

Final Report

Evaluation of Computer Software Packages for RBCA Tier-3 Analysis

Submitted to:

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SUMMARY

The most commonly used three-dimensional (3D) computer software packages, Groundwater Modeling System (GMS) and Visual MODFLOW, plus the two-dimensional (2D) software package, BIOPLUME III were selected to be evaluated for the purpose of the Iowa RBCA Tier 3 analysis. The 3D packages contain the well-established groundwater modeling codes, MODFLOW, MT3D, MT3DMS, and RT3D. The specific features of each of the packages are described and compared. In addition, general data requirements and modeling procedures to use these codes and packages are discussed.

A comparison of the three software packages, which is summarized in Table 1, suggests that GMS is superior to Visual MODFLOW and BIOPLUME III because (1) GMS does everything Visual MODFLOW and BIOPLUME III do and more, and (2) GMS is better documented and more users² friendly. Other factors may have to be considered when selecting a software package. The license prices and training costs for GMS and Visual MODFLOW are similar and excellent technical support are provided. The software BIOPLUME III is free but no technical support and training course are provided by the software developer. All three software

can be run on a Pentium PC with 32 MB RAM and SVGA monitor but only GMS has a UNIX version which can be run on a work station.

Tier 3 modeling of the benzene plumes using GMS at three sites in Iowa: Cook Park in Sioux City, Ida Grove in Ida County, and Climbing Hill in Woodbury County, have been carried out and the results have been written and submitted in a separate report.

1. INTRODUCTION

The three-tiered, risk-based corrective action (RBCA) method of assessment for contaminated sites became a common practice in regulatory programs across the country in the 1990s. The procedures for Tier 1 and Tier 2 assessments in the Iowa underground storage tank program are described in IDNR rules (567 Iowa Admin. Code, Chapter 135) and guidance documents. Tier 3 assessment can be carried out when modeling of a site in Tier 2, with a simple analytical solution, shows contaminant pathways to at-risk receptors exist. In some cases, a Tier 3 effort might involve merely determining a few additional facts, such as construction detail of an apparently threatened drinking water well to show the well and aquifer are not actually threatened. In other cases, Tier 3 analysis might need a greater effort, such as gathering additional site-specific data that are required to run an analytical or a numerical computer code of a fate and transport model of chemicals in soils and aquifers (e.g. MODFLOW and MT3D). The hydrogeological conditions in those cases may be complex, for example, involving a pumping well or a multi-layered aquifer. A computer software package has to be chosen in order to model the fate and transport of the contaminants from leaking underground storage tanks in those sites.

Many numerical computer codes have been developed for ground water modeling during the last thirty years. Today, the codes most commonly used by hydrogeological professionals are MODFLOW, MT3D, MT3DMS, RT3D, and BIOPLUME III. These codes provide numerical solutions to the partial differential equations (see Appendix A) describing ground water flow and the fate and transport of contaminants. Use of these codes for a modeling project involves three major steps: 1) prepare input data sets by following specific instructions provided by the code developers; 2) compile and execute the codes; and 3) plot or graph the numerical results. These

are very time-consuming and tedious processes. Therefore, various software packages with graphical pre- and post-processors have been developed during the last a few years and they have been greatly improved in parallel to the improvement of personal computers and UNIX-based work stations. The pre- and post-processors can be used to generate the input data files to the computer codes automatically and to plot the results in charts and contour maps. These packages make what formerly were time-consuming and tedious tasks of data preparation and result presentation an easy job and maybe even an enjoyable experience.

Among various software packages, three are most commonly used by groundwater professionals and thus they are selected to be evaluated for the purpose of RBCA Tier 3 analysis. These three packages are Groundwater Modeling System or GMS, designed by Engineering Computer Graphics Laboratory at Brigham Young University for the Department of Defense (GMS v3.1 Reference Manual, 2000), Visual MODFLOW, developed by Waterloo Hydrogeologic Software (Guiguer and Fanz, 1999), and BIOPLUME III written by Rifai et al (1997). They are evaluated in this report in terms of their ability and usefulness in addressing Tier 3 fate and transport modeling issues. Data requirements and the general procedures for using these software packages to model the fate and transport of contaminants are also described; and start-up costs, training requirements, and time involved in model preparations are compared.

2. SOFTWARE PACKAGE EVALUATION

In this section the three software packages are reviewed first and then the major differences among them are discussed.

2.1 Groundwater Modeling System (GMS)

GMS software package is designed by Engineering Computer Graphics Laboratory of Brigham Young University, under the direction of the U.S. Army Corps of Engineers and involves support from the Department of Defense, the Department of Energy, and the Environmental Protection Agency. GMS is the most sophisticated and comprehensive groundwater modeling environment available today. It has been used in modeling hundreds of contaminated federal sites and at a large and rapidly-growing number of private and international sites. The availability of a UNIX version of GMS for dedicated work station use is important when a large-scale simulation is needed and computer speed is a significant concern.

GMS provides tools for every phase of a groundwater simulation including site characterization, pre-processing, model development, post-processing, calibration, and visualization. It supports graphical construction of stratigraphy with borehole data, and it is the only system that supports geostatistical analysis, and both finite-element and finite-difference modeling in 2D and 3D. Currently-supported codes include MODFLOW, MODPATH, MT3DMS, RT3D, FEMWATER, SEAM3D, SEEP2D, and UTCHEM. Due to the modular nature of GMS, a custom version of GMS with desired models and model interfaces can be configured, so purchase of the entire software package is not necessary. As needs change or as new model become available, other models can be added. This flexibility translates to economy as one need purchase only the modules necessary for the project at hand.

GMS has been specifically designed to minimize the complexities of modeling and maximize the productivity of the user. Input data files to the modeling code can be automatically created in GMS during the process of building a conceptual model. The GMS program is a graphical user interface capable of realistic 3-D representations. Computer generated graphics can be superimposed over an imported image, such as a scanned-in topographic map or GIS plot to aid in presentation. It allows the user to create a conceptual model of subsurface conditions that can then be used to export aquifer parameters into other groundwater flow and contaminant transport models. GMS contains ten separate modules. These ten modules are: Borehole Module, TIN Module, 2-D Scatter Point module, Map Module, Solid Module, 2-D Mesh Module, 2-D Grid Module, 3-D Mesh module, 3-D Grid Module, and 3-D Scatter Point Module. Each module involves a basic data type supported by GMS. Switching from one module to another can be done instantaneously to facilitate the simultaneous use of several data types when necessary. We review only the four modules (Borehole, TIN, 2-D Scatter Point, and Map Module) that are most commonly used in a groundwater modeling project. For other modules the reader is referred to the GMS v3.1 Reference Manual, 2000.

