MODFLOW and Related Codes

**FUNCTIONAL REQUIREMENTS DOCUMENT**

**Signature Page**

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# OVERVIEW AND SCOPE

| Acronym: | MODFLOW | HISI ID: | 2517 | Software Grade: | C |
| --- | --- | --- | --- | --- | --- |
| Acronym: | MT3DMS | HISI ID: | 2518 |
| Acronym: | GSLIB | HISI ID: |  | Software Grade: | N/A |
| Acronym: | MODPATH | HISI ID: |  |
| Acronym: | PEST | HISI ID: |  |
| Acronym: | GWVISTA | HISI ID: |  |
| Acronym: | SURFER | HISI ID: |  |

This Functional Requirements Document (FRD) is required by PRC-PRO-IRM-309, *Controlled Software Management*, to identify the calculational needs that the CH2M HILL Plateau Remediation Company (CHPRC) intends to meet using the MODFLOW (MODular finite-difference FLOW model) and related codes. CHPRC’s intended use of this software is to calculate short- and long-term subsurface water and contaminant transport in the unconfined aquifer at the Hanford Site at various scales.

This FRD includes an alternatives analysis (Section 1.1) that clarifies why this software has been chosen by CHPRC for the intended use.

Controlled use of this software by CHPRC is directed by the requirements specified in CHPRC-00258, *MODFLOW and Related Codes Software Management Plan* (SMP) (Nichols 2009b). All software addressed by this FRD is acquired, commercial, off-the-shelf (COTS) software applications. This software will run on desktop computers, scientific workstations, and large computer clusters, both within and outside of the Hanford Local Area Network (HLAN).

Multiple software items are addressed by this FRD because these codes have been identified as closely related and functioning to support the numerical implementation of a single groundwater flow and transport model. Therefore, integrated management of these individual software items is preferred to ensure consistent application of quality assurance requirements. The specific software configuration items addressed by this FRD are:

**Calculational Software:**

* **MODFLOW-2000** – the U.S. Geological Survey (USGS) three-dimensional finite-difference groundwater model that simulates steady and non-steady flow in an irregularly shaped flow system in which aquifer layers can be confined, unconfined, or a combination of confined and unconfined.
* **MODFLOW-2000-MST** – the U.S. Geological Survey (USGS) three-dimensional finite-difference groundwater model that simulates steady and non-steady flow in an irregularly shaped flow system in which aquifer layers can be confined, unconfined, or a combination of confined and unconfined. The -MST designation denotes a variant version of MODFLOW adopted by CHPRC that includes source modifications prepared by S.S. Papadopulos and Associates for minimum saturated thickness as part of the 200-ZP-1 Operable Unit groundwater modeling work to handle drying cells. CHPRC deems these modifications essential to enabling use of MODFLOW in the Hanford geologic setting.
* **MT3DMS** – modular three-dimensional, multi-species transport model for simulation of advection, dispersion, and chemical reactions of contaminants in groundwater systems.

