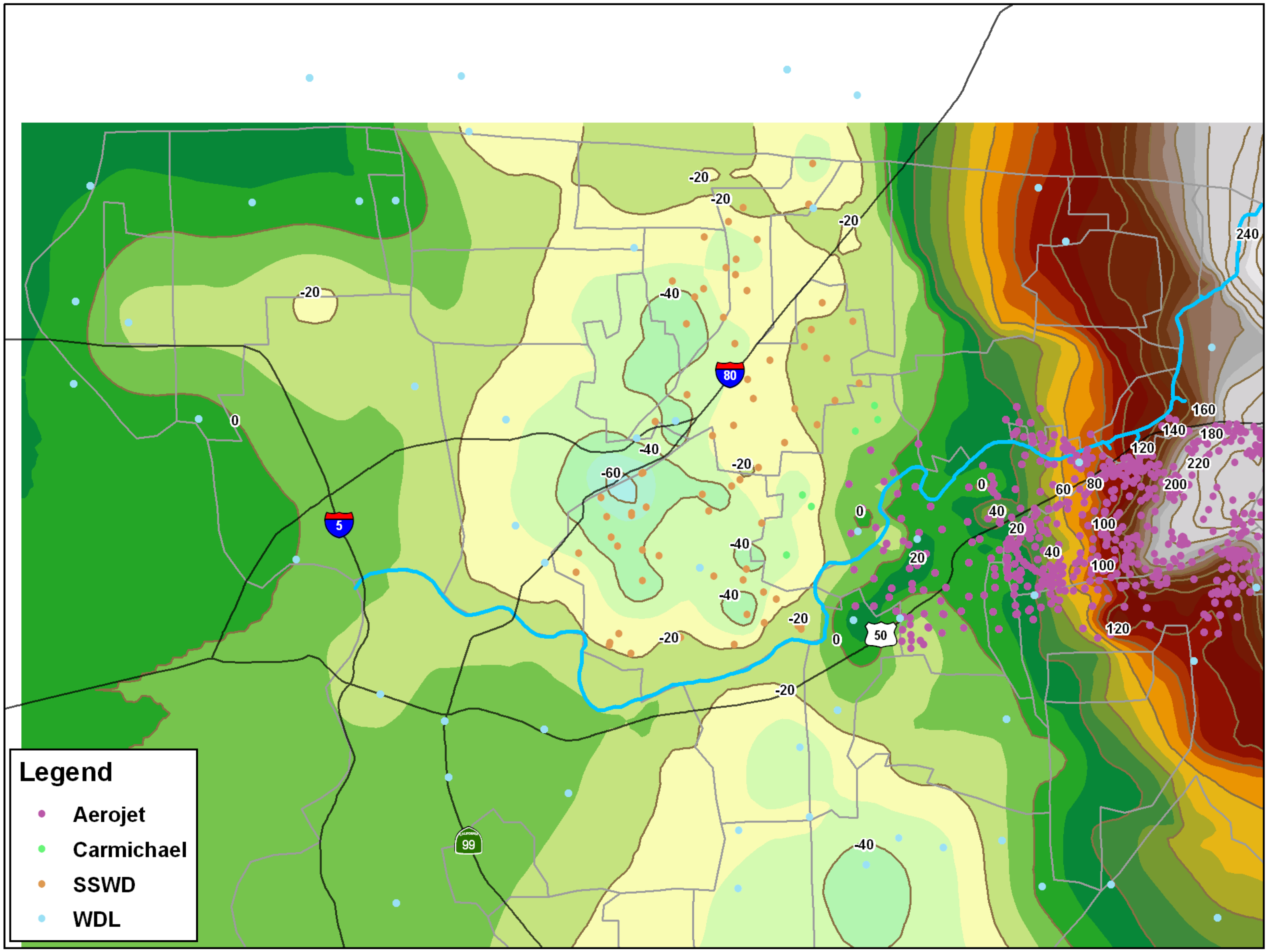


Figure 6: Updated Initial Conditions (Feet above MSL)