2.1.1 Selected Modules in GMS

2.1.1.1 Borehole Module

The Borehole Module is used to manage borehole or well log data. Borehole data can be imported from a text file or entered directly into GMS using the Borehole Editor. The borehole file is comprised of a list of wells. Each geologic layer is assigned a name and color either by importing a material identification file or by utilizing the Borehole Editor. Once the borehole file is imported into GMS, the boreholes can be displayed as 3-D cylinders. The cylinders are

divided into colored segments, which correspond to the different geologic strata penetrated by the borehole. Segments are separated from each other by contacts. Contacts can be selected interactively to generate a triangulated irregular network (TIN) and contour maps. The solid module can be employed in conjunction with the borehole module to create 3-D block modes with geological data displayed on vertical sections.

2.1.1.2 Triangulated Irregular Network (TIN) Module

The TIN Module is used for surface modeling, such as the generation of stratigraphic contour maps. TINs are constructed from selected borehole contacts, using the Contacts TIN command. Each of the selected contacts is represented by an individual vertex in the TIN Module. TINs are formed by connecting the set of vertices with edges to form a network of triangles. The triangulation is performed automatically using the Delaunay criterion, which assures that the triangles are as equiangular as possible. The surface is assumed to vary linearly across each triangle. The display of vertices and triangles can be toggled off in favor of elevations displayed as contours or as colored gradations. TINs can be displayed in 2-D or 3-D.

2.1.1.3 Two-Dimensional Scatter Point Module

The 2-D scatter Point Module is used to interpolate from groups of 2-D scattered data to any of the data types, such as an active TIN. Once the TIN is imported into the 2-D Scatter Point Module, an interpolation scheme must be chosen. GMS supports a variety of interpolation methods including: linear, Clough-Tocher, inverse distance weighted, natural neighbor, and kriging. Of all the various interpolation methods, kriging invariably yielded the most representative contour maps.

2.1.1.4 Map Module

Scanned images, such as TIFF files of topographic maps, can be imported into GMS using the Map Module. Scanned images can be used as background maps to aid in presentation of TINs. The Map Module also contains drawing and text tools. A background map can be created by tracing over the scanned image and highlighting major features of the study area, including major roads, rivers and towns, etc. The drawing tools can also be used to trace contours of one geologic layer to aid in the editing of another layer either above or below it.

2.1.2 GROUNDWATER MODELING CODES ADOPTED IN GMS

GMS adopted the most widely used groundwater modeling codes, e.g., MODFLOW, MT3D, MT3DMS, and RT3D. These codes are described in the following subsections. They also form the basis of Visual MODFLOW, which will be discussed later.

2.1.2.1 MODFLOW

MODFLOW is the most commonly used computer code for groundwater flow modeling. It is a modular, three-dimensional, block-centered finite-difference flow code developed by the U.S. Geological Survey (McDonald and Harbaugh, 1988) to simulate fluid flow in saturated geological materials. MODFLOW was designed such that the user can select a series of modules to be used during a given simulation. Each module deals with a specific feature of the hydrologic system (e.g., wells, recharge, and rivers). MODFLOW is employed by the GMS and Visual MODFLOW packages to create the groundwater flow regime in which the contaminant transport model subsequently operates.

MODFLOW can be used to simulate fully 3-D systems and quasi three-dimensional systems, in which the flow in aquifers is horizontal and flow through confining beds is vertical. The code can also be used for a two-dimensional mode for simulating flow in a single layer, or two-dimensional flow in a vertical cross section. An aquifer can be confined, unconfined or a mixed confined/unconfined. Flow from external stresses, such as flow to wells, area recharge, evapo-transpiration, flow to drains, and flow through riverbeds, can also be simulated. This code has been validated with many real case applications.

2.1.2.2 MT3D

MT3D code (Zheng, 1990) is widely used for simulating transport of one contaminant species at a time (e.g. benzene) in groundwater. It is a modular, three-dimensional transport code for simulation of advection, dispersion, and chemical reactions of contaminants in groundwater systems. Its solute transport simulation is based on the flow field generated with MODFLOW. MT3D can simulate radioactive decay or biodegradation, and linear and nonlinear sorption processes of Freundlich or Langmuir isotherms.

MT3D includes five files that control various aspects of groundwater contaminant transport (basic, advection, dispersion, source/sink, and reaction). The basic package contains basic information for the model, including grid size and timing information; it is required for all model runs. The advection file controls the mathematical solution scheme to be used to represent contaminant movement in ground water. MT3D contains four different solution methods: 1) Method of Characteristics (MOC); 2) Modified Method of Characteristics (MMOC), a particle tracking method that combines ‘backward’ particle tracking with an interpolation scheme to reduce the computational burden of a simulation, but does not handle sharp

contamination fronts very well; 3) Hybrid Method of Characteristics (HMOC), which combines the standard MOC and the MMOC methods, alternating back and forth depending on the presence of sharp concentration fronts; and 4) Upstream Finite Difference, a method not based on particle tracking, but similar to the forward-difference scheme. The dispersion file controls the amount of dispersion introduced by the model at each step in a simulation. The source/sink mixing file controls sources and sinks of concentration due to wells, drains, recharge, rivers/streams, general head boundaries, and evapo-transpiration. MT3D requires only the concentration information for these processes, as the flow characteristics of the sources/sinks are contained in the 'head and flow file' previously created by MODFLOW. The source/sinks, however, must correspond to sources and sinks entered into the MODFLOW model. Finally, the reaction file controls sorption of contaminants by the selected isotherm, and first-order radioactive decay or biodegradation.