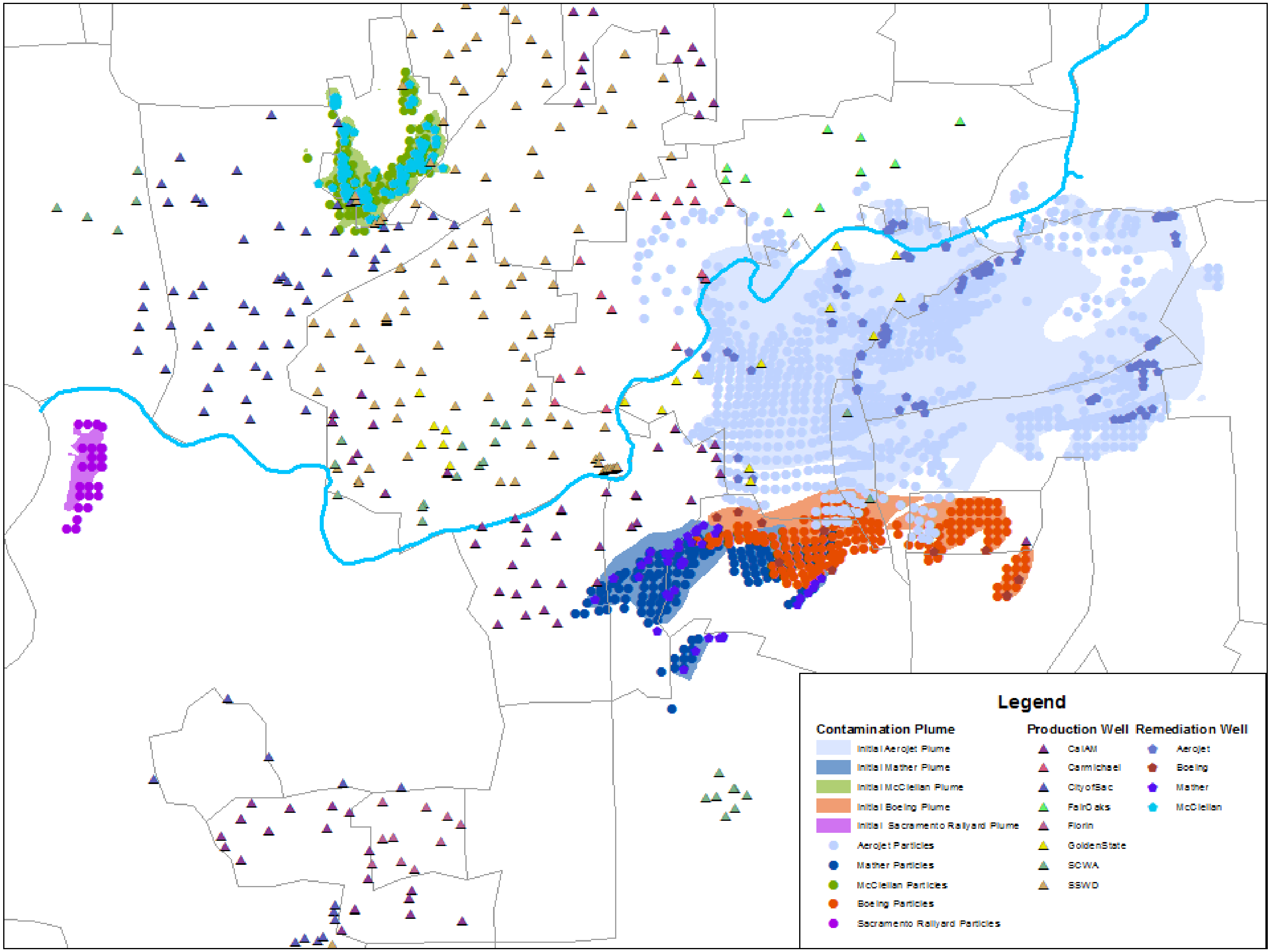


Figure 7: Contamination Plume Particles after 5 Years

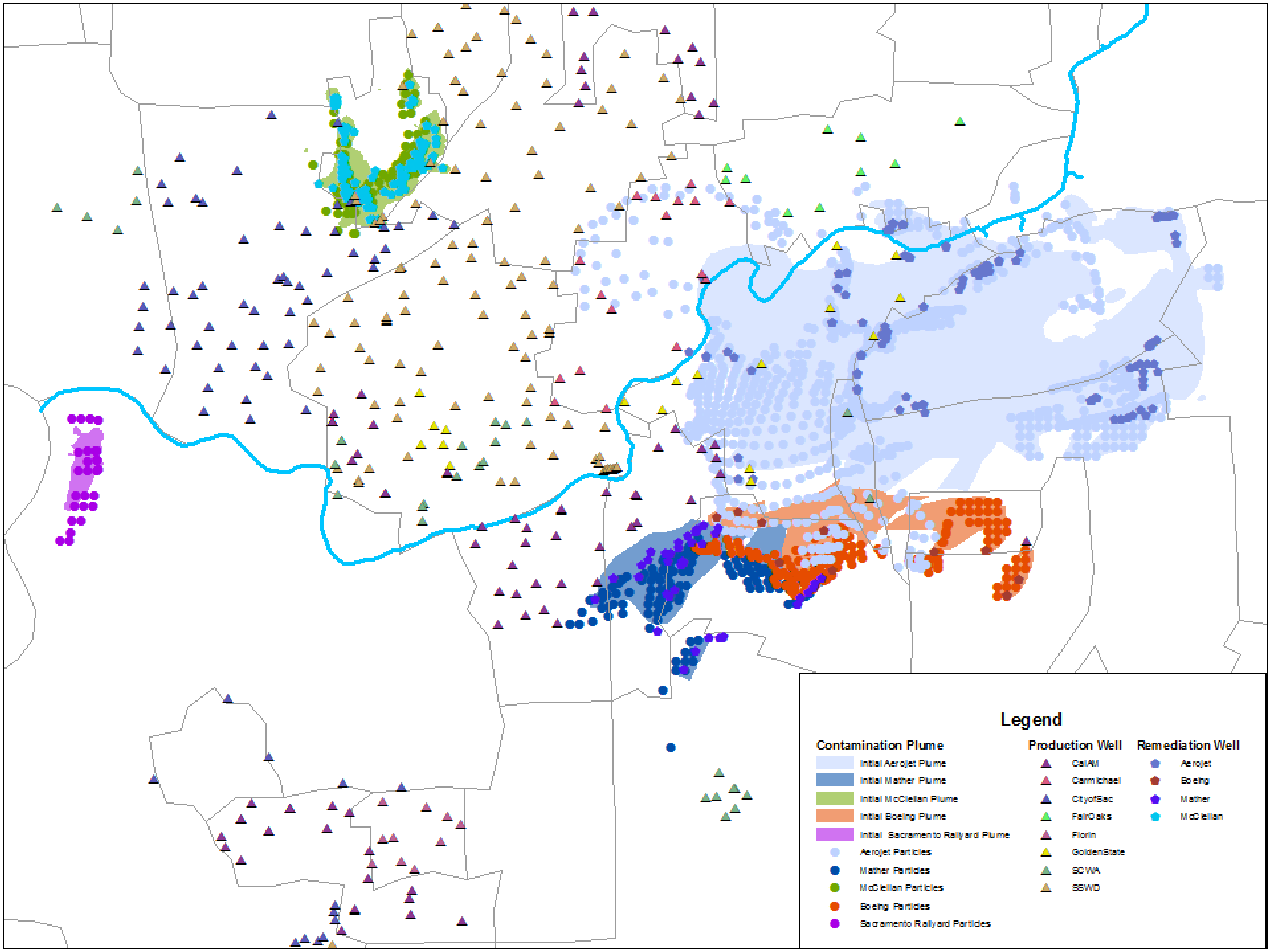


Figure 8: Contamination Plume Particles after 10 Years

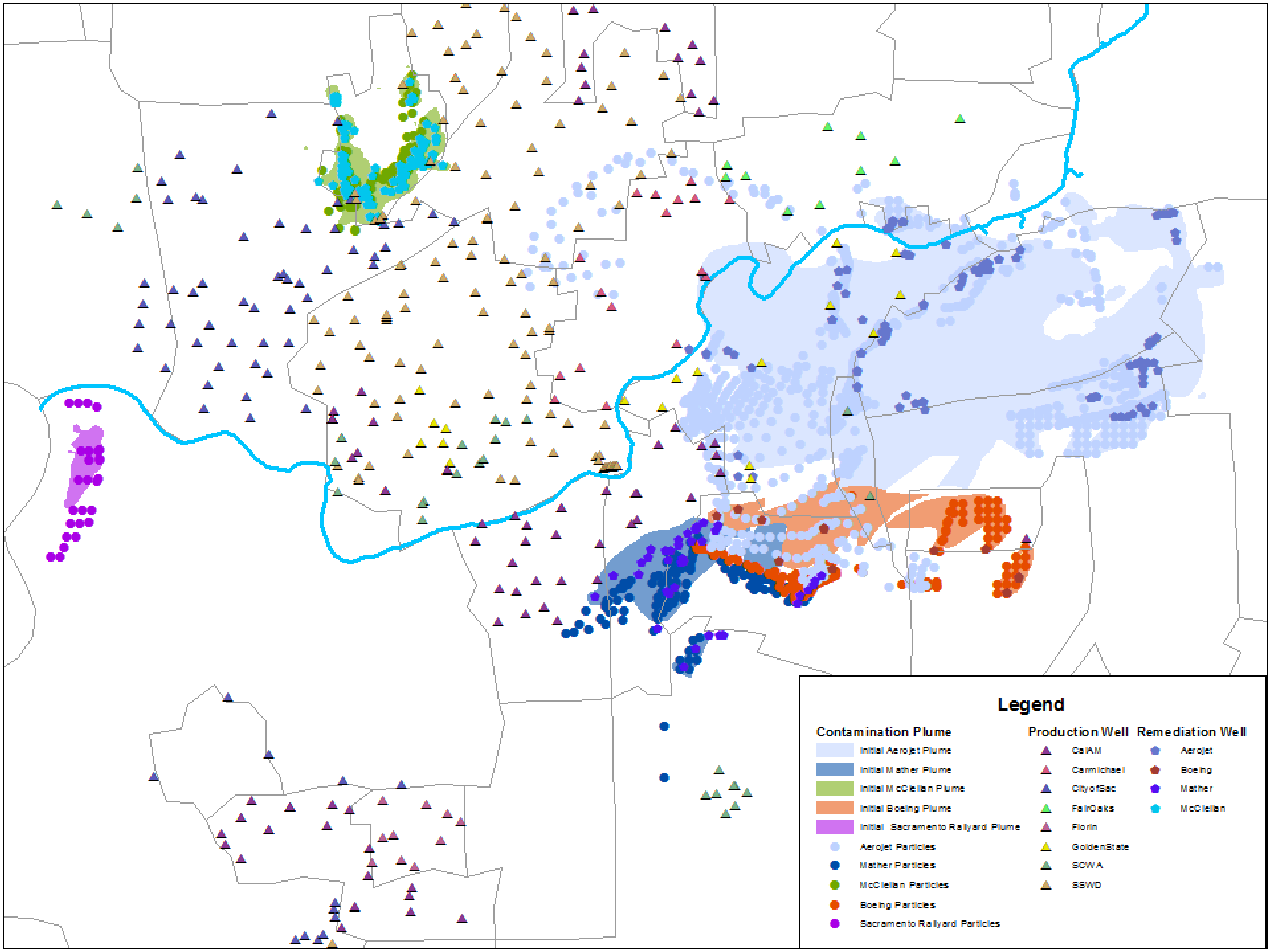


Figure 9: Contamination Plume Particles after 15 Years

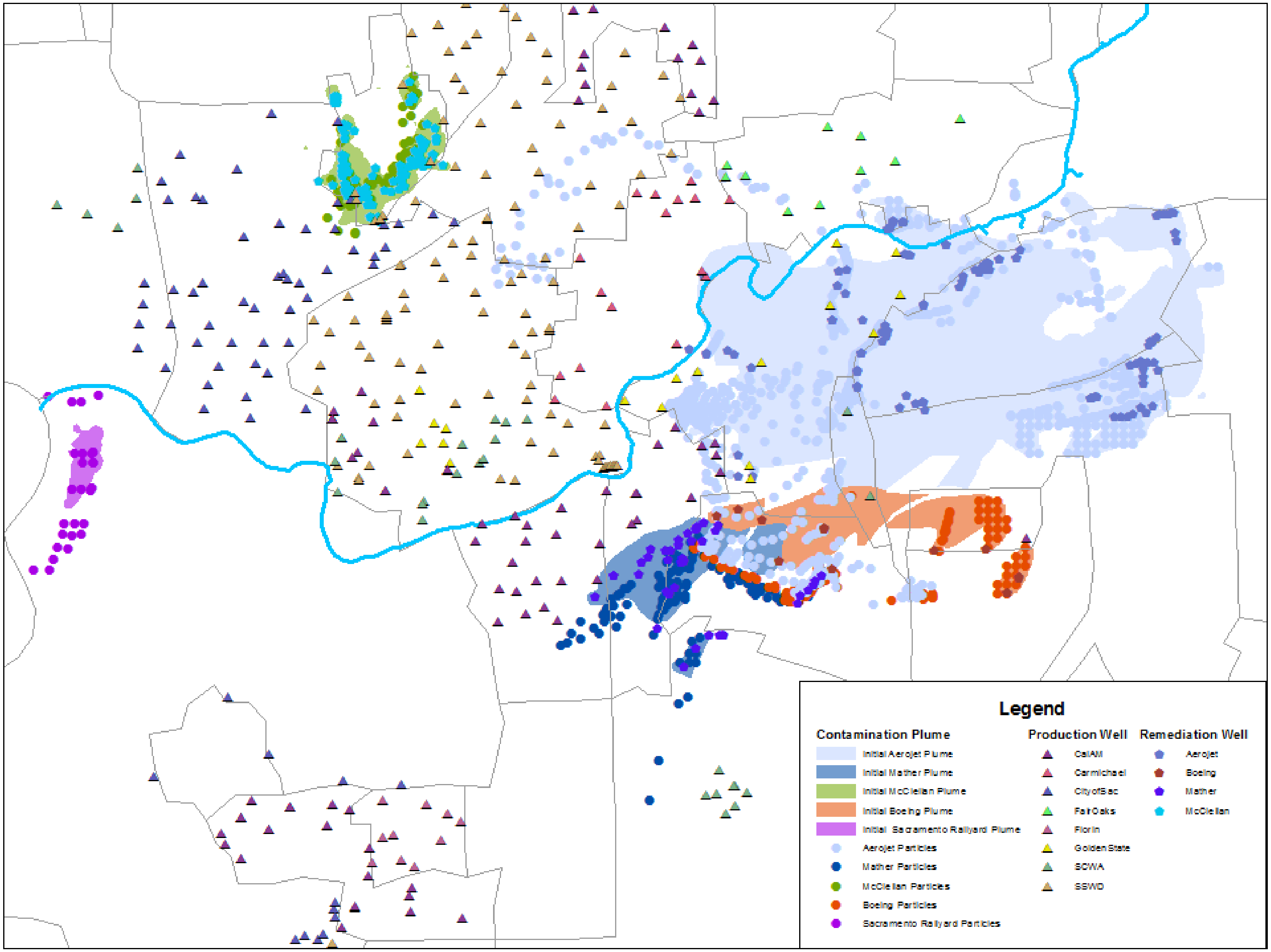


Figure 10: Contamination Plume Particles after 20 Years

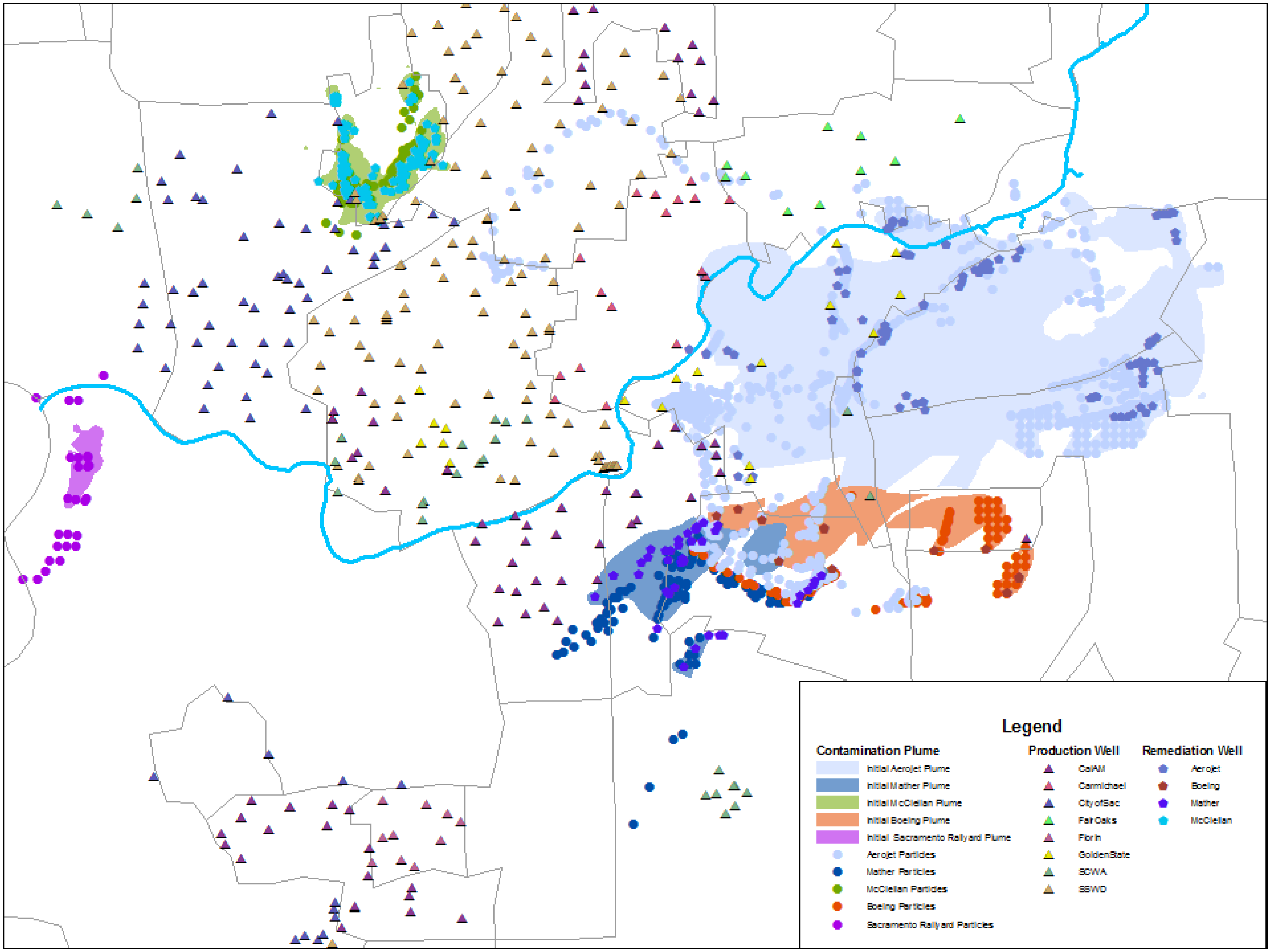


Figure 11: Contamination Plume Particles after 25 Years

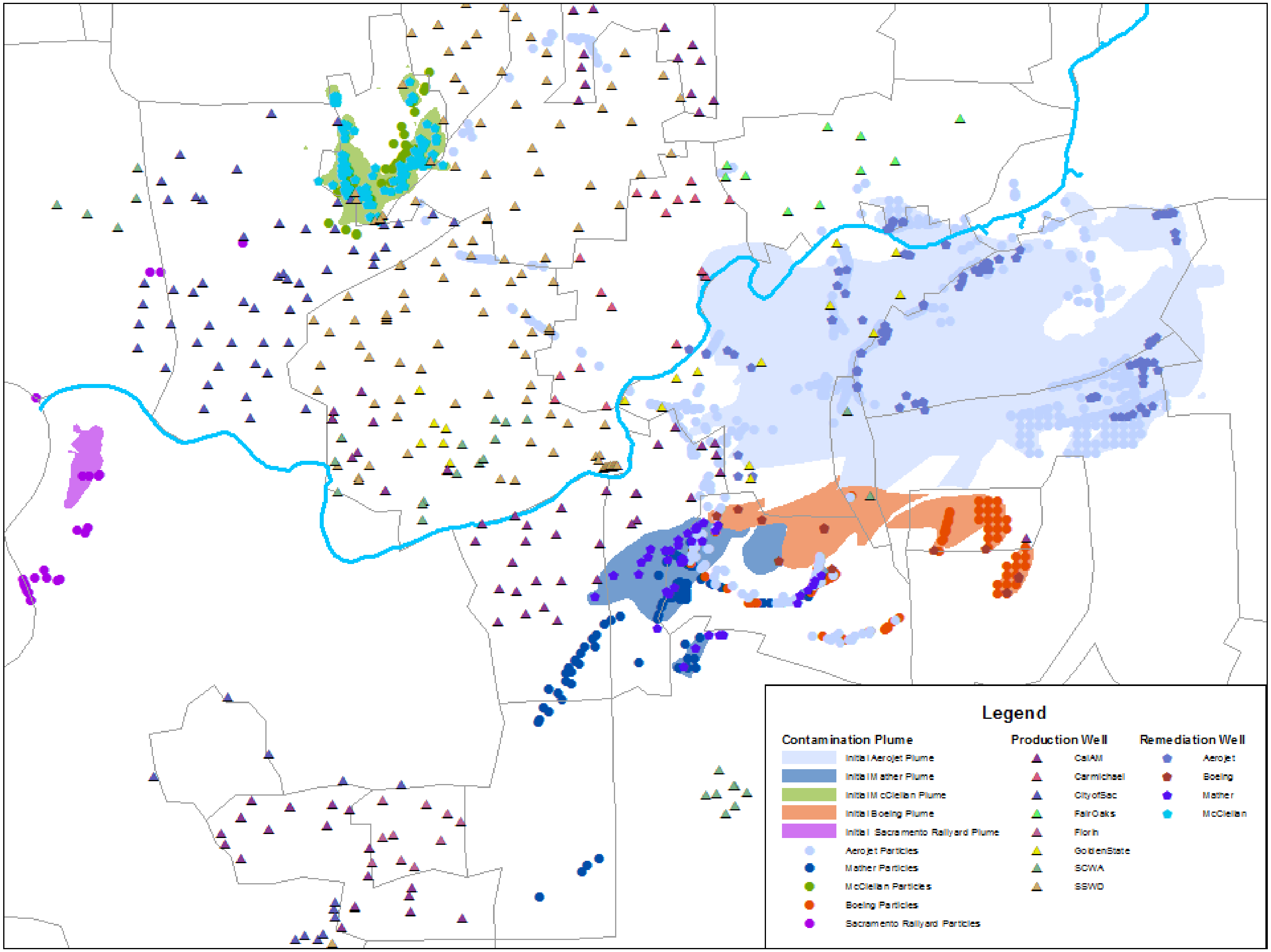


Figure 12: Contamination Plume Particles after 50 Years

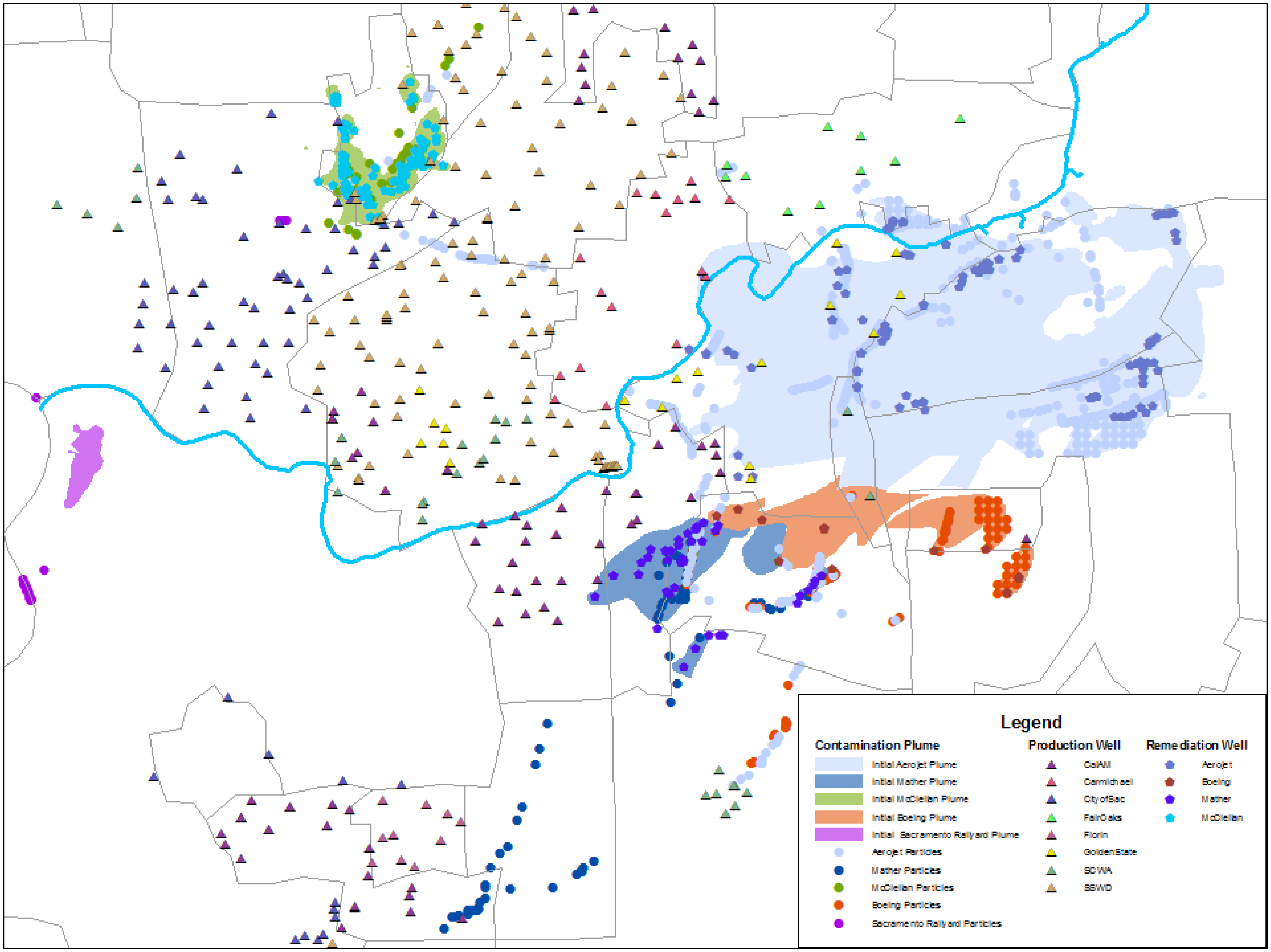


Figure 13: Contamination Plume Particles after 100 Years

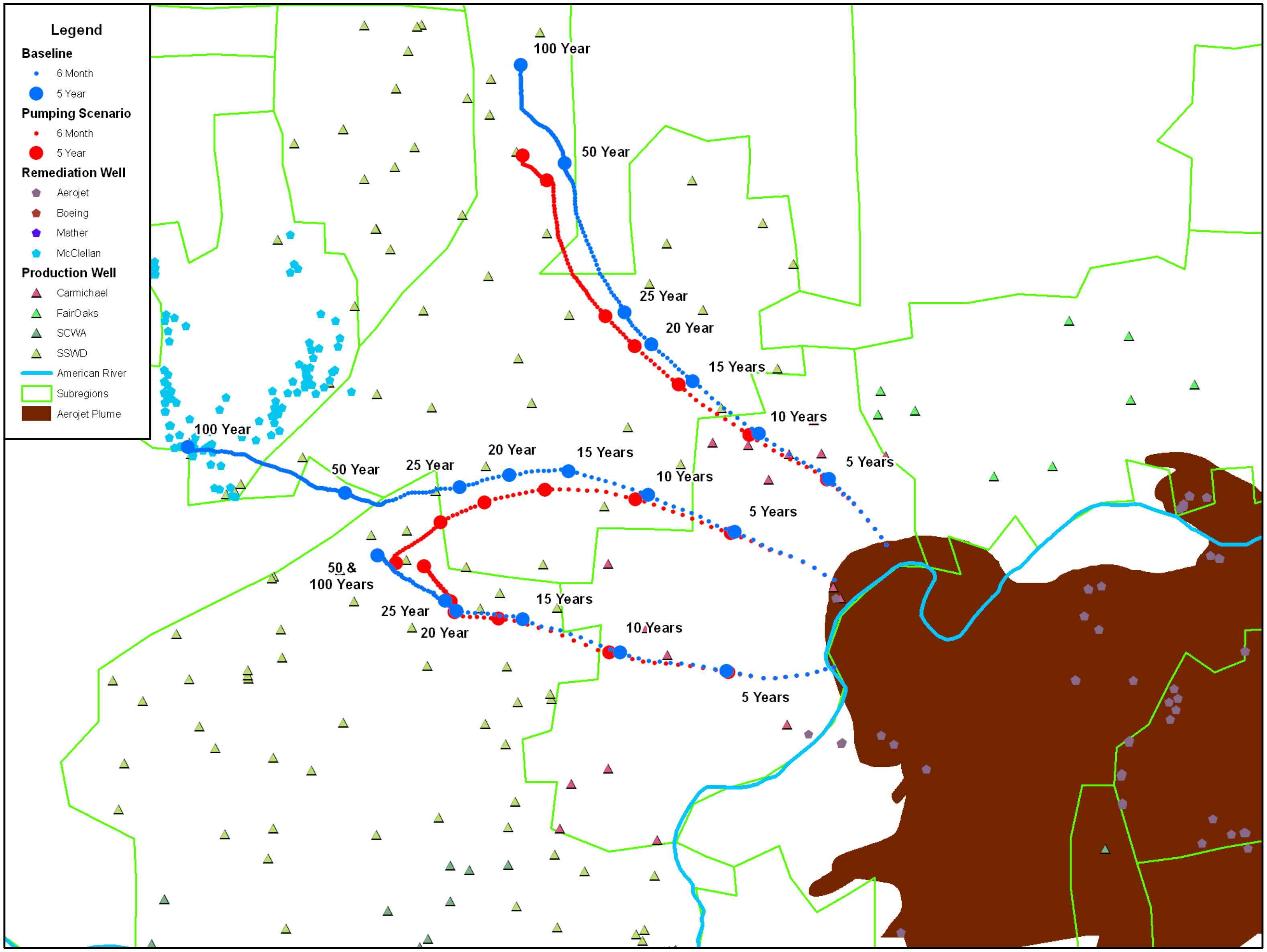


Figure 14: Aerojet Plume Capture Conditions

Table 1: Remediation Operations Simulated in SacIWRM

Facility	Extraction	Recharge via Injection	Recharge via Infiltration	Discharge	Recharge/Discharge Location
	AFY	AFY	AFY	AFY	
Aerojet	**21,240**	**0**	**3,140**	**18,100**	
Get A	640	0	640	0	Rebel Ditch
ARGET	1,900	0	0	1,900	Buffalo Creek
Get B	2,500	0	2,500	0	Rebel Ditch
Get D	1,100	0	0	1,100	Buffalo Creek
Get E/F	5,000	0	0	5,000	Buffalo Creek
Get H-A	1,600	0	0	1,600	Morrison Creek
Get J	4,000	0	0	4,000	Buffalo Creek
Get K	2,300	0	0	2,300	American River
Get L-A	600	0	0	600	American River
Get L-B	800	0	0	800	American River
WRND	800	0	0	800	Buffalo Creek
Boeing	**3,405**	**0**	**0**	**3,405**	
Get H-B	2,670	0	0	2,670	Morrison Creek
SGSA GET	735	0	0	735	Morrison Creek
Mather	**3,023**	**2,938**	**0**	**86**	
Site 7	86	0	0	86	Mather Lake
AC&W	289	289	0	0	4 on-site wells
Main	2,649	2,649	0	0	4 on-site wells
McClellan	**1,569**	**0**	**0**	**1,569**	Magpie Creek
Kiefer Landfill	**2,088**	**0**	**0**	**2,088**	N/A
Elk Grove Landfill	**36**	**0**	**0**	**36**	N/A
Army Depot	**732**	**0**	**0**	**732**	N/A
Sac Regional WWTP	**972**	**0**	**0**	**972**	N/A
Sacramento Railyard	**0**	**0**	**0**	**0**	N/A
Total	**33,065**	**2,938**	**3,140**	**26,988**	

Table 2: Summary of Groundwater Production

Pumping Scenario				
Year Type	SSWD	City of Sac	San Juan Family	**Total**
	(AFY)	(AFY)	(AFY)	**(AFY)**
Wet	44,000	20,000	2,000	**66,000**
Above Normal	44,000	20,000	2,000	**66,000**
Below Normal	44,000	20,000	2,000	**66,000**
Dry	44,000	20,000	2,000	**66,000**
Critical	44,000	20,000	2,000	**66,000**
Baseline				
Year Type	SSWD	City of Sac	San Juan Family	**Total**
	(AFY)	(AFY)	(AFY)	**(AFY)**
Wet	17,000	15,000	500	**32,500**
Above Normal	32,000	18,000	1,500	**51,500**
Below Normal	44,000	22,000	7,000	**73,000**
Dry	44,000	25,000	9,000	**78,000**
Critical	44,000	30,000	10,000	**84,000**

Table 3: Water Supply Mix (Average Annual)

Pumping Scenario			
	SW (AFY)	GW (AFY)	Demand (AFY)
SSWD	0	44,000	44,000
City of Sac	25,000	20,000	45,000
San Juan Family	42,000	2,000	44,000
Total	**67,000**	**66,000**	**133,000**
Baseline			
	SW (AFY)	GW (AFY)	Demand (AFY)
SSWD	8,657	35,343	44,000
City of Sac	24,771	20,229	45,000
San Juan Family	39,643	4,357	44,000
Total	**73,071**	**59,929**	**133,000**

Table 4: Estimated Percent Capture

Plume	Total Number of Particles	Percent Escaped After						
		5 Years	10 Years	15 Years	20 Years	25 Years	50 Years	100 Years
Aerojet Representing Plume (Detection Level)	1166	4%	4%	4%	4%	4%	5%	5%
Aerojet Representing Core Plume (above 4 ppb)	683	0%	0%	0%	0%	0%	0%	0%
Mather Plume	161	4%	7%	9%	11%	13%	17%	20%
Boeing Plume	168	0%	0%	7%	7%	7%	7%	7%
Railyard Plume	26	0%	0%	0%	0%	4%	12%	12%
McClellan Plume	98	0%	0%	0%	0%	0%	1%	3%

APPENDIX A. IWRM_PTM USER MANUAL

1. INTRODUCTION

1.1 Purpose

The purpose of this report is to provide model users with the necessary information to understand the basic operations and simulation capabilities of the Particle Tracking Model (IWRM_PTM) which serves as a post-processor for the Integrated Groundwater and Surface water Model (IWRM).

This report does not include a detailed description of the computer codes from a programming perspective. However, summary level information is provided on the theoretical foundations of IWRM_PTM along with conceptual flowchart of the model code and IWRM implementation. The report also includes a literature review of particle tracking, verification of the code, application and a brief user manual.

1.2 Overview of IWRM_PTM

IWRM_PTM is a particle tracking post-processing package that was developed to compute two-dimensional flow paths using output from steady-state or transient (as small as daily simulations steps) ground-water flow simulations by any finite difference (MODFLOW) or finite element flow model (IWRM, FEMWATER, etc.).

Once the head solutions from IWRM have been obtained at every node, the principal velocity components for each element can be computed using the finite element shape functions and Darcy's Law. In order to compute the path lines, IWRM_PTM uses constant velocity throughout the element to compute particle paths.

IWRM_PTM uses a technique (in-element particle tracking) that traces particles on an element-by-element basis. Given a velocity field, a particle is traced one element by one element until either a boundary, an internal sink/ source is encountered or the available time is completely consumed.

Data input for IWRM_PTM is a combination of data files. IWRM_PTM can compute paths for imaginary particles moving through the simulated ground-water system. In addition to computing particle paths, the model can keep track of the travel time for particles moving through the system. By carefully defining the starting locations of particles, it is possible to perform a wide range of analyses such as delineating capture and recharge areas. Below is a summary table for IWRM_PTM.

Table 1: Summary of IWRM_PTM

		IWRM_PTM
Discretization		Triangular and quadrilateral elements for complicated geometries (and boundaries)
Methodology	**Heads**	calculated at the nodes
	Velocity	calculated for the element and constant within the cell
	Tracking	element-by-element basis
Simulation Type		steady-state or transient-state (daily, monthly, yearly)

Direction of Particle Tracking Computation	forward or backward
Capabilities	computing particle paths keep track of the time of travel delineating capture and recharge areas track multiple particles
Starting Locations & Times	specify starting locations from a file specify a release time for particles from a file
Criteria for Stopping Particles	reaches an external boundary or internal sink/source cell that captures the particle enters a cell with special zone code that is designated as a stopping point is stranded in a dry cell still active at a user-specified stopping time
Output Mode	endpoint mode (initial and final locations) time series mode (locations at all time intervals) element mode (number of particles in elements at specified time steps) pathline mode (locations computed at specific or all time steps for a particle) velocity direction mode (element velocities, directions and magnitudes at specified time step
Limitations	constant velocity within the element the accuracy of velocity calculations the ability to accurately and unambiguously represent internal sinks

1.3 Organization of the Report

Section 1 Introduction: presents the purpose of the report and model overview

Section 2 Literature Review: review of the literature for finite element and finite difference particle tracking methods and models

Section 3 Theoretical Background: presents the summary level theories of numerical methods to track a particle

Section 4 IWRM Implementation: describes what specific issues encountered in implementing IWRM_PTM to IWRM code, what changes were made to IWRM flow code, how IWRM_PTM is organized and a conceptual flowchart of the main program

Section 5 Code Verification: presents two example problems, one analytical and one from MODFLOW user manual, to verify the code

Section 6 Application: represents application of the code to the Sacramento Model and Aerojet Area

Section 7 Program Description: provides documentation for the goals of the program, hardware requirements, array dimension limitations, variable definitions, program file structure, brief explanation of main program and subroutines, description of input/ output files and graphical output options.

2. LITERATURE REVIEW

Particle tracking codes are valuable for post-processing the results of conventional flow models (e.g., MODPATH(Pollock, 1994) for MODFLOW or Particle Tracking Module of GMS for FEMWATER (Yeh, et. al., 1997)) or for visualization of measured velocities or velocities calculated in a flow model. Tracking a particle in a known velocity field results in its path line. An assembly of path lines marked at regular time intervals provides visual information on travel times and flow directions.

Particle tracking models are widely used for either just flow visualization or for simulation of contaminant transport. Advection based concentration (Lagrangian concentration) in solution of advection-dispersion equations is computed by using a particle tracking technique for Eulerian-Lagrangian methods. Therefore, the theory for particle tracking will differ depending on the Eulerian technique, finite difference (FD) or finite element (FEM), used to solve the flow equation or dispersion equation.

MODPATH (Pollock, 1994) is the most popular finite difference particle tracking model available in the literature. MODPATH is a particle tracking code that is used in conjunction with MODFLOW, the U.S. Geological Survey finite-difference ground-water flow model. After running a MODFLOW simulation, the user can designate the location of a set of particles. The particles are then tracked through time assuming they are transported by advection using the flow field computed by MODFLOW. Particles can be tracked either forward in time or backward in time.

MODPATH uses a semi-analytical particle tracking scheme that allows an analytical expression of the particle's flow path to be obtained within each finite-difference grid cell. Particle paths are computed by tracking particles from one cell to the next until the particle reaches a termination criterion. Both steady-state and transient ground-water flow systems can be analyzed with MODPATH.

The biggest limitation of MODPATH is that it cannot be used for other types of numerical approximations of the flow equation, such as finite element models. And also due to finite element formulation, level of detail at which hydrogeologic and system boundaries can be represented are limited. It shares some other limitations of the other particle tracking models such as the accuracy of velocity calculations, and the ability to accurately and unambiguously represent internal sinks.

The in-element particle tracking technique developed by Cheng et al (1996), using an implicit trapezoidal ODE solver to accurately and efficiently trace fictitious particles in the velocity fields, is the basis for particle tracking module of most popular FEM flow or transport models like FEMWATER and FEFLOW (Diersch, 2002).

The technique, named ‘in-element’ particle tracking, traces fictitious particles on an element-by-element basis. Given a velocity field, a fictitious particle is traced one element by one element until either a boundary is encountered or the available time is completely consumed.

This technique also shares the common limitations mentioned above and one common limitation of this method is that this method yields a generally non-conservative flow field at element boundaries and nodal points if the variation of h is other than linear or constant. Despite this disadvantage FEM models are rather popular due to their capability of handling complex geometries.

FEMWATER uses particle tracking for computing advection based concentration in transport module. In order to use its particle tracking module it has to be used in GMS Model in which particle tracking is steady state only. That is, the particles are only influenced by the active time step. In order to use FEFLOW or FEMWATER’s particle tracking module, the whole model should be bought and your input files should be compatible with FEFLOW or GMS, respectively.

3. THEORETICAL BACKGROUND

The particle tracking algorithm used by IWRM_PTM is an extension of Cheng's method (Cheng et al, 1996) as like other numerous existing techniques. In our algorithm tracking is performed in global coordinates, element by element. The exit from an element is starting point for the next one.

The model can track multiple particles with varying starting and ending times either in backward or forward direction. The model also is capable of doing steady state or transient state simulations.

Velocities are calculated using the head values computed from IWRM by the help of the finite element shape functions and Darcy's law. One has to find the point where the particle exits from an element in order to find the next element. In global coordinates the exit point is at the intersection of a linear path line with the straight side of the element.

The algorithm starts from a known initial position $P(X_p,Yp)$, and consists of solving the equation for a path line in global coordinates until the particle exits the element. Once the exit from the element is found it becomes a starting point for the next element and the tracking proceeds in the same fashion until the whole tracking time is reached or the particle has left the flow domain. Therefore the algorithm consists of the following steps:

For convenience, forward particle tracking is considered in the following description. If all velocity terms are multiplied by -1, the tracking algorithm can be operated "in reverse" to track particles backwards along their path lines.

Action 1. Start tracking a particle:

No matter how many particles are considered, each particle can be traced independently.

Action 2. Determine the starting element, say element EP, starting location for the particle and assign the element velocities:

By considering the starting coordinates for the particle, $P(X_p,Yp)$,element configuration data and nodal coordinates data, the starting element and the starting location can be determined. Starting location can be on one of the nodes of the element, it can be on the face of an element or it can be a random point within the element. The tracking will be different for different stating locations. Also, assign element velocities for the current tracking time.

Action 3. Compute the particle tracking in element EP

To compute the particle tracking in an element, the following two steps are taken:

Step 1. Determine the element side on which the particle will end up. This can be accomplished under the consideration explained below.

Determination of the element side where the particle would leave the element in a two-dimensional domain.

As shown in Figure 1, point P is on line L which is determined by points **A** and P. Point **A** represents an element node and P is the starting point. Given the locations and the velocities at both points A and P, the quantity, *Det*, shown in Figure 1 is computed as follows.

Let

$$\Delta X = X_A - X_P \tag{1}$$

$$\Delta Y = Y_A - Y_P \tag{2}$$

then

$$Det = \Delta X \cdot VY - \Delta Y \cdot VX \tag{3}$$

where VX and VY are the velocities in x and y directions respectively for the given element.

By computing Det, the location of point Q, projected end point, can be determined as indicated in Figure 1**.** In a two-dimensional space, we may use quadrilateral and/ or triangular elements to discretize the domain of interest when the finite element method is employed. Point P can be (1) an element node, (2) a point on a side of an element, or (3) a point inside an element during the process of the 'in-element' particle tracking. If the starting point is on an element side, the side will not be eligible to be the ending side. For instance, two element sides are not eligible to be the ending side of the quadrilateral element if point P is a node of the element, while there is one side not eligible for the case of a side point and all sides are eligible for the case of an interior point.

As described above, we can examine the location of the ending point relative to a given line which contains the starting point. Thus, we also can determine whether or not an eligible element side is the ending side by computing the values of Det associated with the two lines determined by the starting point and the two end points of the element side. The two lines are treated the same as line L in Figure 1**.**

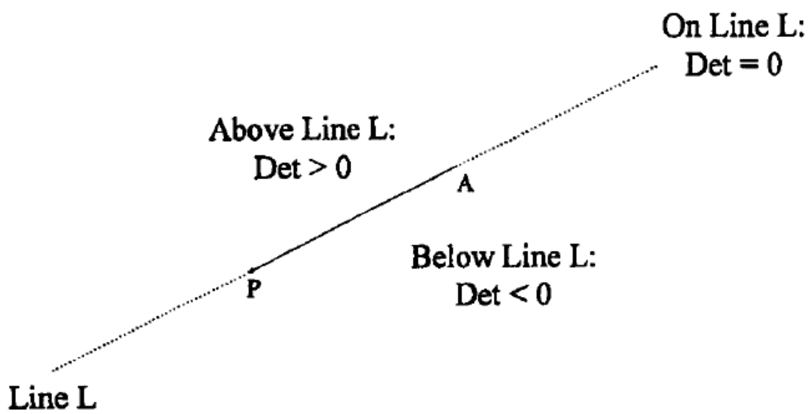


Figure 1: The determination of the tracking direction of fictitious particle in a 2-D space

Step 2. Locate the ending point on the ending side. The basic concept involved in this determination is that the coordinates of the ending point can be interpolated from those of the nodes of the ending side. Thus, there are interpolation parameters to be computed, such that the ending point can be described through interpolation. The interpolation parameters are computed based on the linear velocity-displacement relationship as follows.

For a two-dimension particle tracking path, the ending side is a line segment. Let points 1 and 2 are the end points of this line segment.

Then, the following equations can be written by using linear interpolation:

$$X_Q = X_1 \cdot \xi + X_2 \cdot (1-\xi) = \xi \cdot (X_1 - X_2) + X_2 \tag{4}$$

$$Y_Q = Y_1 \cdot \xi + Y_2 \cdot (1-\xi) = \xi \cdot (Y_1 - Y_2) + Y_2 \tag{5}$$

where ξ is the interpolation parameter used to locate projected end point Q. According to velocity displacement relationship, the following equations can be stated.

$$X_Q - X_p = \Delta t \cdot VX \tag{6}$$

$$Y_Q - Y_p = \Delta t \cdot VY \tag{7}$$

Equating Δt, which is time increment, in both of the equations and replacing $\boldsymbol{X_Q}$ and $\boldsymbol{Y_Q}$ as defined above; one can obtain the interpolation parameter as

$$\xi = \frac{(Y_2 - Y_P) - (X_2 - X_P)VY}{(X_1 - X_2)VY - (Y_1 - Y_2)VX} \tag{8}$$

After computing ξ ($\xi \in [0,1]$)to satisfy both equations (6) and (7) the location of point Q can be calculated using equations (4) and (5). The time consumed for the particle to move along this particle tracking path is then calculated using either equation (6) or (7).

Judgment 1: Is the consumed time smaller than the time increment?

If the consumed time is larger than the time increment, the time increment is the real tracking time for this path and point Q is located as follows.

$$X_Q = X_P + (X_Q - X_P) \cdot \frac{\delta t}{\Delta t} \tag{9}$$

$$Y_Q = Y_P + (Y_Q - Y_P) \cdot \frac{\delta t}{\Delta t} \tag{10}$$

Then, update the starting location P with point Q..

Judgment 2: Is the total tracking time completely exhausted before the particle reaches the element face or edge?

This can be examined by comparing the tracking time with the total tracking time of the particle. If the total tracking time is completely consumed, then the particle has reached the end of tracking. Otherwise, the tracking time is updated by adding time increment to the tracking time, and the next tracking is to proceed from the beginning of Action 3.

Continue with Judgment 1:

If the consumed time is smaller than the time increment, then time increment is updated by using its prior value minus the consumed time.

Action** 4. **Determine the next element, say element** EQ, **which the particle will pass through:

By considering the connectivity list of the elements, the neighboring element that contains the side crossed by the particle can be found.

Judgment 3: Is the particle out of boundary?

If the particle is located on an element side which is on the boundary and the velocity is outward on this boundary, the particle will go out of boundary and end of tracking for that particle has reached.

Judgment 4: Is the new element a strong sink or a special element to stop particle tracking or has zero velocity?

Check if the new element EP is a strong sink or is defined as a special element or has zero velocity. If at least one is satisfied, stop tracking for that particle. Else if continue tracking Action 5.

Action 5. Let EP = EQ:

Update the working element to continue the particle tracking. Reassign the element velocities for the current tracking time to continue the particle tracking And go back to action 3.

Action 6. End tracking a particle:

The end of tracking a particle is reached.

4. IWRM IMPLEMENTATION

The model structure depicting the inter-relationship among IGS_F1, IWRM_F21, IWRM_Q1, and IWRM_PTM is shown in figure 2.

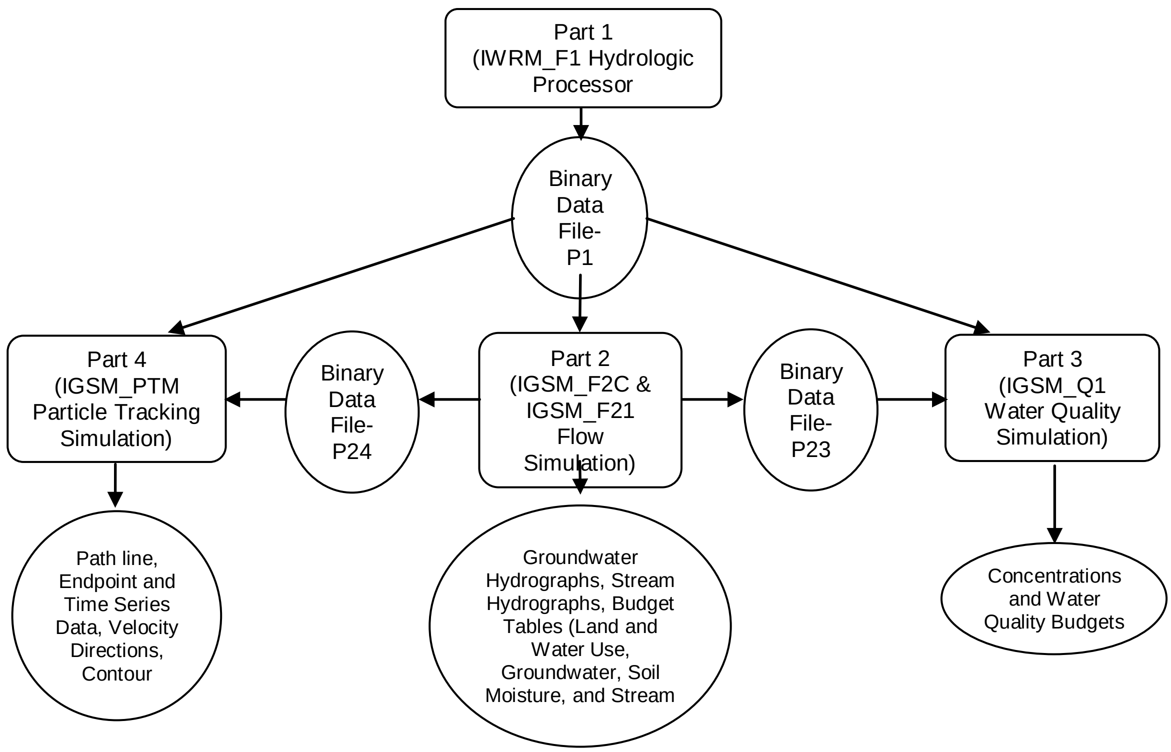


Figure 2 : Model Structure for IWRM

4.1 Issues Encountered in Implementing IWRM_PTM to IWRM Code

In order to develop and run IGMS_PTM as a post processor for IWRM, the following are needed from IWRM.

- Element configuration data
- Nodal coordinates data
- Calculated head values and porosities at all nodes at every time step or velocities for all elements at every time step calculated through Darcy's Law using the nodal heads and porosities.

Among these, first two were decided to be read from the binary file produced after IWRM Part 1 simulations. Subroutines GETG and NODECONF of were adapted to IGMS_PTM code to read these data and prepare the connectivity arrays between the nodes and elements. The third one was taken care of by calculating element velocities in IWRM Part 2 code, then writing the calculated values on a binary file for each time step and finally reading them from the same binary file in the IGMS_PTM code. The details of the velocity calculation in IWRM will be explained in the next section.

Darcy velocity fields obtained from finite element solutions of heads in groundwater flow exhibit discontinuities at element boundaries even if they are calculated at all nodal points. Several methods have been developed to resolve those inaccuracies, mixed hybrid finite element formulations, and stream function formulations. All of these techniques either lead to a considerable increase in the computational effort or are not general enough for all purposes (Cordes and Kinzelbach, 1992). As a result, the biggest challenge in calculating the velocities was to decide whether to calculate the velocities at all the nodes or calculate one velocity for each element that will be constant throughout the element. If there are discontinuity problems with nodal velocity calculations, the problem should be more severe in element velocity calculations. However, IWRM is capable of doing simulations with time steps as small as daily. For a transient simulation with such a small time step, computational effort becomes a bigger problem. On the bright side having a simulation with a daily step makes the effect of inaccuracies and discontinuities negligible. As a result, we decided to calculate velocities for every element rather than the nodes.

4.2 Theoretical Background of Velocity Calculations

For particle tracking purposes we are interested in the pore velocity that a fictitious particle would experience if carried by the fluid through the formation. Pore velocity can be obtained by diving Darcy flux by porosity as

$$V = \frac{K}{\phi} \cdot \nabla h \tag{11}$$

where V is the pore velocity, K is the hydraulic conductivity, ϕ porosity and h is the hydraulic head.

In most finite element work, the Darcy velocity components given in Equation (11) can be calculated numerically by taking the derivatives of the simulated h as

$$V = \frac{K}{\phi} \cdot \sum_{j=1}^{N} (\nabla N_j) h_j \tag{12}$$

where h_j is the amplitude of h at nodal point j, N is the total number of nodes in an element, and N_j is the base function at nodal point j.

For a triangular element the equation (12) can be written explicitly in x and y directions as follows

$$V_x = \frac{K}{\phi} \cdot \left(\frac{\partial N_1}{\partial x} h_1 + \frac{\partial N_2}{\partial x} h_2 + \frac{\partial N_3}{\partial x} h_3 \right) \tag{13}$$

$$V_Y = \frac{K}{\phi} \cdot \left(\frac{\partial N_1}{\partial y} h_1 + \frac{\partial N_2}{\partial y} h_2 + \frac{\partial N_3}{\partial y} h_3 \right) \tag{14}$$

where $\frac{\partial N_1}{\partial x}, \frac{\partial N_2}{\partial x}, .., \frac{\partial N_3}{\partial x}, \frac{\partial N_3}{\partial y}$ are the global derivatives of the base functions at the nodal points defined as

$$\begin{bmatrix}\dfrac{\partial N_1}{\partial x}\\ \dfrac{\partial N_1}{\partial y}\end{bmatrix}=\begin{bmatrix}\dfrac{1}{2A}(y_2-y_3)\\ \dfrac{1}{2A}(x_3-x_2)\end{bmatrix},\quad \begin{bmatrix}\dfrac{\partial N_2}{\partial x}\\ \dfrac{\partial N_2}{\partial y}\end{bmatrix}=\begin{bmatrix}\dfrac{1}{2A}(y_3-y_1)\\ \dfrac{1}{2A}(x_1-x_3)\end{bmatrix},\quad \begin{bmatrix}\dfrac{\partial N_3}{\partial x}\\ \dfrac{\partial N_3}{\partial y}\end{bmatrix}=\begin{bmatrix}\dfrac{1}{2A}(y_1-y_2)\\ \dfrac{1}{2A}(x_2-x_1)\end{bmatrix} \tag{15}$$

where A is the area of the triangular element and x_1, y_1, … , x_3, y_3 are the global coordinates of the nodal points. The details of obtaining the global derivatives for linear triangular elements are discussed in Lapidus and Pinder (1982). After substituting equation (15) into equations (13) and (14), one can obtain final form of the velocity calculations in x and y directions as follows

$$V_x=\frac{K}{2A\phi}\cdot\left[(y_2-y_3)h_1+(y_3-y_1)h_2+(y_1-y_2)h_3\right] \tag{16}$$

$$V_y=\frac{K}{2A\phi}\cdot\left[(x_3-x_2)h_1+(x_1-x_3)h_2+(x_2-x_1)h_3\right] \tag{17}$$

A rectangular element can be considered of consisting of two triangular elements. The velocity components for these triangular elements can be found as described above and the velocity components for a rectangular element can be obtained by summing up these values as

$$V_x=\frac{K}{2A\phi}\cdot\left[(y_2-y_4)(h_1-h_3)+(y_3-y_1)(h_2-h_4)\right] \tag{18}$$

$$V_y=\frac{K}{2A\phi}\cdot\left[(x_4-x_2)(h_1-h_3)+(x_1-x_3)(h_2-h_4)\right] \tag{19}$$

4.3 Flow Chart for IWRM_PTM

The flow chart for IWRM_PTM is presented in Figure 3 as described in Section 3.

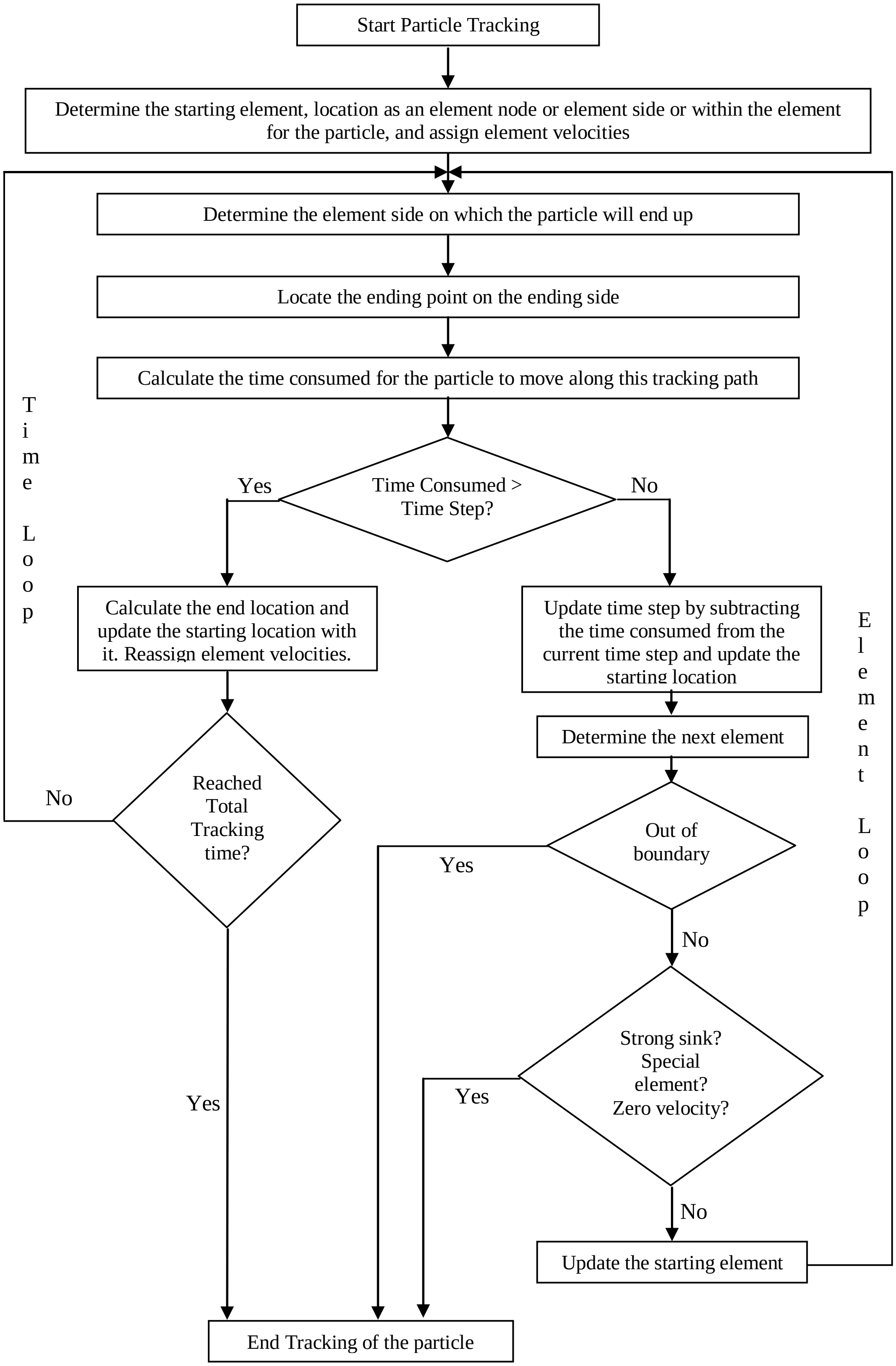


Figure 3: Flow chart for IWRM_PTM

4.4 Changes Made to IGSM Flow Code

In order to calculate and write the element velocities the following changes were made to the IGSM code

- A new binary file with file number 55 was added to the IN2 file.
- Subroutine READCD was modified to accept the new binary file 55
- Modified subroutine OUTFILE to open a binary file and assign the name from the IN2 file.
- A variable EKS was added to subroutine GETGD to define the coefficient in front of the velocity calculations ($K / 2A\phi$).
- Created subroutine WRITEVEL at the end of IGSMSUB to calculate and write the velocities for each element at the end of the time loop as explained above
- Updated subroutines IGSM_F21 and IGSM_F22 to call the subroutine WRITEVEL at the end of each time step if the binary file is necessary. If the name of the new binary file is blank, the output control option KOUTPT will be set to 0 and WRITEVEL won't be called.