2.1.2.3 MT3DMS

MT3DMS code (Zheng and Wang, 1998) is an expanded version of MT3D that can simulate transport of multiple contaminant species at one time. Additional enhancements over MT3D include a new advection solver method called the total variation diminishing scheme (TVD). This solver allows the user to select from three different mathematical methods, depending on the requirements of the system being modeled. Other enhancements are an implicit generalized conjugate gradient solution method, a non-equilibrium sorption option that allows more accurate retardation modeling if certain parameters are known, and the multiple-species structure that will accommodate add-on reaction packages, such as those in RT3D.

2.1.2.4 RT3D

RT3D (Clement et al., 1998) is a FORTRAN 90-based code for simulating multi-species, reactive transport in ground water. RT3D involves a much more detailed modeling of reactive contaminant transport than MT3DMS does. This code is based on the 1997 version of MT3D (DOD Version 1.5), but has extended capabilities of MT3D with the addition of several reaction packages. The code requires the MODFLOW ground water flow code for computing ground water head distributions. It is the first and most widely known of the multi-species models which use the numerical schemes developed in MT3D. RT3D can accommodate multiple sorbed and aqueous phase species with any one of seven pre-defined reaction frameworks, or any other novel framework that the user may define. This allows, for example, natural attenuation processes or an active remediation system to be evaluated, and simulations to be made to consider contaminants such as heavy metals, explosives, petroleum hydrocarbons, and/or chlorinated solvents. RT3D has preprogrammed reaction packages that include: 1) Aerobic decay of BTEX; 2) Degradation of BTEX using multiple electron acceptors; 3) Kinetically limited hydrocarbon biodegradation using multiple electron acceptors; 4) Rate-limited sorption reactions; 5) Double Monod method for biodegradation; 6) Sequential decay reactions (e.g. PCE → TCE → DCE → VC → Ethene) and 7) An aerobic/anaerobic model for PCE/TCE degradation.

Table 1 lists main features of MODFLOW, MT3D, MT3DMS, and RT3D along with BIOPLUME III. The latter model will be described in Section 2.3.

In general, GMS is a very user-friendly software package with strong technical support. It is well documented and has been upgraded numerous times to offer better user interface

features and newly developed modules. The current version of GMS is 3.1. An overview of this software

Table 1 – Selected Ground Water Flow and Contaminant Transport Codes

Name	Description	Processes simulated	Author(s)
MODFLOW 1988	A modular three-dimensional finite-difference groundwater model for simulation of steady-state or transient flow in isotropic or anisotropic and heterogeneous aquifer systems under various stresses.	Darcian Flow, Drain, River, Well, Evapotranspiration Recharge	M.G. McDonald W.A. Harbaugh
MT3D 1990	A modular three-dimensional transport model for simulation of dissolved constituents in groundwater. It uses the flow field generated by MODFLOW to simulate transport of one contaminant species at a time.	Advection, Dispersion, Equilibrium linear and nonlinear sorption, First-order decay	Z. Zheng
MT3DMS 1998	A multiple-species version of MT3D with a new advection solver method, called the total variation diminishing scheme (TVD), a new implicit generalized conjugate gradient solution method, and non-equilibrium sorption.	Advection, Dispersion, Equilibrium linear and nonlinear sorption, Non-equilibrium sorption, First-order decay	Z. Zheng, P.P.Wang
RT3D 1998	A modular three-dimensional reactive transport model. It has the finite difference and TVD solver in addition to the method of characteristics. It uses the numerical technique of MT3D for multiple species and contains several pre-defined reaction schemes, including the two types reactions simulated by BIOPLUME III. User-defined reaction schemes can also be used.	Advection, Dispersion, Equilibrium linear and nonlinear sorption, Non-equilibrium sorption, First-order decay Instantaneous aerobic decay of BTEX Instantaneous dgradation of BTEX Kinetic-limited degradation of BTEX Rate-limited sorption reactions Double Monod model Sequential decay reactions Aerobic/anaerobic model for PCE/TCE degradation	T.P. Clement Y.Sun B.S. Hooker J.N. Petersen
BIOPLUME III 1998	A two-dimensional finite difference model. It has only one solver: the method of characteristics and can simulate two types of multi-species reactions: oxygen-hydrocarbon instantaneous reactions and sequential electron donor-acceptor reactions. It can also simulate reactant-limited biodegradation.	Advection, Dispersion, Equilibrium linear and nonlinear sorption, Non-equilibrium sorption, First-order decay Instantaneous reactions of BTEX Monod kinetic model of BTEX	H.S. Rifai C.J. Newell J.R. Gonzales S. Dendrou B. Dendrou L. Kennedy J.T. Wilson

is presented in Appendix B. A demonstration version of GMS 3.1 can be downloaded from the web-site of the Environmental Simulations Inc. (www.ems-i.com).

The package allows a user to build multi-layer models, with each layer having different hydrogeologic properties (e.g., hydraulic conductivity and porosity). Areal heterogeneities may also be simulated by defining intra-layer zones (polygons) having different properties. This could be used, for example, to model the lateral pinch-out of a sand aquifer between shale beds. The new version of GMS supports automatic calibration and parameter estimation using PEST or UCODE. These important additions enable one to calibrate a model much more efficiently, alleviates much of the tedium of the trial-and-error calibration technique, and is therefore less labor intensive, less frustrating, and less subjective.

Geostatistical analysis in GMS can be conducted using kriging schemes. This tool can be used to obtain the best estimates for parameters at a given point based on limited coverage of observed values in the vicinity. The calibration feature in GMS can be used in either the steady-state or transient mode of the flow model. Calibration is achieved by trial-and-error runs with incrementally varied parameters until observed field data is reasonably reproduced.

2.2 Visual MODFLOW

Visual MODFLOW is another popularly used software package for 3-D groundwater flow and contaminant transport modeling. It was developed by Waterloo Hydrogeologic Software. In many aspects Visual MODFLOW is similar to GMS. They both use the computer code MODFLOW to model groundwater flow, and they use MT3D, MT3DMS, and RT3D codes for simulating fate and transport of contaminants (see section 2.1.2, above, for more details). Visual MODFLOW has also been specifically designed with pre- and post-processing codes to

minimize the complexities of modeling and maximize the productivity of the user. Input data files to MODFLOW can be automatically created with Visual MODFLOW during the process of building a model. However, Visual MODFLOW is not available in a UNIX version.