5. CODE VERIFICATION

In order to verify and test if the model is working, two example cases were chosen. First one is a simple example from Cheng et al, 1996 which has an analytical solution. This example will be used to see if the basic concepts of the model are working properly. Second example is one of the sample problems from MODPATH User Manual. It is a moderately complex example to verify IWRM_PTM and compare its results with MODPATH. These 2 examples together with the next section should help to illustrate basic types of analyses and graphical outputs by IWRM_PTM

Below are the problem definitions and numerical solutions for the example cases with the necessary plots to compare the numerical results.

5.1 Example 1. A two-dimensional particle tracking

A two-dimensional particle tracking is performed under the following flow field:

$$V_X = \frac{-\pi Y}{500} \qquad \text{and} \qquad V_y = \frac{\pi X}{500} \tag{20}$$

A region of [-3000, 3000] x [-3000, 3000] is discretized with 36 elements and 49 nodes. Each element is rectangular with a size of 1000 x 1000. The fictitious particle to be tracked is originally at (0,2000). After a tracking-time period of 500, the fictitious particle will be at (0, - 2000), which can be analytically determined by using the following relationships

$$\int_0^{X_Q} dX = \int_0^{500} V_X dt \qquad \text{and} \qquad \int_0^{Y_Q} dY = \int_0^{500} V_Y dt \tag{21}$$

where $X_Q = 0$ and $Y_Q = -2000$ after solving equation (21) with equation (20).

Figure 4 illustrates the associated particle tracking processes for the case where there are no subelements. Cheng et al (1996) shows in their paper that as the number of the subelements increase their results get smoother. If necessary subelements can be implemented in our model and our model can get better and smoother results with the increasing number of subelements. Dividing elements into smaller subelements can be implemented in the code later depending on the necessity. All need to be done is to divide the elements into subelements and find the heads at new nodes by interpolation (we won't have to interpolate a vector value (velocity) as Cheng et al (1996) were doing, we will be interpolating scalar values (heads) and then calculate the velocity).

When this example was being implemented to our model, only change made was defining the velocities at the center of each element instead of defining the velocities at every node. This change affected the tracking times as expected; however IWRM_PTM duplicated the results successfully as can be seen from the Figure 5. We also added another case where some of the elements are triangular elements in order to see the performance of the code with mix elements. Figure 6 illustrates this case. Figure 6 shows that the model works perfectly with triangular and mix elements, too. In both of the case a second particle was released from X=2500, Y=2000 to see how the model reacts when the particle goes out of the boundary. The model simulated the case successfully and when the particle went out it gave a message that the particle went out and stopped simulation.

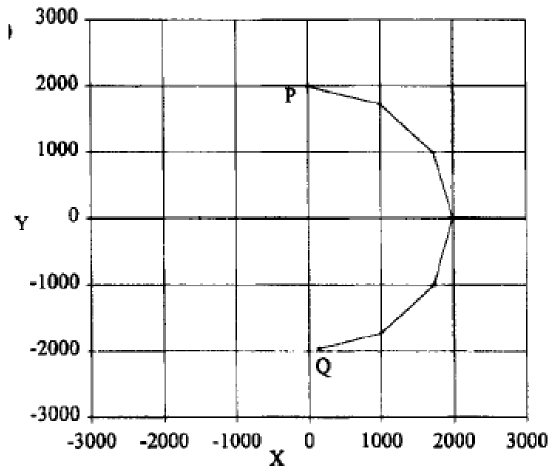


Figure 4. The particle tracking process as in Cheng et al (1996)

5.2 Example 2. MODPATH User Manual Example Problem

The sample problem from is presented to compare the results of MODPATH and IWRM_PTM as well as to illustrate the input and output data from IWRM_PTM. The problem is based on the hypothetical flow system illustrated in Figure 7. The flow system consists of two aquifers separated by a 20-foot-thick confining layer. Recharge to the system is

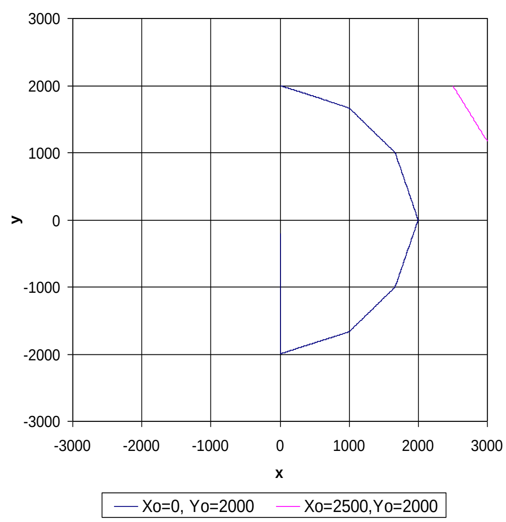


Figure 5. The particle tracking process with the developed model

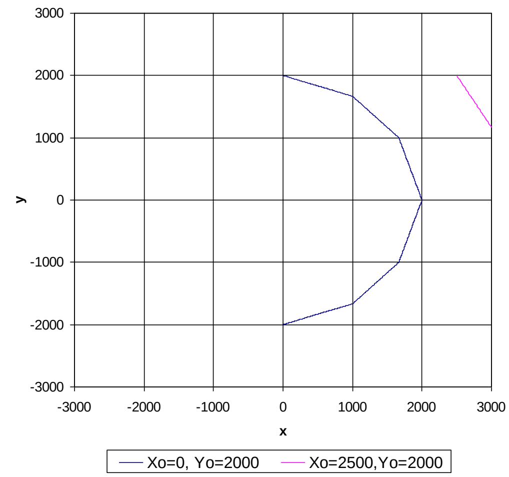


Figure 6. The particle tracking process with the developed model with mix elements

uniformly distributed over the water table at a rate of 0.0045 feet per day for MODPATH. The same amount of recharge is applied in IWRM as deep percolation from precipitation by adjusting and calibrating the necessary parameters. Discharge occurs to a partially-penetrating river along the right side of the flow system in the upper aquifer for. Some water also discharges to wells. Hydrogeologic parameters for these two aquifer layers are listed in Table 2.

Table 2: Hydrogeologic Parameters

	Layer1	**Layer2**
Horizontal Hydraulic Conductivity (ft/ day)	50	25
Specific Yield	0.2	N/ A
Specific Storage	N/ A	1E-4
Porosity	0.3	0.3

The system is simulated using a finite-difference grid containing 27 rows, 27 columns, and 5 layers (Figure 8). Horizontal grid spacing varies from 40 foot by 40 foot squares at the wells to 400 foot by 400 foot squares away from the wells. The upper unconfined aquifer is simulated with one finite-difference layer. A quasi-three-dimensional representation is used for the confining layer. The lower aquifer is represented by four 50-foot-thick layers. Both wells are located in row14, column 14. The well in the lower aquifer is located in model layer 4.

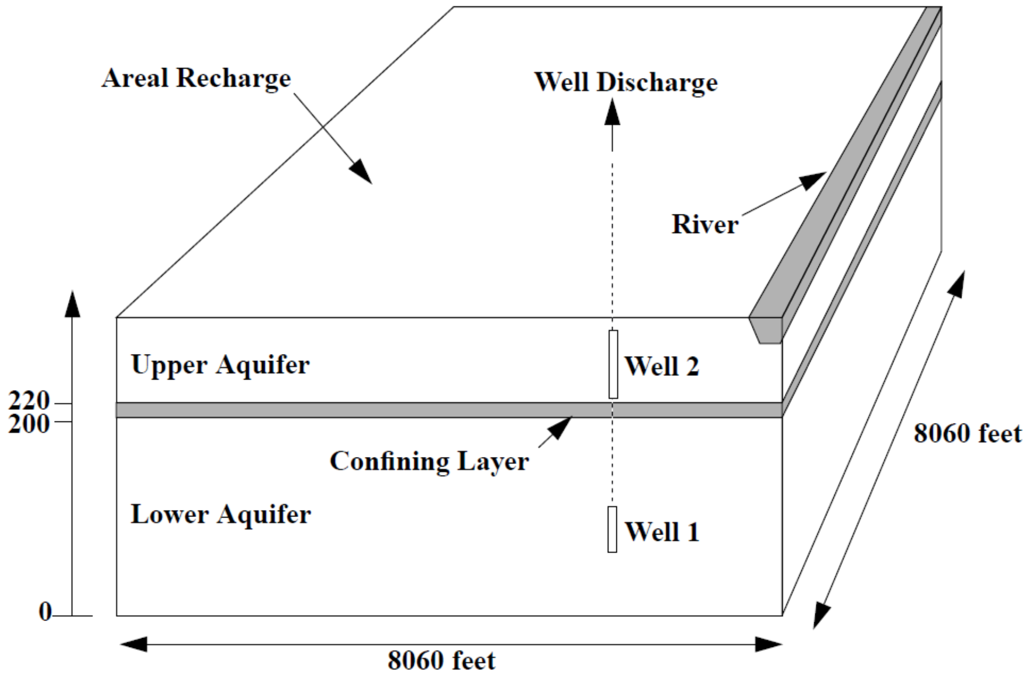


Figure 7. Conceptual model for hypothetical sample problem

The simulation is divided into three stress periods. Stress period 1 is 500 years long with one time step. During stress period 1, only one well is present in layer 4 and all stresses are identical to those of the steady state simulation. Stress period 2 is 30 years long and consists of eight time steps for MODFLOW and MODPATH. IWRM and IWRM_PTM use monthly simulation option. During stress period 2, wells are present in layers 1 and 4, each discharging at 80,000 cubic feet per day. Stress period 3 is 1,250 years long and contains one time step. Both wells continue to discharge at 80,000 cubic feet per day during stress period 3.

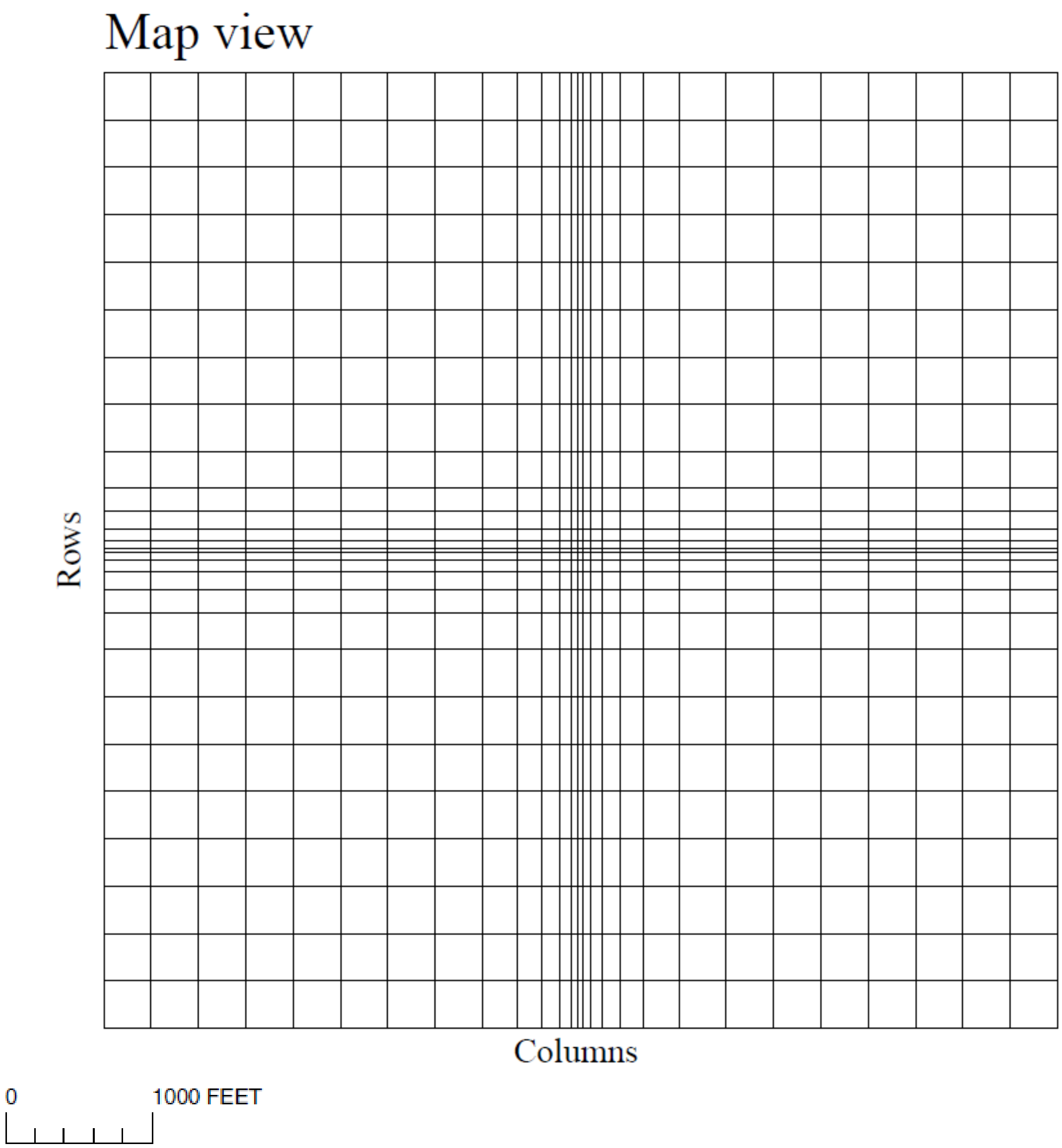


Figure 8. Finite-difference grid of the hypothetical system of the problem

5.2.1 IWRM Verification

In order to verify IWRM_PTM, IWRM results have to be verified with MODFLOW results first. In this manner necessary IWRM input files were prepared and necessary variables were calibrated like amount of precipitation to obtain 0.0045 feet per day of deep percolation, or stream input flow to maintain the constant head at the stream or its rating curve, or etc.

Here only the comparison of the heads for both of the models are provided, since velocity calculations depends on the heads calculated from the flow model. Figures 9, 10, 10, 11, and 12 below show the results and comparison of the models at different time steps and stress periods.

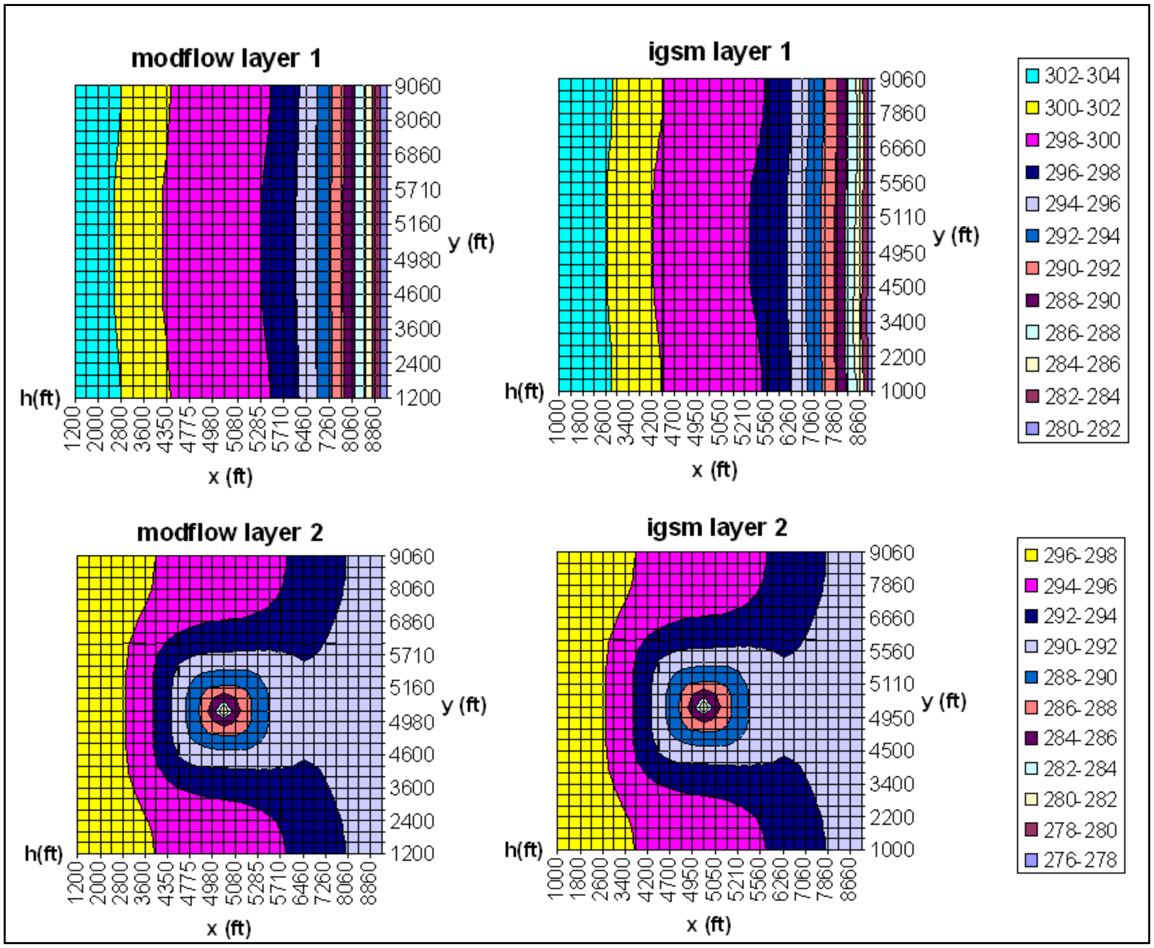
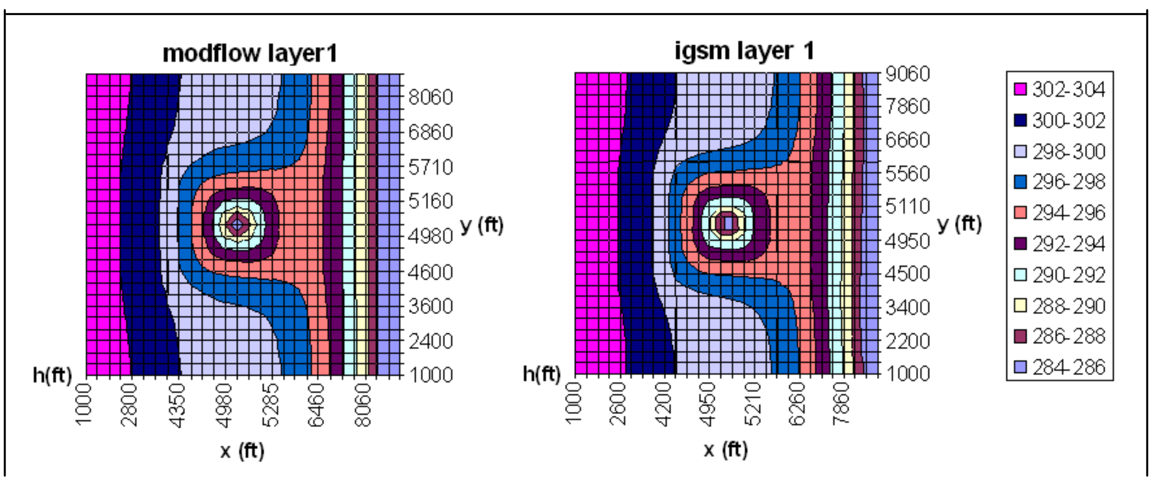


Figure 9: Comparison of heads calculated at the end of stress period 1



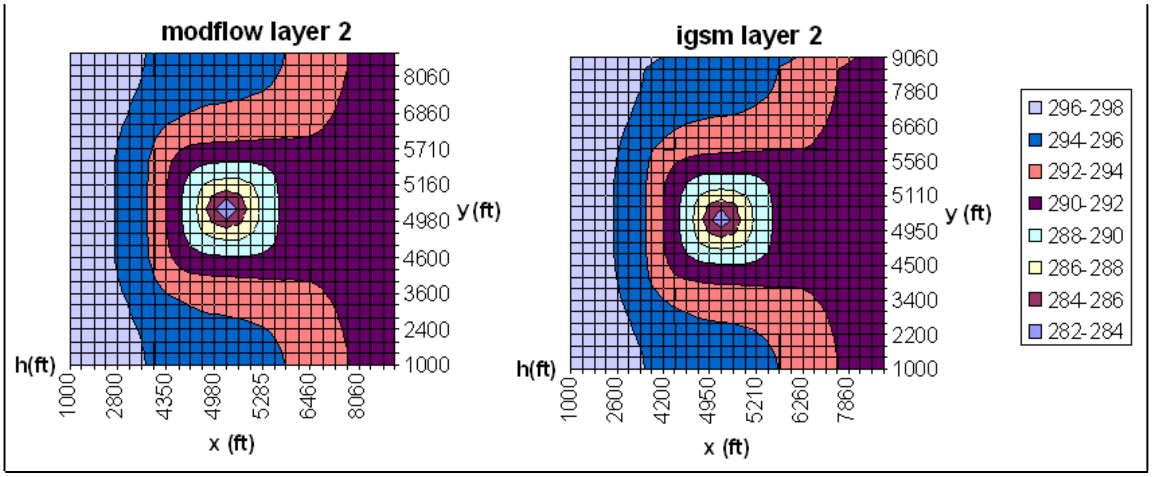


Figure 10: Comparison of heads calculated at the end of time step 1 at stress period **2**

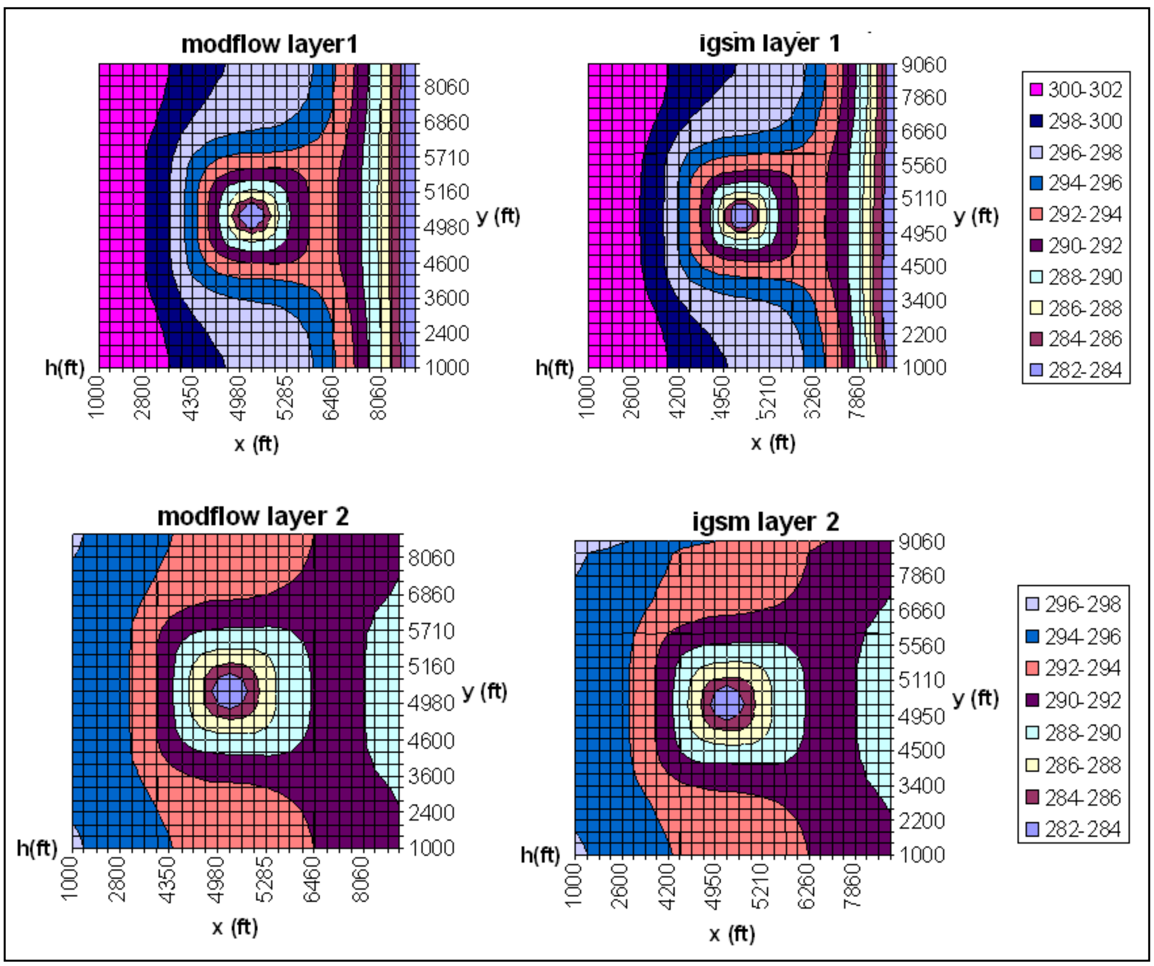


Figure 11: Comparison of heads calculated at the end of time step 3 at stress period 2

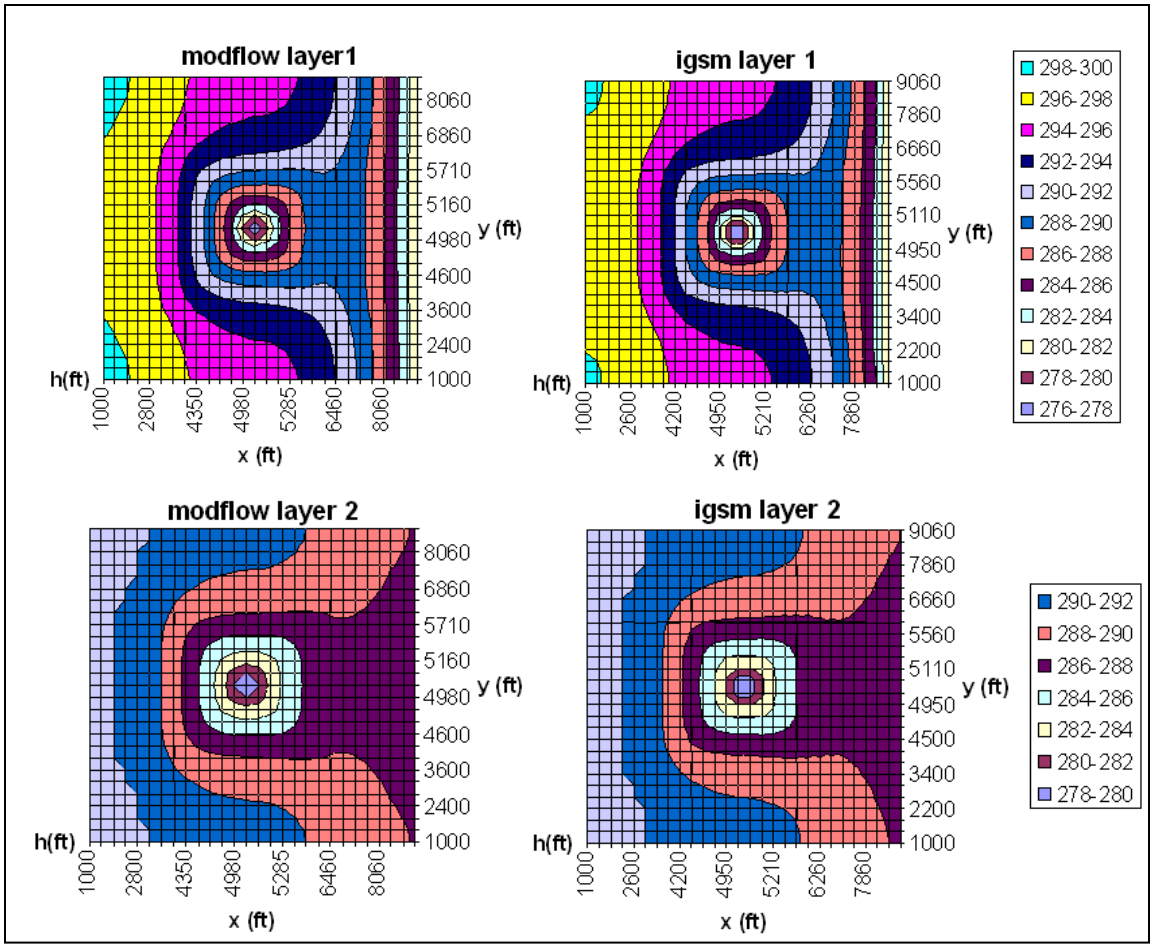
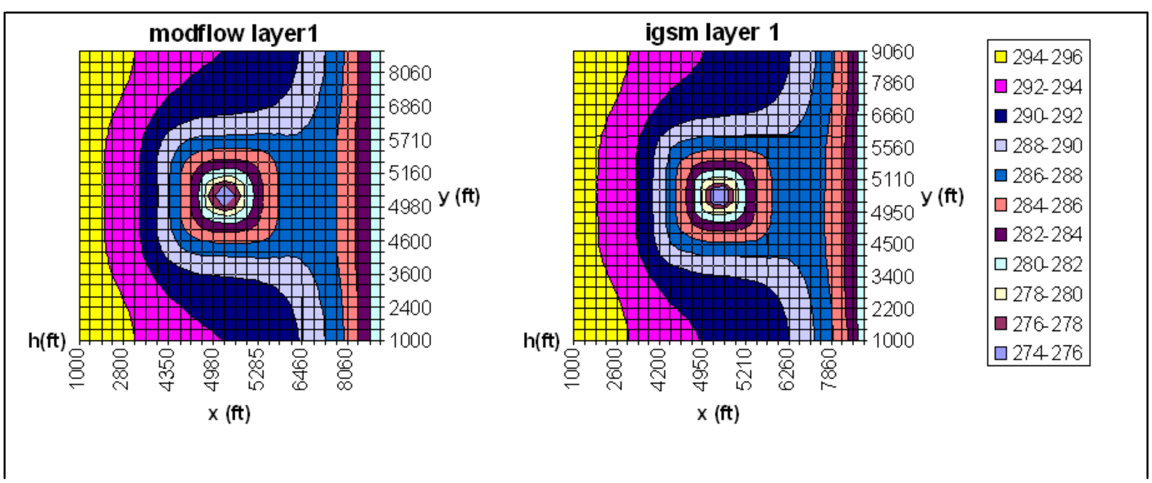


Figure 12: Comparison of heads calculated at the end of time step 6 at stress period 2



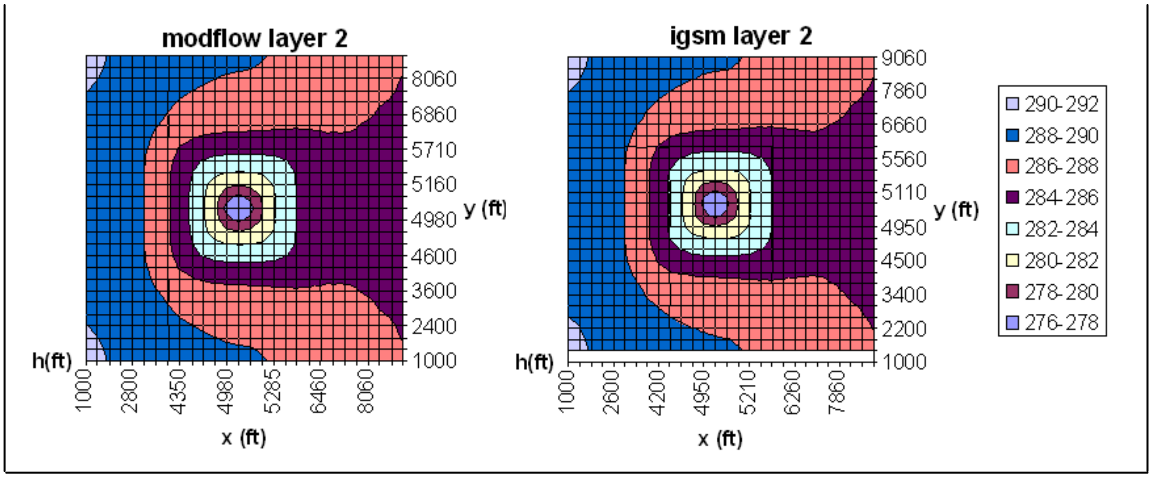


Figure 13: Comparison of heads calculated at the end of time step 8 at stress period 2, and stress period 3 (second steady state)

5.2.2 Verification of Tracking Time

In order to compare the tracking time of the models two different tests were done. First test was done in layer 1 with 7 particles at stress period 1. Second test was done in the first layer, too. Again 7 particles were used but this time the test was done at stress period 3 and at a different location. The results are plotted in Figure 14 and 15. As can be seen from the plots, tracking time for both of models are very close.

5.2.3 Backward Tracking Endpoint Analysis for the Well in Layer 1

The evolution of the capture area for the well in layer 1 was examined by placing 28 particles on the faces of the cell containing the well and tracking them backward to their recharge locations. MODPATH and IWRM_PTM simulations were compared with a run where the particles were started after around 17.7 years of pumping. For MODPATH analyses, the particles were stopped tracking when they reached the water table to find recharge locations. Particles started on the faces of the cell containing the well, almost at the bottom of the aquifer, ended at the recharge locations (at the water table). IGMS_PTM tracked the particles for 17.7 years. Model results are compared and shown in Figure 16.

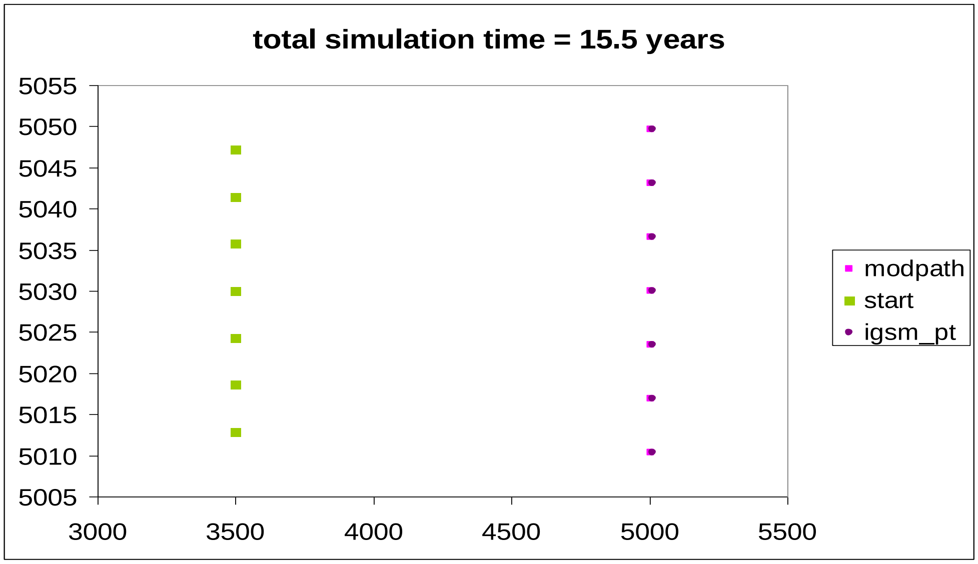


Figure 14. Comparison of tracking time during stress period 1

5.2.4 Forward Tracking Endpoint Analysis for the Well in Layer 1 and Stream

This run will delineate the new steady state capture areas for the well and the stream in layer 1. The capture areas are most easily delineated with forward tracking. Because the system has attained a new hydraulic steady state by the end of stress period 2, a 2*2 array of particles are placed at the water table in all cells in layer 1 at the beginning of stress period 3. The particles that start from the water table and would pass the confining layer and reach the well in the second layer were excluded in this example. These particles can be tracked completely through the system because the 1,250 year length of stress period 3 is much longer than the residence time of any of the particles in the system. Results for MODPATH are plotted in Figure 17 and for IWRM_PTM in Figure 18.

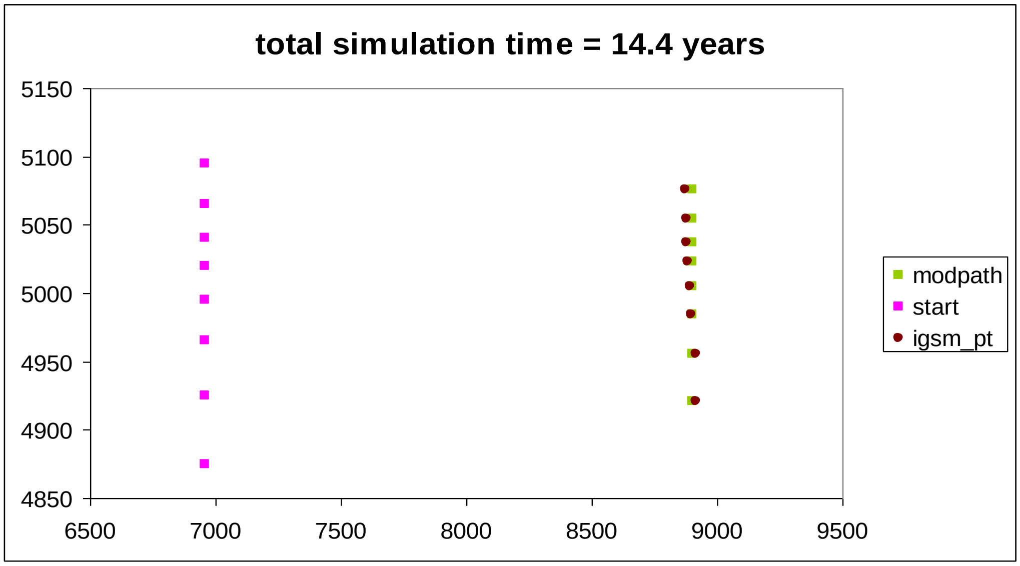


Figure 15. Comparison of tracking time during stress period 3

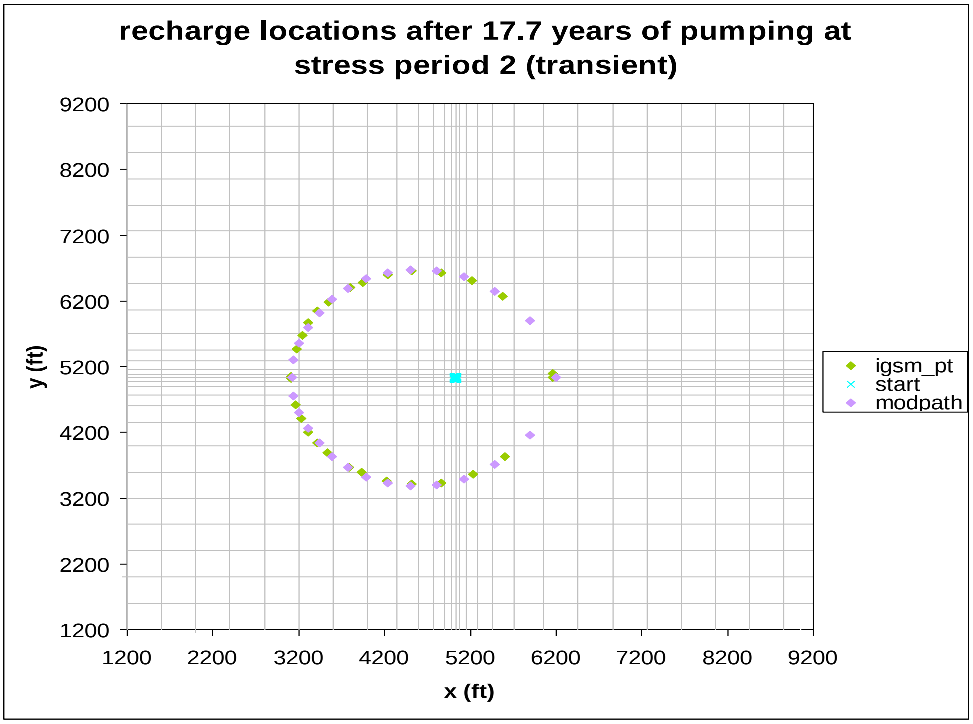


Figure 16. Capture area for the well located in layer 1

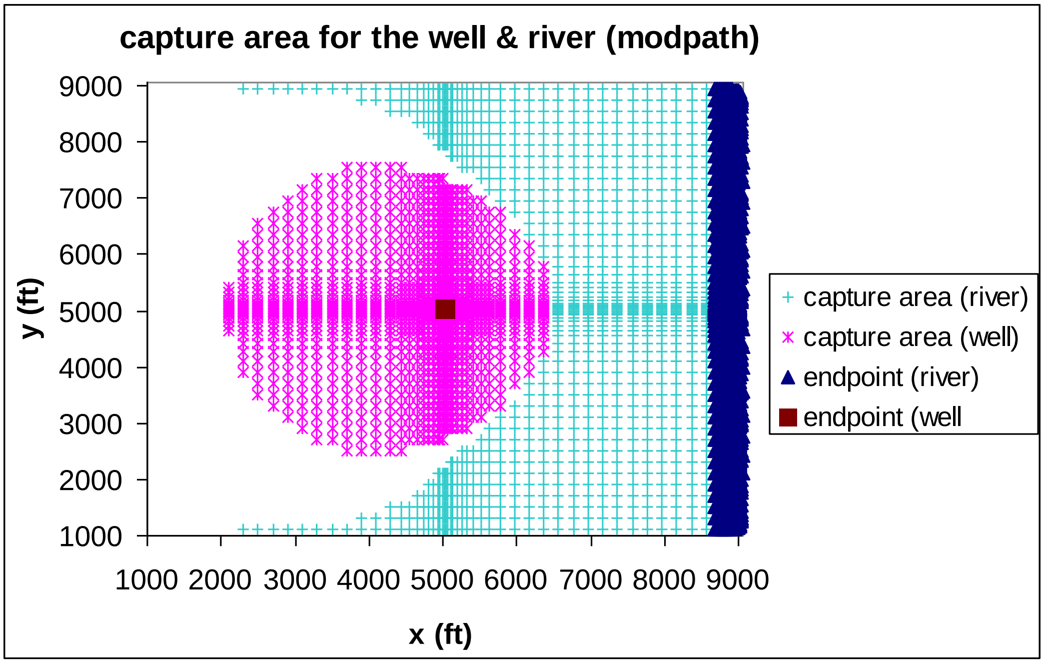


Figure 17. Capture areas for the well located in layer 1 and the stream

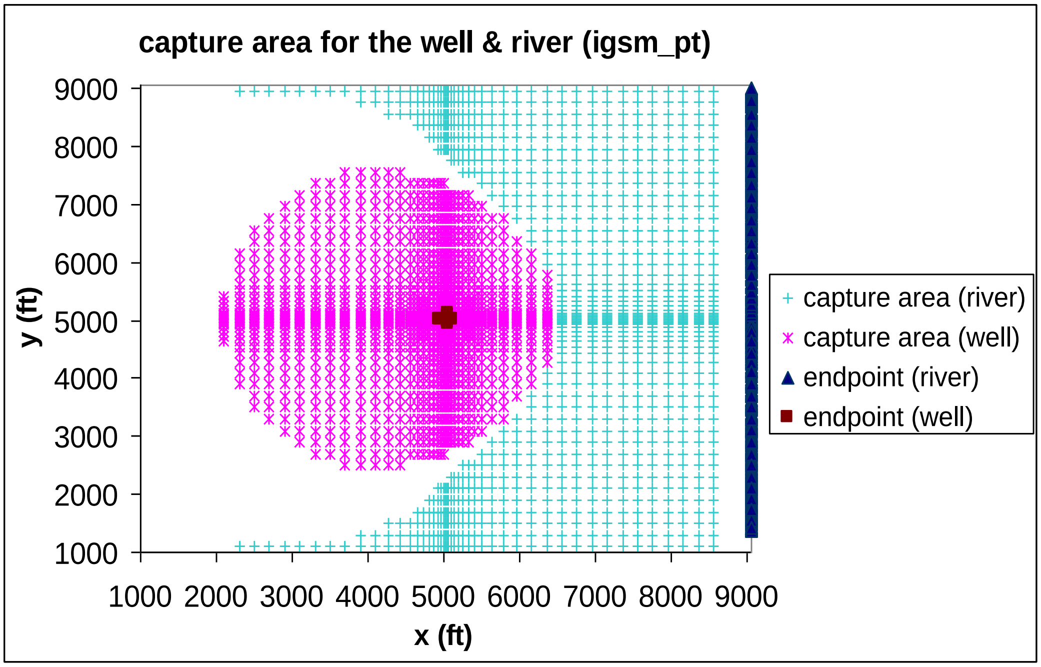


Figure 18. Capture areas for the well located in layer 1 and the stream

6. APPLICATION

In order to see the performance of the model, IWRM_PTM should be applied to an example case with a more complex velocity field. In that manner, Sacramento Valley IGMS flow model's results were used to test the performance of the model. In both of the test cases, the release locations were picked randomly to see the performance of the code.