Similar to GMS, Visual MODFLOW modeling environment allows the user to assign all of the necessary flow and transport parameters interactively, to run the flow and transport simulation, calibrate the model, and to visualize and print results in plan view and full-screen cross-section. Heterogeneous layered sequences and heterogeneities within layers can be readily simulated. Visual MODFLOW also support automatic calibration and parameter estimation using WinPEST, the only true Windows version of PEST (Parameter EStimation Technology). The Visual MODFLOW interface contains a logical menu structure that guides a user through the steps required to build, calibrate and evaluate a groundwater flow and contaminant transport model. A demo version of Visual MODFLOW can be downloaded from the web-site of the Scientific Software Group (www.scisoftware.com).

The VisualMODFLOW Pro package includes a graphical display module known as 3D-EXPLORER. This latter product enables the user to show AutoCAD files (.dxf) and bitmaps (.bmp) of a project, plus borehole data, surface topography and geologic cross-sections. Modules for seepage analysis (SEEP) and vadose zone modeling (FEMWATER) are not currently available in Visual MODFLOW, but can be purchased separately from Waterloo Hydrogeologic, Inc. The software developer also has a separate package called FRAC3DVS that can simulate groundwater flow and contaminant transport in a fractured aquifer. These products may be viewed at www.flowpath.com.

2.3 BIOPLUME III

The BIOPLUME III software package was written by Rifai et al.(1997) as a collaborative effort between the U.S. EPA and the U.S. Air Force. EPA staff contributed conceptual guidance in the development of the model and field data collection. BIOPLUME III is a window-based program and can not be run on a UNIX machine. It is written to model in one layer the intrinsic remediation of organic contaminants due to the natural processes of advection, dispersion, sorption, and ion exchange. Intrinsic remediation studies are data intensive and must include extensive field studies for model verification. To help the environmental professional with the management, visualization, and decision-making tasks involved, the EIS Graphical User Interface Platform is included in the software. EIS is the latest integrated software platform under Windows 95 in which to register, sort, and evaluate the site-specific data of the physical processes influencing the ground water migration of organic contaminants.

BIOPLUME III is not as comprehensive as either GMS or Visual MODFLOW. BIOPLUME III cannot simulate intra-layer heterogeneity, and there is no provision for model calibration. The incapability to model multiple layers limits the usefulness of this program. BIOPLUME III cannot simulate flow or transport in the vadose zone. But it is offered without cost and can be downloaded from EPA's website (<http://www.epa.gov/ada/csmos>). BIOPLUME III can be useful for designing bioremediation systems in more-or-less homogenous, unconfined aquifers.

BIOPLUME III is based on the U.S. Geological Survey Method of Characteristics (MOC) Model dated July 1989 (Konikow and Bredehoeft, 1989). It simulates the biodegradation of organic contaminants using a number of aerobic and anaerobic electron acceptors: oxygen,

nitrate, iron (III), sulfate, and carbon dioxide. To accomplish this, and to determine the fate and transport of the hydrocarbons and the electron acceptors/reaction by-products, the model solves the transport equation six times per computer run. For the case where iron (III) is used as an electron acceptor, the model simulates the production and transport of iron (II) or ferrous iron. Three different kinetic expressions can be used to simulate the aerobic and anaerobic biodegradation reactions. These include: first-order decay, instantaneous reaction, and Monod kinetics. The principle of superposition is used to combine the hydrocarbon plume with the electron acceptor plumes.

BIOPLUME III reasonably assumes that biodegradation occurs sequentially in the following order:

Oxygen → Nitrate → Iron (III) → Sulfate → Carbon Dioxide

The model can also be used to simulate bioremediation of hydrocarbons in ground water by injecting electron acceptors (except for iron (III)) and can also be used to simulate air sparging for low injection air flow rates. Finally, the model can be used to simulate advection, dispersion, and sorption without including biodegradation.

There are two limitations imposed by the biodegradation expressions incorporated in BIOPLUME III. First, the model does not account for selective or competitive biodegradation of individual hydrocarbons species. This means that hydrocarbons are generally simulated as a lumped organic, which represents the sum of benzene, toluene, ethyl benzene or xylene. If a single component is to be simulated, the user would have to determine how much electron acceptor would be available for the component in question. Secondly, the conceptual model for biodegradation used in BIOPLUME III is a simplification of the complex biologically mediated redox reactions that occur in the subsurface.

The main differences between BIOPLUME III and the RT3D code are:

- (1) BIOPLUME III is a two-dimensional code while RT3D can handle three dimensions;
- (2) BIOPLUME III is based on the USGS MOC transport code which has only one transport solver: the method of characteristics; whereas RT3D is based on MT3DMS code which has the finite-difference and TVD solvers in addition to the method of characteristics;
- (3) BIOPLUME III can simulate two types of multi-species reactions, instantaneous reactions and sequential electron donor-acceptor reactions, while in addition to these two, RT3D can simulate other types of reactions, including a user-definable reaction.

2.4 Comparison of Software Packages

2.4.1 Comparison of Software Functions

There are some major differences among the three software packages described above. First of all, both GMS and Visual MODFLOW can simulate 3-D flow and solute transport while BIOPLUME III can only model 2-D cases. Secondly, Both GMS and Visual MODFLOW use MODFLOW to model groundwater flow and thus can handle the multi-layer heterogeneity of aquifer materials which BIOPLUME III can not. Thirdly, GMS has both PC and UNIX version, and thus can be run on a personal computer as well as a dedicated work station, whereas Visual MODFLOW and BIOPLUME III do not have UNIX version and thus can not run on a work station. This is important when a large-scale simulation is needed and the speed of a computer is a significant concern. Fourthly, GMS contains more solvers than the other two. Fifthly, GMS is building a conceptual model using GIS objects, which the other two packages do not. This feature is especially convenient when the hydrology and geology of the modeling area are

complex. Sixthly, GMS contains a finite element code FEMWATER, which the other two packages do not. FEMWATER is a three-dimensional model for simulating fluid flow and contaminant transport in a vadose zone, such as soil.

The GMS package also has useful tools to conduct geostatistical analysis with Kriging schemes. These tools can be used to obtain the best estimates for the parameter values on each cell based on the limited number of the observed values of these parameters. In addition, GMS contains useful Borehole and Solid modules. These modules can be used to construct three-dimensional models of stratigraphy based on well logs.