6.1 Application to Depression Zones in Sacramento Valley

For this case study three batches of particles (each having 10 particles) were released at three different upstream locations. These locations are at the upstream of two depression zones located at both sides of the Cosumnes River where it intersects with Highway 99. The particles were released on Oct 1969 and were tracked daily for 30 years.

The pathline plots showing dissipation of the plumes are shown in Figure 19 at twelve different time steps. Although groundwater levels for 1977 were used as a background, the general flow pattern is similar with similar depression zones. As can be seen the particles follow the general pattern of the flow. Most of the particles continue moving in the direction of the dispersion zones which will be their end point. Also some of the particles got caught at local depression zones temporarily and than moved forward when the flow conditions had changed. This is very difficult to see in Figures 19. As a result, a pathline plot that shows the movement of one of the particles on *x-y* space for every time step is presented in Figure 20. In the figure the black dots show the path of the particle. If the particle stays at the same location more than one day there is a colored bubble around that location and the size of the bubble increases with the increasing number of days the particle spent at that location. IWRM_PTM has a control parameter defined in master control file that specifies the amount of time a particle can stay at the same location. If this parameter is exceeded the tracking for this particle stops at that specific location. This parameter was assigned really high in this example to see if the particle would still move after a long wait.

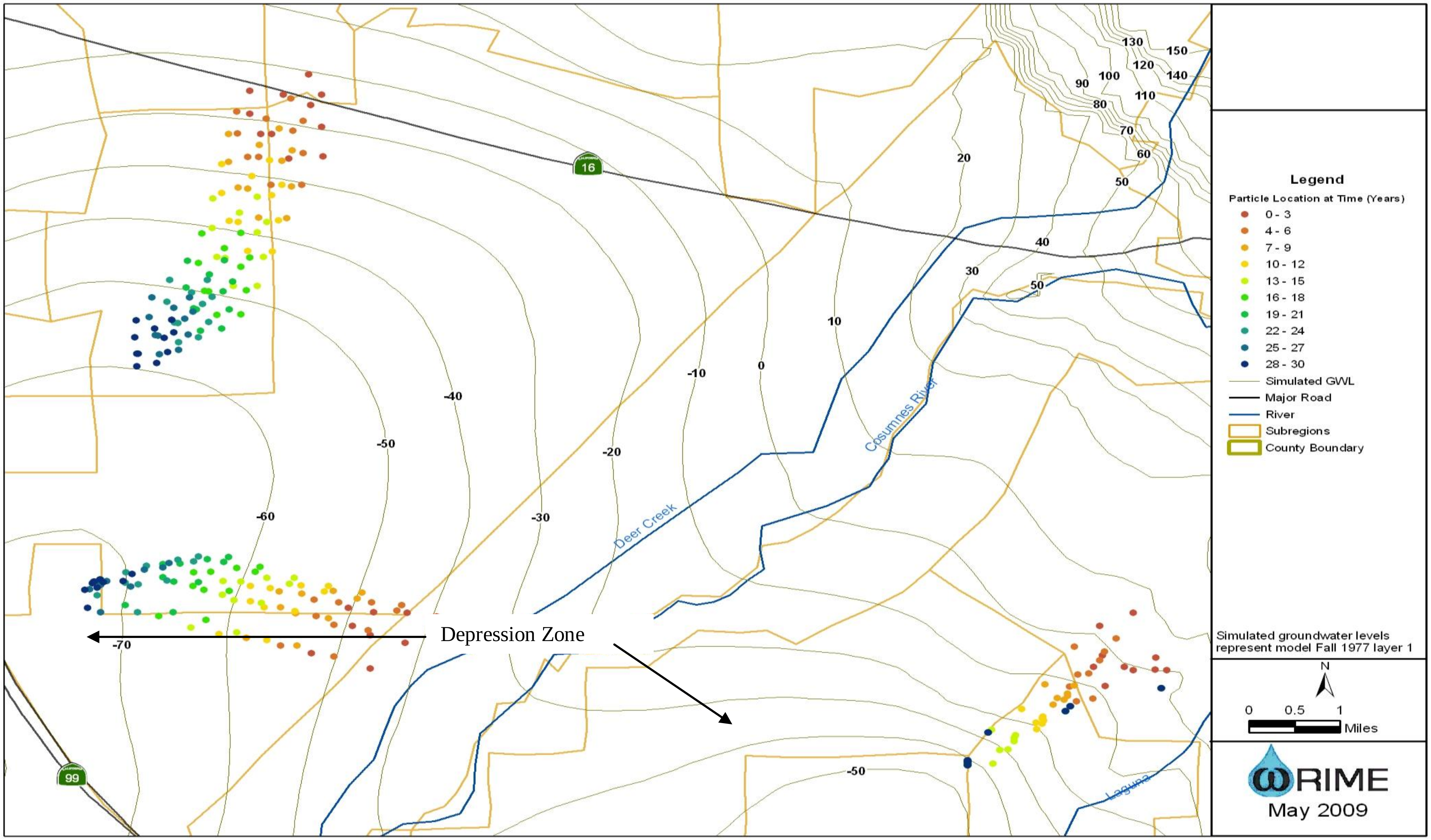


Figure 19. Time series plot showing dissipation of the different plumes in 30 years of time to depression zones.

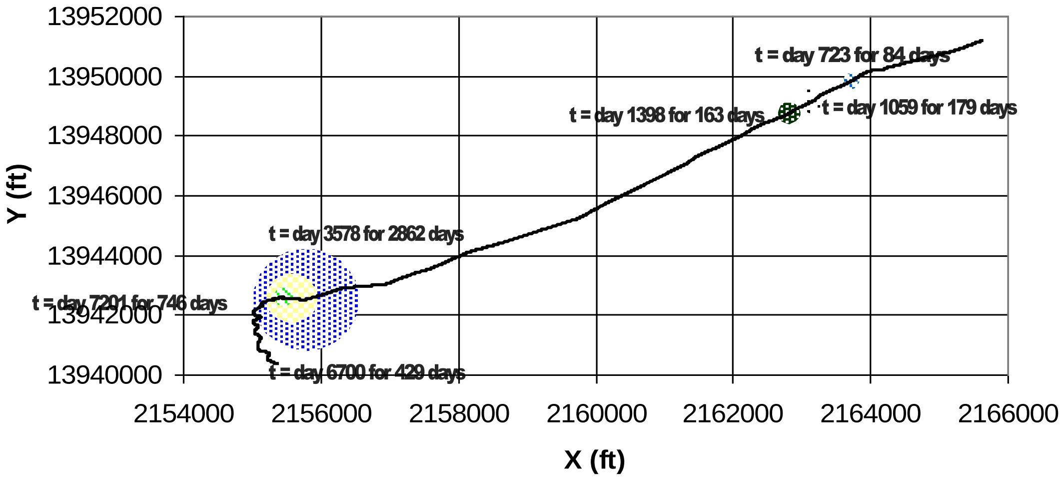


Figure 20. The path of the particle with the bubbles showing how long the particle stayed at that location

6.2 Application to Aerojet Area

Two different case studies were done in Aerojet area. In the first case 1000 particles were released from two different locations close to east boundary of the region. In the second case, again 1000 particles were released from three different locations around the center of the region. The aim of these runs were to see how the particles, that were already produced and arrived to these specified locations by Oct 1969 or produced at these location on Oct 1969, had moved in 30 years time.

While these cases were being developed, the locations were picked randomly and they might or might not be possible sources of contamination. Their intention was to see the performance of the code. They don't represent any conclusive results. However, realistic case studies can be created for any location and time interval in the Aerojet Area or any region to see the dissipation of contamination. Also particles can be released cautiously from one or more different sources if necessary for different cases.

The pathline plots showing dissipation of the plumes are shown in Figure 21 and 23 at twelve different time steps for cases 1 and 2, respectively. Figures 22 and 24 show the starting locations (on Oct 1st 1969) and end points (on Sep 30th 1999) for cases 1 and 2, respectively. Although groundwater levels for 1977 were used as a background, the general flow pattern is similar.

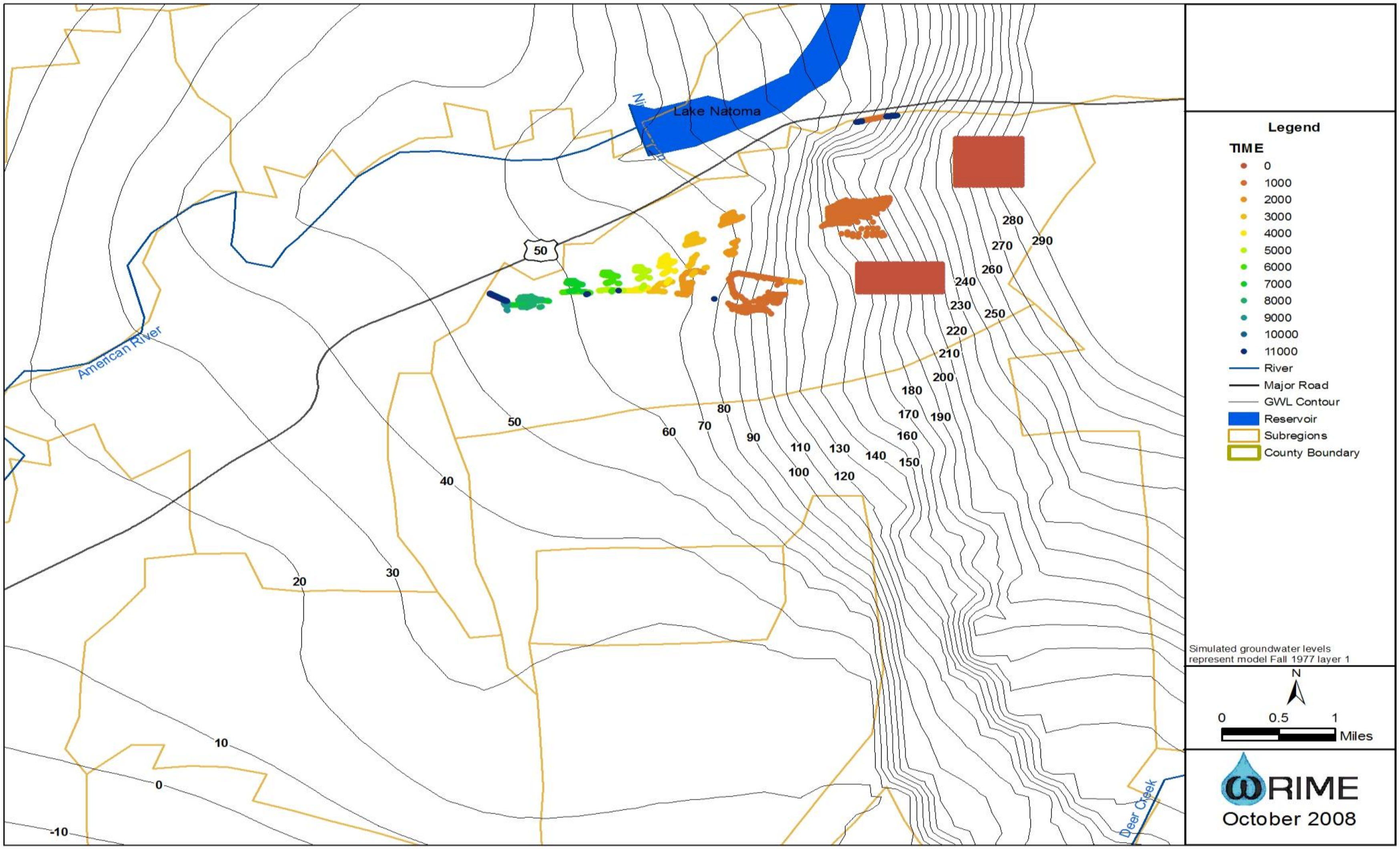


Figure 21. Time series plot showing dissipation of the different plumes in 30 years of time in Aerojet Area.

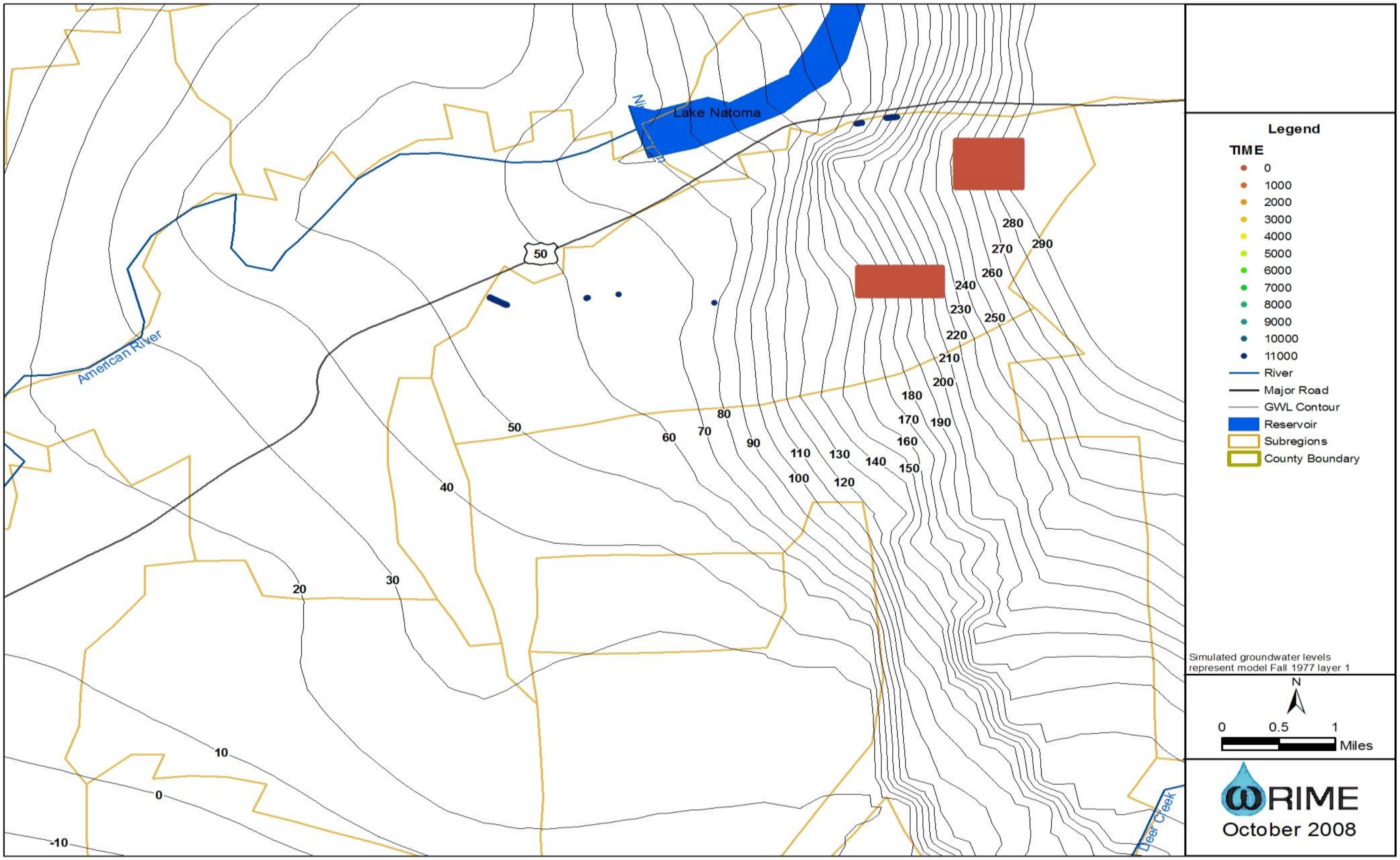


Figure 22. Time starting and end locations of different plumes in 30 years of time in Aerojet Area.

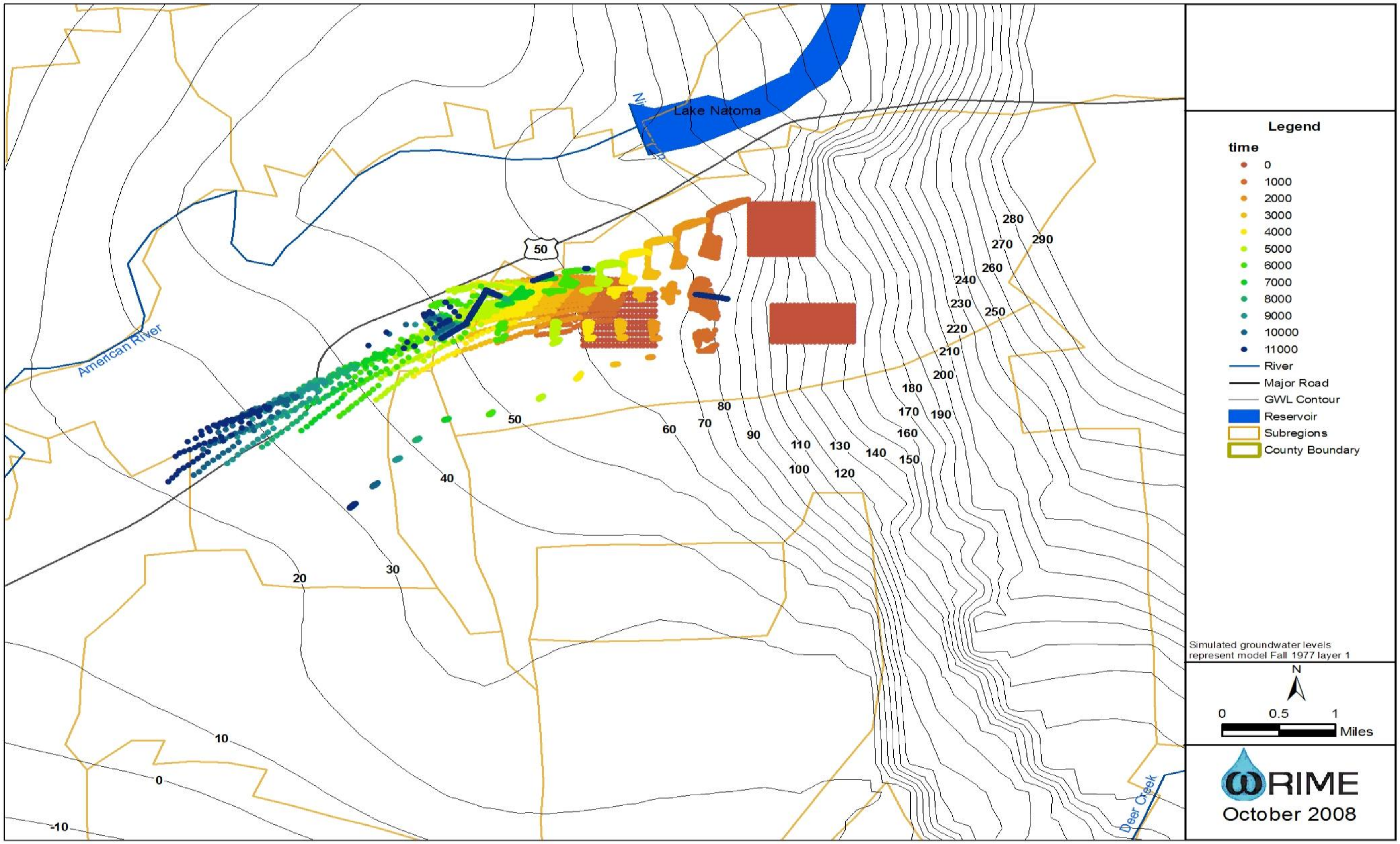


Figure 23. Time series plot showing dissipation of the different plumes in 30 years of time in Aerojet Area.

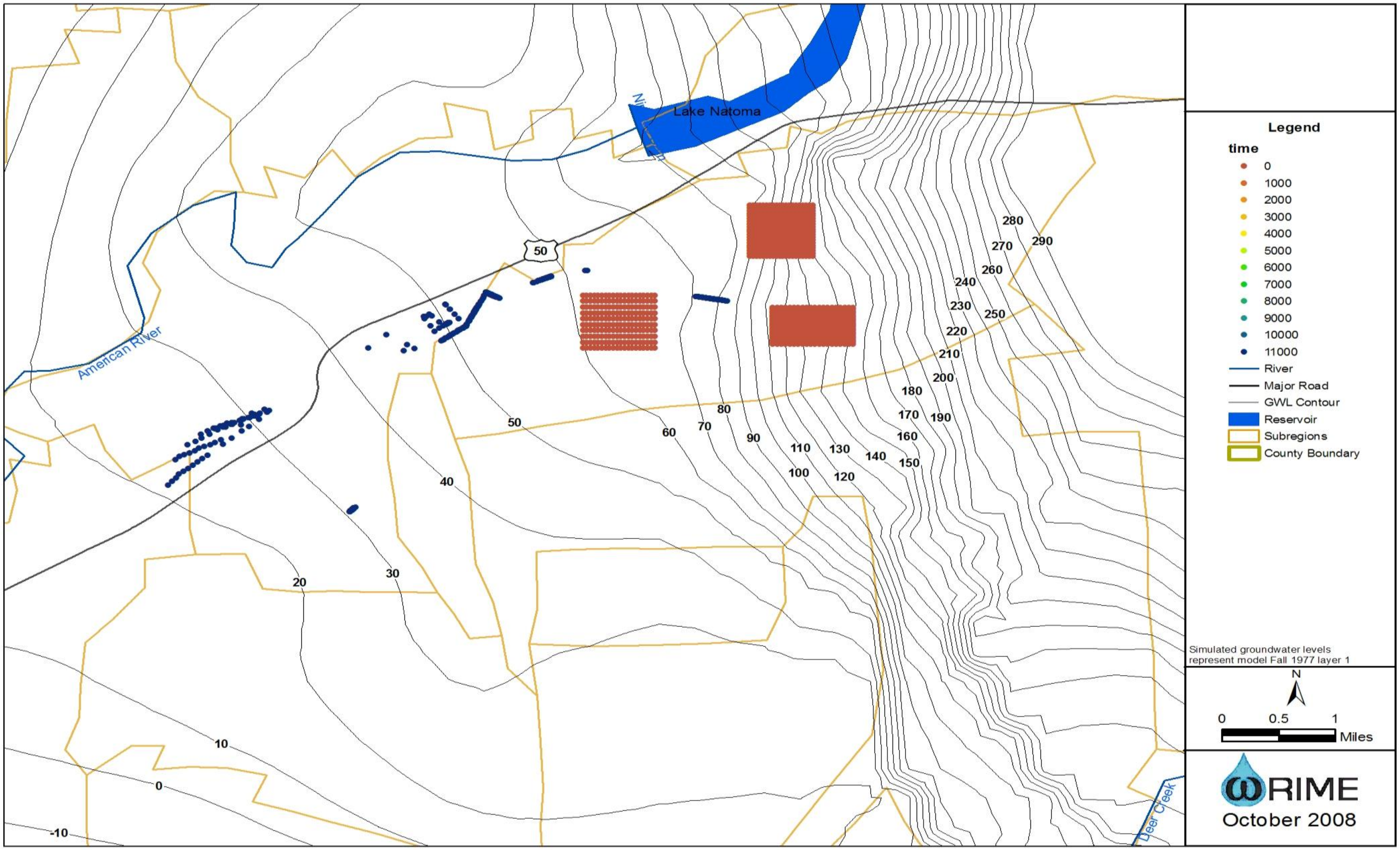


Figure 24. Time starting and end locations of different plumes in 30 years of time in Aerojet Area.

7. PROGRAM DESCRIPTION

7.1 Program Concept

7.1.1 Goal of the Program

The IWRM_PTM, written in American National Standard Institute (ANSI) FORTRAN 90, has major goals vis-à-vis program coding:

1. Effective data management routines for easy input data preparation.
2. Minimization of computer memory requirements and execution time.

7.1.2 Hardware Requirements

The IWRM is set-up to operate on IBM compatible PCs. The program is currently compiled with LAHEY FORTRAN™ extended memory compiler, F95L_WIN32. The minimum hardware requirements to run the program are as follows.

1. ***Processor*:** Pentium based or faster PC.
2. ***Memory*:** 128 MB or more of random access memory (RAM).
3. ***Disk Space:*** 500 MB or more of available hard disk space. The actual disk space requirement depends on the size and details of the specific project.
4. ***Operating System*:** Windows NT, 2000, XP, or Vista.

7.1.3 Array Dimension Limitations and Variable Definitions

The present version of the program can simulate a system with the following *maximum dimensions:*

- Nodes: 6,000
- Triangular Elements: 4,000
- Quadrilateral Elements: 5,000
- Particles: 10,000

These limits are set in the current version of the IWRM_PTM. However, these limits can be modified by changing the array dimension parameters in the main code and re-compiling the program.

All the variables used in IWRM_PTM code and their definitions are presented in Table 3.

Table 3. Variables and their definition for IWRM_PTM

Variable	Definition of Variables
DELT	Simulation time step size in months or days(restricted to 1)
DELTPT	Simulation time step for particle tracking (0 = daily, 1 = monthly)
endSP	Last day of the month during daily simulation
EPS	Error Term
H	Groundwater head for each node in the current time

IDE	Node numbers surrounding each element
IDPRN	Array that holds the dates to print times series output files
IELCNT	Number of times each particle visited each element during the shifting process
IEP	Element for the particle at the beginning of the time step or subtime step
IEPAR	Element for each particle in the current time
IEQ	Element for the particle at the end of the time step or subtime step
ILAST	Ending time of the simulation
IMO	Month during the simulation
INIT	Beginning time of the simulation
IOUTFLG	Flag to help output that specifies the status of simulation for each particle in the current time
IPART	Particle number to be simulated in the current time
IPRNEP	Total number of particles in an element
IRELT	Release time for each particle
ISIMON	Flag to specify if there will be simulation for each particle in the current time
ISPEL	Array to hold the special elements
ISTOPT	Simulation end time for each particle
ITIME	Time during the simulation
IYR	Year during the simulation
JND	Node numbers surrounding each node
KTRACK	Flag to specify the simulation type (backward or forward)
ND	Number of nodes
NDAY	Number of days during within a month daily simulation
NE	Number of elements
newSP	First day of the month during daily simulation
NJD	Cumulative no. of nodes surrounding each node
NN	Array to specify the starting location at the beginning of the time step or subtime step
NP	Number of particles
NPAREL	Total number of particles for each element in the specified time step
NSHIFT	Maximum number of shifts when a particle enters a shifting process
NSPEL	Number of special elements in which the particle will be stopped
NWRTEP	Number of dates to print the times series output files
SHIFT	Shifting distance in the case of a channel flow in a shifting process
SHIFTCHN	Shifting distance if not a channel flow in a shifting process
VPX	Velocity in X-direction for the particle at the beginning of the time step or subtime step
VPY	Velocity in Y-direction for the particle at the beginning of the time step or subtime step
VX	Groundwater velocity in X-direction for each node in the current time
VY	Groundwater velocity in Y-direction for each node in the current time
X	X-coordinate for all nodes
XP	X-coordinate for the particle at the beginning of the time step or subtime step
XPAR	X-coordinate for each particle in the current time
XQ	X-coordinate for the particle at the end of the time step or subtime step
Y(I)	Y-coordinate for all nodes
YP	Y-coordinate for the particle at the beginning of the time step or subtime step
YPAR	Y-coordinate for each particle in the current time
YQ	Y-coordinate for the particle at the end of the time step or subtime step

7.2 Program File Structure

Input/ Output of the model is streamlined by using a number of files that generally contain one type of data only. This allows each file to be structured in a unique, tabular format suitable for a given type of data. Within each input file, any number of lines can be used to write comments such as project name, file name, date of revisions, sources of data and other notes as described by the model user. The only requirement is that all comment cards must start with a 'c' or 'C' or '*' in the first column. The program will automatically recognize these lines and skip the corresponding lines while reading the input data. This innovative and flexible feature allows the input data files to be fully documented without limiting the number of comment cards or their locations. Each input/ output file is linked to a unit number and is referenced internally. As such, the unit numbers cannot be changed arbitrarily. The list and description of input and output files used in the IWRM_PTM are presented in Table 4.

Table 4. List and Description of Input and Output Files Used in IWRM_PTM

File Unit	Name	Description	File Type	Required/Optional
5	Master Control File	Title of the simulation run, names of all input/output files for, and other control parameters for output options.	Input	Required
7	Element Configuration Data	Element configuration for the finite element mesh, including user specified element numbers with connecting node numbers which define the elements.	Input	Required
8	Nodal Coordinates Data	X-Y spatial coordinates for each node.	Input	Required
9	Initial Condition Data	Particle starting locations at initial time step of the given simulation as well as particle release and simulation end times.	Input	Required
10	Binary Time Series Velocity Data From IWRM Part 2	Binary output of time series velocities generated by Part 2	Input	Required
6	Standard Output File	Standard output of shifting process, its location and reason and possible error messages.	Output	Required
11	Particle Status Output	Output file of particle locations, elements, and status for each particle.	Output	Required
12	Element Particle Count Output	Output for the number of the particles for each element for chosen time steps.	Output	Optional
13	Particle Endpoint Output	Output file for the locations of the particles at the end of simulation.	Output	Optional
14	Particle Location Output	Output for locations of particles and their status at specified time steps.	Output	Optional

15	Velocity Direction Output	Output velocities, their magnitudes, and directions for each element at specified time steps.	Output	Optional

7.3 Main Program and Subroutines

7.3.1 IWRM_PTM

The IWRM_PTM does the following

- Processes IWRM_PTM master control file (Unit 5);
- Specifies the size of all the adjustable arrays;
- Opens and reads the Part 2 binary file for velocities (Unit 10)
- Generates the standard output file (Unit 6);
- Generates the particle status output file (Unit 11);
- Generates element particle count output file (Unit 12);
- Generates the particle endpoint output file (Unit 13);
- Generates the particle location output file (Unit 14);

A flow chart representing the program structure for IWRM_F1 (Part 1) is shown in Figure 25. The subroutines included in IWRM_PTM, as shown in Figure 25, are described below.

7.3.2 Subroutine GETG_PTM. This subroutine opens and processes all the input data (except unit6 and 10) in the following order:

- Unit 7 : Element configuration data
- Unit 8: Nodal coordinate data
- Unit 9: Initial condition data

Subroutine GETG_PTM calls subroutines NODECONF and CCW_JND.

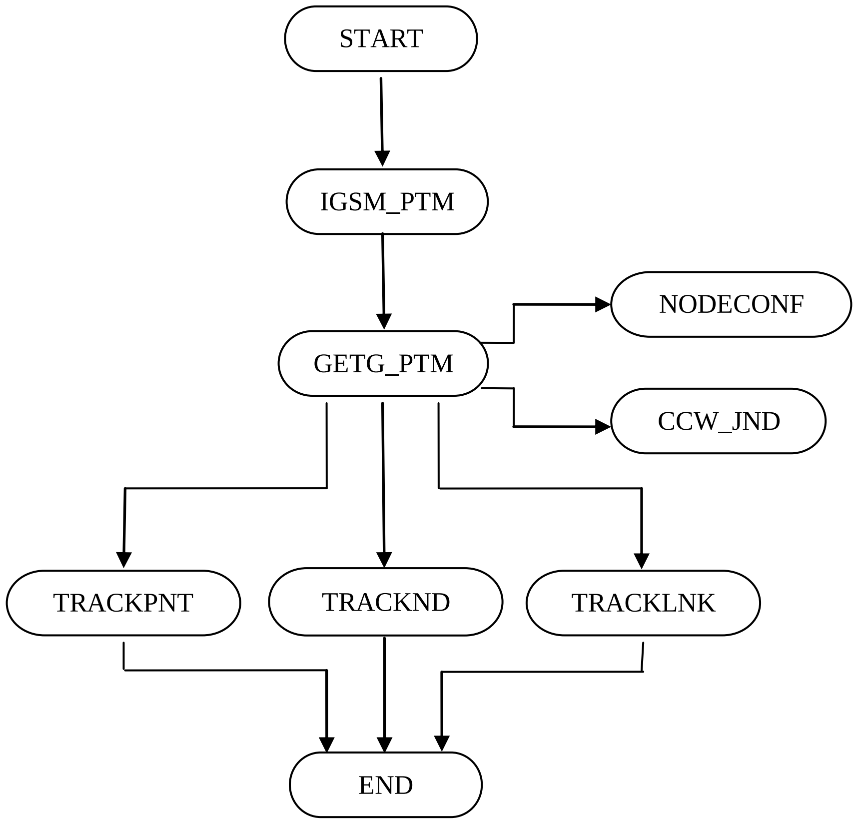


Figure 25. IGMS_PTM Program Structure

7.3.3 Subroutine NODECONF. This subroutine defines following arrays:

- JDE = Node numbers surrounding each element;
- JND = Node numbers connected to each individual node;
- NJD = Cumulative number of nodes connected to each node.

The relationship between JDE, JND, and NJD is given in IWRM User Manual.

7.3.4 Subroutine CCW_JND. This subroutine rearranges the array JND in a way that the nodes connected to each individual node are ordered in a CCW. If there are boundary nodes surrounding a node, this subroutine puts the boundary node connected to the that node in CCW order in first position.

7.3.5 Subroutine TRACKPNT. This subroutine accomplishes the particle tracking for a particle that starts from a random within an element (this point cannot be a node or on a link connecting two nodes). The subroutine checks all the faces of the element as described in Section 3 one by one and decides in which direction the particle will go in that current time step.

7.3.6 Subroutine TRACKND. This subroutine accomplishes the particle tracking for a particle that starts from a node on an element. The subroutine first finds which element will the particle move in and then checks all the faces of the element as described in Section 3 one by one and decides in which direction will the particle go in that current time step.

7.3.7 Subroutine TRACKLNK. This subroutine accomplishes the particle tracking for a particle that starts on a link between two nodes of an element. The subroutine first finds which of the two neighboring element will the particle move in and then checks all the faces of the element as described in Section 3 one by one and decides in which direction will the particle go in that current time step.

7.4 IWRM_PTM Input/ Output Files

The input files used in IWRM_PTM are already shown in Table 4 and example of each follows.

7.4.1 UNIT = 5: Master Control File

Purpose of the File

This is the main control file for IWRM_PTM. It contains the following data blocks.

***Title of the Project Run*:** Three lines are reserved for this.

***Names of the Input/ Output Files*:** The file names must be less than 20 characters and inserted in the first 20 columns of the line.

***Model simulation period*:**

- The initial time of simulation (INIT) (initial year * 100 + initial month)
- The final time of simulation (LAST) given in the same format as INIT (last year * 100 + last month)
- Simulation time step (DELTPT).
- Simulation type flag for steady or transient simulation

Note on Simulation Time:

IWRM_PTM uses should have the same initial date of the simulation which corresponds to the first day (or month for monthly simulation) of the IGMS flow simulation. Similarly, final date of simulation should be the same as the final date of the simulation which corresponds to the last day (or month for monthly simulation) of the IGMS flow simulation. Similarly, the simulation time step should be the same as the gw simulation time step (DELTGW) of the corresponding IWRM simulation. If simulation time step is chosen as daily the first day of simulation will be the first day of the initial month and the last day of the simulation will be the last day of the last month.

***Output Control Options*:** These options help monitor the program execution as well as debug any input data errors.

***Input/ Output Unit Control*:** This option allows model input and/ or output to be provided or written in British and/ or SI unit, as desired.

***Model simulation period*:** This option lists the particle shifting parameters, such as

- Maximum number of shifts
- Shifting distance if not a channel flow
- Shifting distance in the case of a channel flow.

***Simulation Option*:** This option specifies whether the simulation will be forward or backward.

***Special Element Option*:** This option specifies Number of special elements to stop the particle tracking, followed by the elements.

***Output Option*:** Number of dates for printing time series data, followed by the dates in year and month format. In the case of the daily simulation the values will be written for the last day of the specified month. Similarly, number of dates for printing element velocity directions is defined and followed by the dates in year and month format. In the case of the daily simulation the values will be written for the last day of the specified month.

Note: File Naming Convention

It should be noted that a file name beginning with a 'C' or 'c' inserted in the first column, may be read as a comment card and therefore, the line will be skipped, and the input file name will be ignored. This problem can be handled in two ways:

- Ensure no file names start with a 'C' or 'c'.
- Enter the filename beginning on the 2nd column of the line, leaving a blank in the first column. This should solve the problem; however, it has been found that some compilers read the preceding blanks in a character string as characters. This will add blanks to the file name, and will cause a failure when attempting to open the input file. If this is the case with the compiler, a filename should not be started with a 'C' or 'c'.
- In the sample files included in this User's Manual, the first column is left blank.

```
C*****************************************************************************
C
C          INTEGRATED GROUND AND SURFACE WATER MODEL  (IWRM)
C
C----------------------------------------------------------------------------
C
C                    MASTER CONTROL FILE
C                  PARTICLE TRACKING MODULE
*                   Filename: PT.IN3
C
C
C*****************************************************************************
C              Titles To Be Printed in the Output
C
C  Enter 3 lines for the title. Do not use '*' , 'c' or 'C' in the first
C  column.
C----------------------------------------------------------------------------
                        REGIONAL GROUNDWATER MODEL
                       NAME OF PROJECT, CALIFORNIA
                               PART 3
C*****************************************************************************
```

```
C                  File Description
C
C  The following lists all of the input and output file names used in
C  running PART 1.  If no file exists (i.e. no lakes are being modeled ),
C  leave  the filename blank.
C---------------------------------------------------------------------------
C   FILE NAME              DESCRIPTION
C---------------------------------------------------------------------------
SACPT.IN3                      / 5: control input file
SACOUT1.OUT                    / 6: standard output file
SACELEM.DAT                    / 7: element configuration file
SACXY.DAT                      / 8: node x-y coordinate file
SACINIT.DAT                    / 9: initial condition data file
SACVEL.BIN                     /10: time series velocity data file from pass 2
SACSTAT.OUT                    /11: particle status output
SACELPAR.OUT                   /12: element particle count output
SACENDPNT.OUT                  /13: particle endpoint output
SACLOC.OUT                     /14: particle location output
SACVDIR.OUT                    /15: velocity field output file
C*****************************************************************************
C                   Model Simulation Period
C
C   The following lists the first  and last year of model simulation and the
C   simulation time step either daily or monthly.
C   INIT;  Initial date of model simulation  (should be the same as INIT of  IWRM simulation)
C   LAST;  Last date of model simulation (should be the same as LAST  of IWRM simulation)
C   DELPT;  Simulation time step (should be the same as DELTGW of IWRM simulation)
C
C-----------------------------------------------------------------------------
C      VALUE                DESCRIPTION
C-----------------------------------------------------------------------------
          196910          /INIT
          200409          /LAST
           0              /DELTPT   simulation time step: 1 MONTHLY, 0 DAILY
           0              /IFLAGS simulation type: 1 --> steady, 0 --> transient
C*****************************************************************************
C                 Output Control
C    KOUT; Enter 1 - to print geometric and stratigraphic information
C             Enter 0 - otherwise
C
C    KDEB; Enter 2 - to print messages on the screen to monitor execution
C             Enter 1 - to print non-zero Finite Element Stiffness Matrix Components
C             Enter 0 - otherwise
C---------------------------------------------------------------------------
C  VALUE                    DESCRIPTION
C---------------------------------------------------------------------------
   1                     /KOUT
   2                     /KDEB
C*****************************************************************************
C*****************************************************************************
C               Input / Output Unit Control
C
C    KUNIN;  Enter 0 - For English input
C               Enter 1 - For Metric input
C
C    KUNOUT; Enter 0 - For English output
```

```
C                    Enter 1 - For Metric output
C---------------------------------------------------------------------------
C VALUE                    DESCRIPTION
C---------------------------------------------------------------------------
   0                       /KUNIN
   0                       /KUNOUT
C*********************************************************************************
C                         Particle Shifting Options
C
C   The following lists the particle shifting parameters. These parameters should be
C   changed depending the simulation time step and simulation units
C
C   NSHIFT;     Maximum number of shifts ( should be different for monthly and daily sim)
C   SHIFT;         Shifting distance in not a channel flow (should be different for ft and m)
C   SHIFTCHN; Shifting distance in the case a channel flow (should be different for ft and m)
C-----------------------------------------------------------------------------
C   VALUE                   DESCRIPTION
C-----------------------------------------------------------------------------
   50                       /NSHIFT
   1.0                      /SHIFT
   10.0                      /SHIFTCHN
C*********************************************************************************
C                  Simulation Options
C    KTRACK;  Enter 1  - For Forward Tracking
C                    Enter -1 - For Backward Tracking
C
C---------------------------------------------------------------------------
C VALUE                    DESCRIPTION
C---------------------------------------------------------------------------
   1                       /KTRACK
C*********************************************************************************
C        Defining Special elements in which the particle will be stopped
C
C   NSPEL;   Number of special elements
C-----------------------------------------------------------------------------
C   VALUE                   DESCRIPTION
C-----------------------------------------------------------------------------
   0                      /NSPEL
C-----------------------------------------------------------------------------
C   ELEMENT
C-----------------------------------------------------------------------------
C     121
C     154
C*********************************************************************************
C                  Output Options
C
C   NWRTEP;   Number of days for printing the time series data
C-----------------------------------------------------------------------------
C   VALUE                   DESCRIPTION
C-----------------------------------------------------------------------------
   10                      /NWRTEP
C-----------------------------------------------------------------------------
C   YEAR   MONTH
C-----------------------------------------------------------------------------
     2004    9
     2005    3
```

```
    2005    9
    2006    3
    2006    9
    2007    3
    2007    9
    2008    3
    2008    9
    2009    3
C-----------------------------------------------------------------------------
    C   NDVD;   Number of days for printing velocities, their magnitude, and their
    C           directions for each element for velocity direction output file
    C-----------------------------------------------------------------------------
    C   VALUE                   DESCRIPTION
    C-----------------------------------------------------------------------------
       10                     /NWRTEP
    C-----------------------------------------------------------------------------
    C   YEAR   MONTH
    C-----------------------------------------------------------------------------
    2004    9
    2005    3
    2005    9
    2006    3
    2006    9
    2007    3
    2007    9
    2008    3
    2008    9
    2009    3
    C*******************************************************************************
    C  End of file
    C*******************************************************************************
```

7.4.2 UNIT = 7: Element Configuration File

7.4.3 UNIT = 8: Nodal Coordinate File

These files are already defined in IWRM user manual. Nothing has been changed from the IWRM format.