A model needs to be calibrated before it can be used for prediction. Both GMS and Visual MODFLOW support automatic calibration tools. Considering that model calibration with trial and error is labor intensive (therefore expensive), frustrating (therefore often left incomplete), and subjective (therefore biased and leading to results the quality of which is difficult to evaluate), GMS and Visual MODFLOW are much superior than BIOPLUME III in this regard.

Table 2 Comparison of the Software Packages for the Tier-3 RBCA Analysis

	GMS	Visual MODFLOW	BIOPLUME III
Dimension	3-D	3-D	2-D
Flow Code	MODFLOW	MODFLOW	BIOPLUME III
Transport Code	MT3D/MT3DMS/RT3D	MT3D/MT3DMS/RT3D	BIOPLUME III
Numerical Methods	FDM,FEM,MOC,TVD	FDM,MOC	FDM,MOC
Model calibration	YES	YES	NO
PC Version	YES	YES	YES
Unix Version	YES	NO	NO
Modeling heterogeneity	YES	YES	NO
Building conceptual models with GIS objects	YES	NO	NO
Geostatistics Analysis	YES	NO	NO
Simulating Vadoze Zone	YES	NO	NO
Building Stratigraphy	YES	NO	NO

2.4.2 Comparison of Software Cost, Support, and System Requirements

Some of the important factors in selecting a software package are their prices, training costs, technical support, and system requirement. Comparative cost, training, and support information is provided in Table 3 (current as of July, 2001). The price of GMS varies depending on modules and codes included. The MODFLOW/MODPATH/MT3D package is recommended for a Tier 3 evaluation. The price of this package is \$2600 and it includes codes MODFLOW, MODPATH, and MT3DMS as well as modules Borehole, TIN, SOLID, 2D Scatter Point, and MAP, plus Geostatistical tools. This package of GMS costs more than that of Visual MODFLOW Pro package because the GMS package offers the GIS tools that Visual MODFLOW does not have. The Visual MODFLOW Pro package includes codes MODFLOW, MODPATH, MT3DMS,

Table 3 Comparison of Cost and Support

	GMS	Visual MODFLOW	BIOPLUME III
Price	\$2600	\$1995	Free
Codes and Modules included	MODFLOW MODPATH MT3DMS GEOSTATISTICS MAP, GRID, TIN, SOLIDE BOREHOLE	MODFLOW MODPATH MT3DMS RT3D WinPEST 3D-EXPLORER	BIOPLUME III
Training Cost	\$1195 (4 days)	\$1075 (3 days)	N/A
Tech Support	Provided	Provided	N/A
System Requirement	Pentium PC 32 MB RAM SVGA Monitor	Pentium PC 32 MB RAM SVGA Monitor	Pentium PC 32 MB RAM SVGA Monitor

	Unix Work Station	
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RT3D, and WinPEST as well as 3D-Explorer. The latter is a 3-D graphic animation module that is part of the standard GMS package. Excellent technical support is provided for both GMS and Visual MODFLOW. A four-day and three-day training courses are offered for GMS and Visual MODFLOW, respectively, and the costs for attending those courses are usually more than \$1000. The software BIOPLUME III is free and can be downloaded from the web-site: <http://www.epa.gov/ada/csmos>. However, no technical support and training course are provided by the software developer. All three software can be run on a Pentium PC with 32 MB RAM and SVGA monitor but only GMS has a UNIX version which can be run a work station.

3. DATA REQUIREMENTS

The data needed to run these software packages are described in this section. This discussion serves only as a guideline for data collection and preparation in order to make better use the software packages evaluated and to obtain more accurate simulation results. This is an overview of the data requirements pertaining to the computer programs and by no means is all the data described in the following required for a Tier 3 analysis. It should be understood that probably no site in Iowa would have such a complete data set available after tier 2 assessment.

Data needed to run groundwater flow and solute transport codes, MODFLOW and MT3D/MT3DMS/RT3D, are summarized in Table 4. The data can be grouped into three general categories. Data under category A, the physical framework, define the geometry of the system, including the thickness and area extent of each hydrostratigraphic unit. Under category B, hydrogeologic data include information on hydrologic heads and fluxes (items B.1 and B.2 in Table 4), which are needed to formulate the conceptual model and check model calibration. Hydrogeologic data also include aquifer properties and hydrologic stresses such as pumping wells. In addition, the distribution of effective porosity is required when calculating average linear velocities from head data for input to particle tracking codes. Under category C chemical data are needed to define a contaminant plume and its fate and transport by groundwater and its attenuation by natural processes.

Table 4 Data needs for a groundwater flow and solute transport model

A. Physical framework

1. Geologic map and cross sections showing the areal and vertical extent and boundaries of the geological formations.
2. Topographic map showing surface water bodies, divides, and wells.
3. Contour maps showing the elevation of the base of the aquifers and confining beds.
4. Isopach maps showing the thickness of aquifers and confining beds.
5. Maps showing the extent and thickness of stream and lake sediments.

B. Hydrogeologic properties

1. Water table and potentiometric maps for all aquifers.
2. Hydrographs of groundwater head and surface water levels and discharge rates.
3. Maps and cross sections showing the hydraulic conductivity and/or transmissivity distribution.
4. Maps and cross sections showing the storage properties of the aquifers and confining beds.
5. Hydraulic conductivity values and their distribution for stream and lake sediments.
6. Spatial and temporal distribution of evapotranspiration, groundwater recharge; Surface water-groundwater interaction, groundwater pumping, and natural groundwater discharge.

C. Chemical properties

1. Initial concentration distribution of the contaminants in all aquifers.
2. Source dimensions and source concentration.
3. Changes of Source concentrations with time and flux rates.
4. Spatial distribution of transport parameters, such as dispersivities and rate coefficient.

(modified from Anderson and Woessner, 1992)

Obtaining the information necessary for modeling is not an easy task. Some data may be obtained from existing reports, but in most cases additional on-site field work may be necessary. A discussion of the field techniques for acquiring these data is beyond the scope of this report. A separate report entitled “Guidelines to Determine Site-Specific Parameters for Modeling the Fate and Transport of Monoaromatic Hydrocarbons in Contaminated Aquifers” by Lovanh, et.

al. (2000) is currently available on the IDNR website: www.state.ia.us/epd. A brief overview of selected field techniques is presented below.