7.4.4 UNIT = 9: Initial Condition Data File

This is the initial conditions data file. It contains the following data block.

- Number of particles to be simulated
- A conversion factor to convert the stating locations data from any unit to feet
- The particle number, the x and y coordinates of each particles starting location and starting element for each particle

Note: If the element number is not known, just enter 0 for element number, the code should find the element

- The particle number, release and end date of each particle. The release date is specified in year and month format. In the case of daily simulation the release date is the first day of the month. The end date is specified in year and month format, too. In the case of daily simulation the end date is the last day of the month.

```
C*************************************************************************
C
C          INTERGRATED GROUND AND SURFACE WATER MODEL (IWRM)
C
C-------------------------------------------------------------------------
C
C                 INITIAL CONDITION FILE
C                     PART 1
C
C-------------------------------------------------------------------------
C                        REGIONAL GROUDNWATER MODEL
C                       NAME OF PROJECT, CALIFORNIA
C                                PART 1
C*************************************************************************
C                     File Description
C
C   This file contains the starting locations and the release times of all
C   the particles. A factor is also included to convert the x-y- coordinates
C   to feet.
C*************************************************************************
C                 Particle Starting Locations
C
C   NP;     Number of Particles
C-------------------------------------------------------------------------
   10               /NP
   3.2808           /FACT
C-------------------------------------------------------------------------
C
C  The following lists the particle number number, x-y coordinates
C  and elements for each particle
C  ID;     Particle number
C  X,Y;  Coordinates of  particle release location (UTM)
C  E;       Element Number of  particle release location
C
C-------------------------------------------------------------------------
C   Part     -------Coordinates-------  Element
C    ID          X            Y       E
C-------------------------------------------------------------------------
1      656203  42758810
2      656203  42759270
3      656203  42759730
4      656203  42760190
5      656203  42760650
6      656203  42761110
7      656203  42761570
8      656203  42762030
9      656203  42762490
10    656203  42762950
C-------------------------------------------------------------------------
C
C  The following lists the particle number and release times
C  for each particle
```

```
C  ID;    Particle number
C  Rel;   Release time of the particle
C  End;  End time of the particle tracking
C----------------------------------------------------------------------
C   Part     Release Time   End Time
C    ID      Year  Month    Year  Month
C----------------------------------------------------------------------
1     2004     10       9          2109
2     2004     10       9          2109
3     2004     10       9          2109
4     2004     10       9          2109
5     2004     10       9          2109
6     2004     10       9          2109
7     2004     10       9          2109
8     2004     10       9          2109
9     2004     10       9          2109
10    2004     10       9          2109
C***************************************************************************
C End of file
C***************************************************************************
```

7.4.5 UNIT = 6: Standard Output File

The standard output file (Unit 6) is produced in ASCII format and contains much information of the model run and can also utilized for debugging errors during the simu lation. It contains the following output information:

Model Run Time: The date and time of the model run.

Input File Names: Names of all the input files used along with the dates and times they were last modified.

Debugging Errors: Any debugging errors occurred during the simulation.

Particle Shifting Information: The location, element, time and reason of the shift in the case a particle is shifted due to channel flow or if the direction of the particle was chosen wrong. Also prints when the simulation for a particle is over either since a boundary, an internal sink/ source is encountered or the available time is completely consumed

```
*****************************************************************************************
                              REGIONAL GROUNDWATER MODEL
                             NAME OF PROJECT, CALIFORNIA
                                      PART 3
*****************************************************************************************

 THIS RUN IS MADE ON 03/03/09  AT    5:16p

 THE FOLLOWING FILES ARE USED IN THIS SIMULATION:
  5  SACPT.IN3              03/03/2009  05:16 PM          8,189
  6  SACOUT1.OUT
  7  SACELEM.DAT            04/04/2006  12:31 PM        147,726
  8  SACXY.DAT              03/29/2007  10:55 AM        116,126
  9  SACINIT.DAT            03/02/2009  06:07 PM         39,253
 10  SACVEL.BIN             03/02/2009  04:39 PM    520,501,328
 11  SACLOC.OUT             03/03/2009  05:15 PM      4,481,460
```

```
 12  SACELPAR.OUT                03/03/2009  05:15 PM              823
 13  SACENDPNT.OUT               03/03/2009  05:15 PM           90,621
 14  SACTMSRS.OUT                03/03/2009  05:15 PM           58,582
 ENGLISH IN
 ENGLISH OUT
 THE PARTICLE 632 AT X= 2156095.003889801 Y= 14024539.09624803 ON THE LINK B/W 1174 AND 1173
IS STUCK B/W ELEMENTS 1205 AND 1301 AT TIME 200410
 THE PARTICLE 663 AT X= 2156502.203563602 Y= 14023452.15480395 ON THE LINK B/W 1174 AND 1177
IS STUCK B/W ELEMENTS 1302 AND 1303 AT TIME 200411
 THE PARTICLE 648 AT X= 2156309.705282939 Y= 14024132.13951649 ON THE LINK B/W 1174 AND 1173
IS STUCK B/W ELEMENTS 1205 AND 1301 AT TIME 200412
 THE PARTICLE 661 AT X= 2156559.712671483 Y= 14023222.66091118 ON THE LINK B/W 1174 AND 1177
IS STUCK B/W ELEMENTS 1302 AND 1303 AT TIME 200712
 THE PARTICLE 663 AT X= 2156502.203563602 Y= 14023452.15480395 ON THE LINK B/W 1177 AND 1174
IS STUCK B/W ELEMENTS 1303 AND 1302 AT TIME 200812
 THE PARTICLE 664 AT X= 2156479.925575232 Y= 14023541.05658773 ON THE LINK B/W 1177 AND 1174
IS STUCK B/W ELEMENTS 1303 AND 1302 AT TIME 200912
THE PARTICLE 432 AT X= 2151617.633104235 Y= 14025807.83277904 ON THE LINK B/W 1346 AND 1347
IS STOPPED AT TIME 202001
 THE PARTICLE 661 AT X= 2156559.712671483 Y= 14023222.66091118 ON THE LINK B/W 1177 AND 1174
IS STUCK B/W ELEMENTS 1303 AND 1302 AT TIME 202001
 THE PARTICLE 662 AT X= 2156537.261301083 Y= 14023312.25458740 ON THE LINK B/W 1177 AND 1174
IS STUCK B/W ELEMENTS 1303 AND 1302 AT TIME 202001
 THE PARTICLE 663 AT X= 2156502.203563602 Y= 14023452.15480395 ON THE LINK B/W 1174 AND 1177
IS STUCK B/W ELEMENTS 1302 AND 1303 AT TIME 202001
 THE PARTICLE 664 AT X= 2156479.925575232 Y= 14023541.05658773 ON THE LINK B/W 1174 AND 1177
IS STUCK B/W ELEMENTS 1302 AND 1303 AT TIME 202001
 THE PARTICLE 661 AT X= 2156559.712671483 Y= 14023222.66091118 ON THE LINK B/W 1174 AND 1177
IS STUCK B/W ELEMENTS 1302 AND 1303 AT TIME 202002
```

7.4.6 UNIT = 11: Particle Status Output

The particle status output file (Unit 11) is produced in ASCII format and contains *x* and *y* coordinates, and element of the location and status of the simulation at the end of each month both for daily and monthly simulation. For a chosen time step the information for each particle is listed in a line and particles are listed next to each other from the first particle to the last particle.

```
*                    ****************************************
*                    *     PARTICLE TRACKING(FT,DAY)       *
*                    ****************************************
*                    *       PARTICLE STATUS OUTPUT        *
*                    ****************************************
* PART #              1                                    2                                     3    ……
-------------------------------------------------------------------------------------------------------------------------
   TIME     X        Y      ELEMENT   STATUS     X        Y      ELEMENT   STATUS     X
 Y           ELEMENT  STATUS     ……
-------------------------------------------------------------------------------------------------------------------------200410
2152855.7  14028309.8    1296      1   2152855.7  14028460.8    1296      1   2152855.7  14028611.7    1296      1
……
200411   2152840.6  14028308.9    1296      1   2152840.6  14028459.8    1296      1   2152840.6  14028610.7
1296      1    ……
200412   2152825.4  14028307.9    1296      1  2152825.4  14028458.8    1296      1   2152825.4  14028609.7
1296      1    ……
```

200501 2152810.3 14028306.9 1296 1 2152810.3 14028457.8 1296 1 2152810.3 14028608.7
1296 1 ……
200502 2152795.2 14028305.9 1296 1 2152795.2 14028456.8 1296 1 2152795.2 14028607.7
1296 1 ……
200503 2152780.0 14028304.9 1296 1 2152780.0 14028455.8 1296 1 2152780.0 14028606.7
1296 1 ……
200504 2152764.9 14028303.9 1296 1 2152764.9 14028454.8 1296 1 2152764.9 14028605.8
1296 1 ……
200505 2152749.7 14028302.9 1296 1 2152749.7 14028453.8 1296 1 2152749.7 14028604.8
1296 1 ……
200506 2152734.6 14028301.9 1296 1 2152734.6 14028452.8 1296 1 2152734.6 14028603.8
1296 1 ……
200507 2152719.5 14028300.9 1296 1 2152719.5 14028451.8 1296 1 2152719.5 14028602.8
1296 1 ……
200508 2152704.3 14028299.9 1296 1 2152704.3 14028450.8 1296 1 2152706.2 14028601.8
1295 1 …… 200509 2152689.2 14028298.9 1296 1 2152689.2 14028449.8 1296 1
2152705.5 14028601.7 1295 1 ……
200510 2152674.1 14028297.9 1296 1 2152686.7 14028449.5 1295 1 2152704.8 14028601.5
1295 1 ……
200512 2152667.8 14028297.4 1295 1 2152685.9 14028449.3 1295 1 2152704.1 14028601.3
1295 1 ……

7.4.7 UNIT = 12: Element Particle Count Output

The element particle count output file (Unit 12) is produced in ASCII format and contains the element numbers that contains at least one particle and the number of the particles in that element at the end of the month for each time specified in the master control file. The initial element particle count will always be printed at the beginning of the file. The date for the initial element particle count should be the last day of the month before the start of simulation. If the initial date is 200410, the date for the initial element particle count would be 09/ 30/ 2004.

```
*        ****************************************
*        *     PARTICLE TRACKING(FT,DAY)        *
*        ****************************************
*        *   ELEMENT PARTICLE COUNT OUTPUT      *
*        ****************************************
-------------------------------------------------------------------------------------
   TIME  ELEM
-------------------------------------------------------------------------------------
```

200409	1198	1199	1200	1205	1206	1296	1300	1301	1302	1303	1400	1484	1485
# OF PRT	106	91	93	98	1	110	122	52	38	68	21	49	51
200503	1100	1196	1197	1293	1294	1295	1391	1392	1393	1394	1395	1396	1482
# OF PRT	97	86	66	64	77	10	2	39	32	7	24	79	12
200509	1196	1287	1288	1292	1293	1390	1391	1392	1393	1395	1481	1482	1483
# OF PRT	188	1	3	81	4	5	16	59	27	182	3	43	24
200603	1291	1292	1390	1391	1392	1393	1394	1481	1482	1483	1485	1568	1569
# OF PRT	192	3	25	21	59	1	205	40	31	2	251	2	1
200609	1290	1291	1387	1388	1390	1391	1392	1393	1394	1478	1479	1480	1481
# OF PRT	6	181	4	5	25	24	10	179	218	1	27	12	44
200703	1290	1291	1387	1388	1390	1391	1393	1478	1479	1480	1481	1482	1483
# OF PRT	176	13	18	4	19	4	461	26	36	20	36	2	32
200709	1386	1387	1392	1393	1478	1479	1480	1481	1565	1566	1567	1569	1570
# OF PRT	6	3	445	206	19	9	23	18	2	30	9	77	101

200803	1288	1390	1391	1392	1477	1479	1481	1482	1565	1566	1569	1570	1662
# OF PRT	3	209	140	48	1	118	256	1	26	75	43	3	5
200809	1390	1479	1481	1564	1565	1661	1662	1663	1769	1770	1774		
# OF PRT	137	148	517	14	97	1	15	2	3	4	62		
200903	1478	1479	1564	1565	1661	1662	1769	1774	1882	1883			
# OF PRT	1	765	50	15	10	46	11	98	1	3			
200909	1477	1478	1479	1661	1662	1768	1769	1882	1883	1887			
# OF PRT	1	11	754	42	68	7	11	7	1	98			
201003	1386	1477	1478	1479	1660	1661	1767	1768	1769	1881	1882	2010	2011
# OF PRT	1	2	10	753	1	77	3	24	21	6	4	1	97

7.4.8 UNIT = 13: Particle Endpoint Output

The particle endpoint output file (Unit 13) is produced in ASCII format and contains the release time, end of tracking time, *x*-*y* coordinates and element of the location and status of the simulation for each particle at the end of the simulation.

```
*                ****************************************
*                *     PARTICLE TRACKING(FT,DAY)        *
*                ****************************************
*                *     PARTICLE ENDPOINT OUTPUT         *
*                ****************************************
-------------------------------------------------------------------------------
   PART#   REL TIME   END TIME       X          Y        ELEMENT   STATUS
-------------------------------------------------------------------------------
     1     20041001   20341014   2113649.1  14050233.8     444       5
     2     20041001   20800924   2110077.7  14055739.2     285       8
     3     20041001   20740110   2110029.1  14054670.1     360       8
     4     20041001   20730710   2110043.2  14054183.7     360       8
     5     20041001   20731204   2110064.0  14054156.3     361       8
     6     20041001   20730801   2110065.2  14054116.7     361       8
     7     20041001   20981124   2110108.6  14056389.1     285       5
     8     20041001   20890801   2104992.7  14049045.6     519       5
     9     20041001   20750507   2100053.7  14041489.4     868       5
    10     20041001   20751003   2096764.3  14038429.7    1059       5
    11     20041001   21090930   2094250.6  14037662.9    1152       1
    12     20041001   20460124   2102659.5  14032558.0    1162       5
    13     20041001   20250830   2105619.8  14031796.5    1163       5
    14     20041001   20250315   2105768.5  14031792.1    1067       8
    15     20041001   20250805   2105633.3  14031795.2    1163       5
```

7.4.9 UNIT = 14: Particle Location Output

The particle location output file (Unit 14) is produced in ASCII format and contains *x*-*y* coordinates and element of the location and status of the simulation for each particle at the end of the month for the times specified in the master control file. The initial location of the particles will always be printed at the beginning of the file. The date for the initial location of the particles should be the last day of the month before the start of simulation. If the initial date is 200410, the date for the initial location of the particles would be 09/ 30/ 2004.

```
*                    ****************************************
*                    *     PARTICLE TRACKING(FT,DAY)       *
*                    ****************************************
*                    *      PARTICLE LOCATION OUTPUT       *
*                    ****************************************
```

TIME	PART#	X	Y	ELEMENT	STATUS
200409	1	2119068.8	14041824.4	789	0
200409	2	2119068.8	14041004.2	789	0
200409	3	2119068.8	14040184.0	883	0
200409	4	2119068.8	14039363.8	883	0
200409	5	2119068.8	14038543.6	978	0
200503	1	2118886.5	14041836.8	789	1
200503	2	2118886.5	14041016.6	789	1
200503	3	2118863.1	14040180.6	883	1
200503	4	2118863.1	14039360.4	883	1
200503	5	2118836.6	14038588.2	978	1
200509	1	2118698.4	14041855.3	789	1
200509	2	2118698.4	14041035.1	789	1
200509	3	2118637.9	14040188.9	883	1
200509	4	2118637.9	14039368.7	883	1
200509	5	2118559.0	14038707.2	978	1

7.4.10 UNIT = 15: Velocity Field Output

The velocity direction output file (Unit 15) is produced in ASCII format and contains *x-y* coordinates of velocity, their direction and their magnitudes for each element at the end of the month for the times specified in the master control file. If no dates is defined in the master control file, the velocities for the first month of the simulation will be written as a default. If number of dates is not defined zero, the velocities for the first month will only be written if the first month is defined in the master control file.

```
*                    ****************************************
*                    *     PARTICLE TRACKING(FT,DAY)       *
*                    ****************************************
*                    *      VELOCITY DIRECTION OUTPUT      *
*                    ****************************************
```

TIME	ELEM#	Vx	Vy	FLOW DIR(DEG)	FLOW MAGNITUDE
200410	1	-0.149	0.020	262.329	0.150
200410	2	-0.127	0.153	219.558	0.199
200410	3	-0.121	0.232	207.526	0.261
200510	1	-0.018	0.315	183.351	0.315
200510	2	0.059	0.373	170.937	0.378
200510	3	0.142	0.364	158.662	0.390
200610	1	0.280	0.393	144.553	0.483
200610	2	0.286	0.370	142.293	0.467
200610	3	0.493	0.454	132.636	0.670

7.5 Post Processing: Graphical Output

It is possible to generate different graphical outputs based on the results generated by IWRM_PTM. Microsoft Excel, GIS or any other software can be used as a post-processer to plot the necessary graphics. Following types of plots can be generated using IWRM_PTM output:

7.5.1 **Pathline**

Locations computed at specific times (can be obtained from particle location output file (unit = 14)) or at all times (can be obtained from particles status output file (unit = 11)) for a specific particle can be plotted along the pathlines as in Figure 20.

7.5.2 Endpoint

Possible endpoint plot types are

1. Stating locations from a forward tracking analysis
2. Final locations from a forward tracking analysis
3. Final locations from a backward tracking analysis

These plot types are called endpoint plots because they plot either starting or final locations of particle paths based on data in the particle endpoint output file (unit = 13). These plots are useful in delineating sources of water to major discharge points and (or) to hydrogeologic units within a flow system.

Plot type 1 displays starting coordinates from a forward tracking analysis. This type of plot can be used to produce a map of source areas by placing particles at the top of cells receiving areal recharge. Figures 18, 22, and 24 are examples for this kind of plot.

Plot type 2 displays data points marking the final locations from a forward tracking analysis. This type of plot is useful for showing the distribution of recharge entering a model layer or a designated hydrogeologic zone. Figures 18, 22, and 24 are examples for this kind of plot.

Plot type 3 displays data points marking the final locations from a backward tracking analysis. If particles are placed around a discharge point, this type of plot maps source areas for the discharge point. Figure 16 is an example for this kind of plot.

7.5.3 Time Series

Time series plot displays a snapshot of particle locations at specific values of tracking time. Time series plots require a time series file generated by IWRM_PTM. Time series plots may be drawn in using the particle location output file (unit = 14). Points may be drawn in a single color specified by the user, or colors may be allowed to cycle according to the time step number, so that multiple time steps can be distinguished. Figures 19, 21, and 23 can be examples to this kind of plot.

REFRENCES

Cheng, J. R., Cheng, H P., Yeh, G. T. (1996). “A particle tracking technique for the Lagrangian–Eulerian finite element method in multi-dimensions.” *Int JNumer Meth Eng*, 39, 1115–36.

Diersch, H.-J. G. (2002). *“FEFLOW Reference Manual”, Finite Element Subsurface Flow & Transport Simulation System*. WASY Institute for Water Resource Planning and Systems Research Ltd., Berlin, 278 p.

Lapidus, L., and Pinder, G. F. (1982). *Numerical Solution of Partial Differential Equations in Science and Engineering*. John Wiley & Sons, Incorporated, New York.

Pollock, D.W., (1994). *User's Guide for MODPATH/ MODPATH-PLOT, Version 3: A particle tracking post-processing package for MODFLOW, the U.S. Geological Survey finite-difference ground-water flow model*. U.S. Geological Survey Open-File Report 94-464.

Yeh, J., Lin, H. J., Richards, D. R., Cheng J., Cheng, H., and Jones, N. L. (1997). *FEMWATER: A three-dimensional finite element computer model for simulating density dependent flow and transport*. TR CHL-97-12, U.S. Army Engineer Waterways Experiment Station, Vicksburg, MS. Cheng et al 1996.