Transmissivity and storage coefficient are typically obtained from pumping test results (Domenico and Schwartz, 1998; Dawson and Istok, 1991). For modeling at a local scale, values of hydraulic conductivity can be determined by pumping tests if volume-averaged values are desired or by slug test if point values are required (Bouwer, 1989; Bouwer and Rice, 1976). For unconsolidated sand-size sediment, hydraulic conductivity may also be obtained from laboratory grain size analyses or from laboratory permeability tests using permeameters. Permeameter results must be used with caution because hydraulic conductivity values obtained from permeameter tests can be several orders of magnitude smaller than values measured in situ. The discrepancy is caused by rearrangement of grains during repacking the sample into the permeameter. Furthermore, large-scale features such as fractures, gravel lenses, or other types of bedding that may impart transmission characteristics to the hydrogeologic unit as whole are not captured in a sample the size of a laboratory column. Hence, even intact core samples taken from the field for laboratory analyses tend to yield lower hydraulic conductivity values than are measured in the field.

Laboratory measurements of specific yield suffer from the same scale problems as hydraulic conductivity measurements. Field measurements of specific yield from pumping tests are also uncertain, as are estimates of effective porosity measured by tracer experiments (De Marsily, 1986). While hydraulic conductivity ranges over 13 orders of magnitude, specific yield and effective porosity vary mainly within 1 order of magnitude. Consequently, there is less uncertainty associated with specific yield and porosity estimates relative to hydraulic conductivity. In the absence of site-specific field or laboratory measurements, initial estimates

for aquifer properties may be given based on literature. The thickness and vertical hydraulic conductivity of stream channel and lake bottom sediments are needed for leakage calculations. These values can be estimated from field measurements or during model calibration.

Hydrologic stresses include pumping, recharge, and evapotranspiration. Of these, pumping rates may be the easiest to estimate. Recharge is one of the most difficult parameters to estimate. Likewise, field information for estimating evapotranspiration (ET) is likely to be sparse. Actual or published field measurements using lysimeters and studies of the vegetation may be helpful in estimating ET rate or areal patterns of ET.

Other parameters appearing in equation (A.1) are the dispersion coefficients, the biodegradation rate coefficient, and retardation factor. Values for these parameters must also be defined before these models can be employed for a specific site in tier 3 risk assessment. The Tier 3 guidelines (Lovanh et. al., 2000) provides a comprehensive review of these parameters and one is referred to that document.

4. MODELING PROCEDURES

The most comprehensive modeling protocol is described in the book written by Anderson and Woessner (1992). For a RBCA Tier 3 analysis, one should proceed according to the following six steps:

1. Data collection Data as listed in Table 3 are collected as previously discussed;
2. Conceptual model development Hydrostratigraphic units and system boundaries are identified. Field data are assembled including information on the water balance and data needed to assign values to aquifer parameters and hydrologic stresses. During this stage a field visit to the site is highly recommended. A field visit will help keep the modeler tied into reality and will exert a positive influence on the subjective decisions that will be made during the modeling study.
3. Model design The conceptual model is put into a form suitable for modeling. This step includes design of the grid, selecting time steps, setting boundary and initial conditions, and preliminary selection of values for aquifer parameters and hydrologic stresses.
4. Model calibration and sensitivity analysis The purpose of calibration is to establish that the model can reasonably reproduce field-measured heads and flows. During calibration a set of values for aquifer parameters and stresses is found that approximates field-measured heads and flows. Calibration is done by trial-and-error adjustment of parameters or by using an automated parameter estimation code. A sensitivity analysis is performed for poorly constrained parameters by varying their values over a likely range, one at a time, and taking note of how the modeling result is affected.

5. Prediction The model is run with calibrated values for parameters and stresses.

Estimates of future stresses are needed to perform a predictive simulation. Uncertainty in a predictive simulation arises from uncertainty in the calibrated model and the inability to estimate accurate values for the magnitude and timing of future stresses.

6. Presentation of modeling results. Clear presentation of model results is essential for effective communication of the modeling effort. The resulting report should contain figures showing the conceptual model and the mathematical grid, as well as maps and cross sections showing the model result. Tables should be included listing all input parameters and settings, and justifications for each. Calibration and sensitivity analysis results should be included. Having all of this readily accessible in the report gives any reader confidence in the modeler's interpretations and conclusions.

The steps described above represent generally accepted procedures for model design and application. The reader must be aware that the applicability of the general modeling procedures discussed herein to a specific modeling problem requires a large component of judgment on the part of the modeler. In many cases some of the steps may need to be repeated, such as the first step: data collection.

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APPENDIX A

The three selected packages, GMS, Visual MODFLOW, and BIOPLUME III, utilize solutions to the following partial differential equation describing transport of contaminants in groundwater (e.g., Javandel, et. al., 1984)

$$\frac{\partial C_k}{\partial t} = \frac{\partial}{\partial x_i} \left(D_{ij} \frac{\partial C_k}{\partial x_j} \right) - \frac{\partial}{\partial x_i} (v_i C_k) + \frac{q_s}{\theta} C_{ks} + r_c \quad \text{where } k=1,2,\dots,m \quad (\text{A.1})$$

$$\frac{dC_{im}}{dt} = r_{im} \quad \text{where } im=1,2, \dots, (n-m) \quad (\text{A.2})$$

where

- n is the total number of species;
- m is the total number of aqueous-phase (mobile) species;
- n-m is the total number of solid-phase (immobile species);
- C_k is the aqueous-phase concentration of k^{th} species dissolved in groundwater, ML^{-3} ;
- C_{im} is the solid-phase concentration of im^{th} species, ML^{-3} ;
- t is time, T;
- x_i is the distance along the respective Cartesian coordinate axis, L;
- D_{ij} is the hydrodynamic dispersion coefficient, L^2T^{-1} ;
- v_i is the seepage or linear pore water velocity, LT^{-1} ;
- q_s is the volumetric flux of water per unit volume of aquifer representing sources (positive) and sinks (negative), T^{-1}
- C_s is the concentration of the sources of sinks, ML^{-3} ;
- θ is the porosity of the porous medium, dimensionless;
- r_c is the rate of all reactions that occur in the aqueous phase, $MM^{-1}L^{-3}$ or ML^3T^{-1}

r_{im} is the rate of all reactions that occur in the solid-phase, $\text{MM}^{-1}\text{L}^{-3}$ or ML^3T^{-1}

The transport equation (A.1) is linked to the flow equation through the relationship:

$$v_i = -\frac{K_{ii}}{\theta} \frac{\partial h}{\partial x_i} \quad (\text{A.3})$$

where K_{ii} is a principal component of the hydraulic conductivity tensor, LT^{-1} and h is the hydraulic head, L.

The hydraulic head is obtained from the solution of the three-dimensional groundwater flow equation:

$$\frac{\partial}{\partial x_i} \left(K_{ii} \frac{\partial h}{\partial x_j} \right) + q_s = S_s \frac{\partial h}{\partial t} \quad (\text{A.4})$$

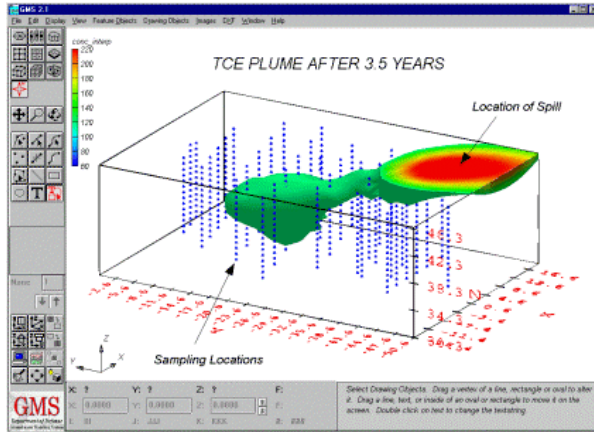
where q_s is the source or sink and S_s is the specific storage of the porous materials, L^{-1} .

Note that the hydraulic conductivity tensor (K_{ij}) actually has nine components. However, it is generally assumed that the principal components of the hydraulic conductivity tensor (K_{ii} , or K_{xx} , K_{yy} , K_{zz}) are aligned with the x , y and z coordinate axes so that non-principal components become zero. This assumption is incorporated in most commonly used flow models, including MODFLOW.

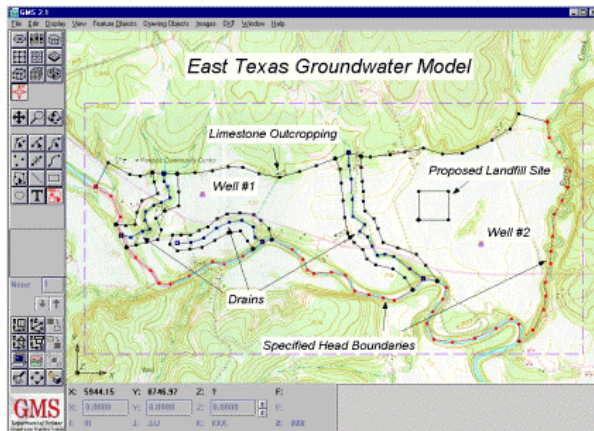
As with many partial differential equations that describe the fate and transport of a contaminant, equation (A.1) can be solved analytically with simplified assumptions to obtain exact and closed-form solutions, such as those used in Tier 2 assessments. Those analytical solutions are generally limited to steady and uniform flow, and should not be used for groundwater flow or solute transport problems in heterogeneous and/or an-isotropic aquifers with irregular boundaries. In the latter cases numerical solutions to equation (A.1) have to be derived. The numerical solutions can simulate more complex systems, such as unsteady flow

and contaminant transport affected by multiple reactions for which reaction rates or chemical properties vary spatially. These solutions are programmed in groundwater modeling codes.

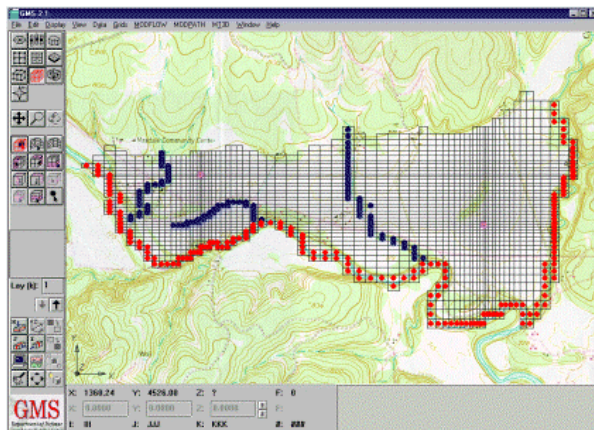
APPENDIX B: GMS Overview



GMS is a comprehensive package which provides tools for every phase of a groundwater simulation including site characterization, model development, post-processing, calibration, and visualization. GMS is the only system which supports TINs, solids, borehole data, 2D & 3D geostatistics, and both finite element and finite difference models in 2D & 3D. Currently supported models include MODFLOW, MODPATH, MT3D, RT3D, FEMWATER, and SEEP2D.



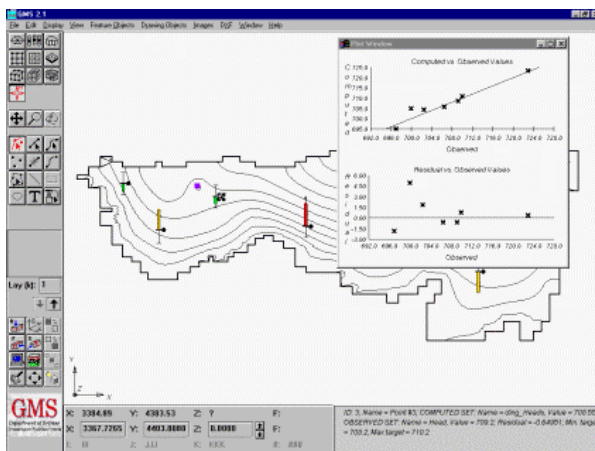
GIS TOOLS The Map module can be used to construct a conceptual model directly on top of a scanned map of a site using GIS objects. Boundary conditions and parameter values can be assigned directly to the GIS objects. The conceptual model can be used to automatically generate a MODFLOW/MODPATH/MT3D grid and assign all stresses, sources/sinks, and material properties to the appropriate cells.



MODFLOW GMS includes MODFLOW interface. Models can be defined and edited at the conceptual model level or on a cell-by-cell basis at the grid level. All model parameters are easily defined. MODFLOW can be launched from a GMS menu. All popular packages are supported including the Horizontal Flow Barrier package and the Stream/Aquifer Interaction package. GMS reads/writes native MODFLOW files.

MT3D/M3DMS Using a previously computed MODFLOW flow solution, MT3D/MT3DMS can be used to perform a contaminant transport simulation. The MT3D/MT3DMS input data can be defined either at the conceptual model level using GIS objects or at the grid level. Advection, dispersion, diffusion, sorption, and decay can all be simulated. Output can be viewed using color-shaded contour plots or 3D iso-surface plots. Animations can also be generated to clearly illustrate the fate of a plume over time.

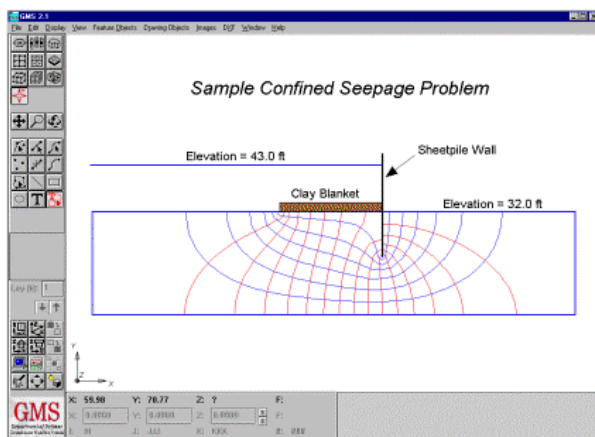
RT3D is a new reactive transport model developed by Batelle at the Pacific Northwest National Laboratories. RT3D is a modified version of MT3D which can be used to model multi-species transport and complex chemical reactions including bioremediation and natural attenuation. Numerous pre-defined reactions are available and an option is provided for linking to user-defined reactions.



CALIBRATION TOOLS GMS includes a suite of tools to aid in model calibration. One or more observed values (typically head) can be defined at observation points. With each value a confidence can be assigned. When a computed solution is imported to GMS, the residual error is plotted on a calibration target at each point and a variety of plots can be generated showing calibration statistics. The calibration tools can be used with any of the models in GMS.

MODPATH Once a flow solution is computed by MODFLOW, a particle tracking analysis can be performed with MODPATH. MODPATH can be used to compute capture zones for wells and to estimate travel times for contaminants in groundwater. Starting locations for particles can be defined graphically. A variety of options for post-processing MODPATH solutions are available. Particle tracking can be performed with either a steady state or transient flow field.

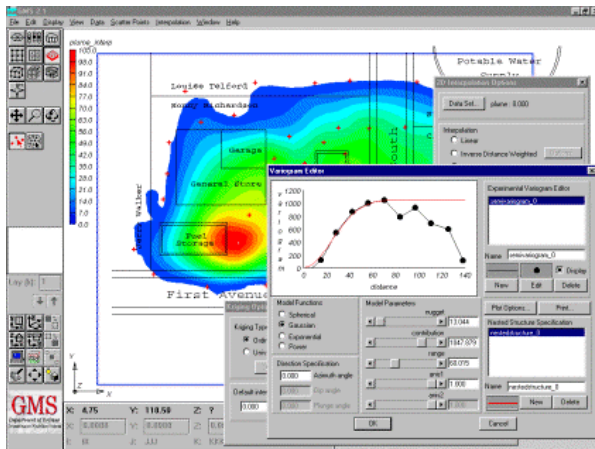
FEMWATER is a fully 3D finite element model. It can be used to simulate density driven, coupled flow and contaminant transport in both the saturated and unsaturated zone. Complex stratigraphy can be directly represented in the model rather than hidden in transmissivity and leakage terms. Solutions can be displayed using highly realistic 3D plots and animation sequences. Well-suited for general purpose flow and transport modeling and salinity intrusion studies.



SEEP2D is a 2D finite element model which can be used to simulate flow in confined or unconfined profile models or for confined areal models. For unconfined models, flow can be modeled in both the saturated and unsaturated zone. Solutions can be displayed using plots of

flow vectors and head contours. For many problems, a complete flow net with equipotential lines and flow lines can be generated. SEEP2D is perfect for analyzing flow through earth dams and levees.

SITE CHARACTERIZATION The borehole module in GMS can be used to import various types of site characterization data. Traditional borehole logs can be imported and used to plot stratigraphy or to build TINs or solid models. Geophysical data including data from cone penetrometer tests (CPT) can also be imported and plotted. The geophysical data can be processed to infer stratigraphy or they can be filtered and converted to scatter points for 3D interpolation.



GEOSTATISTICS GMS supports a sophisticated suite of 2D and 3D geostatistical tools. These tools can be used to generate a 2D contour map or a 3D iso-surface plot of an existing contaminant plume. They can also be used to interpolate elevations and other model parameters such as starting head. Numerous interpolation methods are supported including Kriging, Natural Neighbor, and Inverse Distance Weighted. A graphical editor is provided for creating variograms for Kriging.

STRATIGRAPHY MODELING GMS provides an extensive set of tools for modeling the stratigraphy at a site. Borehole, scatter point, and geophysical data can be used to construct stacked surface models using TINs, or fully 3D volumetric models using boundary representation solid models. Solid models can be sliced interactively to construct simple cross section plots or complex fence diagrams. The volume of each solid can be computed.

ANIMATION When visualizing the results of a transient simulation, there is simply no substitute for animation. Any transient data set can be converted to an animation film loop in GMS in seconds. The animations are generated and saved in the Microsoft Video for Windows (*.AVI) format. The resulting AVI files can be played back at a later time inside GMS or as a stand-alone object simply by double-clicking on the file. AVI files can also be imported to Powerpoint presentations or placed on web pages.