**Support Software:**

* **ArcGIS™[[1]](#footnote-1)** – acquired software visualization tool (typically used to assess validity of interpolated hydrostratigraphic surfaces and extents and to visually identify locations to place control points to constrain the hydrostratigraphic surfaces)
* **allocateQ** – utility code that constructs a MODFLOW well package (“WEL”) file; identifies water table elevations at proposed remedy well locations, and processes the hydraulic conductivity and saturated thickness data so that, so that flow for fully-penetrating wells that penetrate multiple model layers can be properly apportioned according to layer transmissivity
* **Calcthick** –utility code that determines saturated thickness from MODFLOW layer definitions and calculated heads
* **HeadTargDry** – utility code that retrieves and interpolates simulated heads allowing for dry model cells. It is used for model calibration; performs linear interpolation between model nodes to the coordinates of the monitoring location; includes options to ‘hunt’ down through dry layers for the water table
* **GSLIB** – geostatistical software library
* **MakeGHB3** – utility code that prepares the general head boundary (“GHB”) input file for MODFLOW
* **MakeRecharge** – creates the recharge (“RCH”) input files for both the historic and predictive model simulations, specifying recharge values from natural, artificial, and overland flow data sets
* **MODPATH/MODPATH-PLOT** – particle-tracking post processing code for MODFLOW
* **NRDWL\_conc** – utility code that replaces contaminant concentrations from QuantVar program with specified concentrations at specific cell locations
* **PEST** – for model calibration, parameter estimation and predictive uncertainty analysis
* **Read-lst-budget** – utility code that creates a file “prefix”-budget.out that will be brought into a spreadsheet to tabulate and plot (a) the volumetric budget terms (IN and OUT), and (b) the mass balance error of the MODFLOW simulation, as reported by MODFLOW at the end of each interval specific in the output control (OC) file
* **Read-MT3D-Out-Budget** – utility code that compiles mass balance reports generated by MT3D into a single readable file, in a manner similar to READ-LST-BUDGET for MODFLOW
* **Starthead** – utility code that creates the initial head conditions for the predictive flow calculations by plucking the last time step head result from historic run heads output
* **Groundwater Vistas™[[2]](#footnote-2)** – Windows®[[3]](#footnote-3) graphical user interface for 3-D groundwater flow & transport modeling
* **Surfer™[[4]](#footnote-4)** - Graphical interpolation and display for preparing geostatistical distributions of contaminants to support definition of initial conditions
* **Well-layers** – utility code that determines the layers in the model that a well screen of a particular well overlaps

Calculational software is distinguished from supporting software because these two groups of software are classified and graded differently in the SMP. The basis for the difference is that the first three codes, MODFLOW-2000, MODFLOW-2000-MST, and MT3DMS, calculate results that will be used to support decision making and as such, these items constitute safety software graded to level C. In contrast, support software includes graphical interfaces, visualization, and input preparation support but not calculation of results that directly support decision making, and are therefore not rated as safety software and are graded to N/A (that is, none of the software grading checklist questions are answered affirmatively).

## Alternatives Analysis

MODFLOW is a computer code that solves the groundwater flow equation. The program is the most widely used by hydrogeologists in the world to simulate the flow of groundwater through aquifers. Related codes solve for flow pathlines, contaminant transport, and other aspects controlled by groundwater flow. The code is free software, written primarily in Fortran, and can compile and run on Windows®, Linux®[[5]](#footnote-5), or other operating systems. It is developed and distributed by the USGS.

MODFLOW is a computer program that numerically solves the three-dimensional ground-water flow equation for a porous medium by using a finite-difference method. MODFLOW is designed to be modular in that different functionalities such as wells, rivers, evapotranspiration, etc. can be added as modules to the basic groundwater flow solutions. Although MODFLOW was designed to be easily enhanced, the design was oriented toward additions to the ground-water flow equation. Frequently there is a need to solve additional equations; for example, transport equations and equations for estimating parameter values that produce the closest match between model-calculated heads and flows and measured values. The version of MODFLOW that is the basis for the version addressed in this SMP, MODFLOW-2000, is designed to accommodate the solution of equations in addition to the ground-water flow equation. The user’s manual for MODFLOW-2000 (Harbaugh et al. 2000) contains an overview of the old and added design concepts, documents one new package, and contains input instructions for using the model to solve the groundwater flow equation.

Alternatives are restricted given DOE’s direction to use MODFLOW software for groundwater simulation at the Hanford Site (Klein 2006). Other software tools exist; examples include

* The Coupled Fluid, Energy, and Solute Transport (CFEST) (Gupta 1997) – previously used for groundwater flow and transport modeling at Hanford (Cole et al. 2001a, Cole et al. 2001b, Cole et al. 2001c, Vermeul et al. 2001, Vermeul et al. 2003a, Vermeul et al. 2003b, Bergeron and Cole 2005, Freedman et al. 2005). CFEST’s finite-element formulation provided certain advantages including better capability to represent the complex flood-deposition formation geology at Hanford than most finite-difference formulations can provide. However, use of CFEST is currently severely limited due to consistency and transparency concerns and well as past quality assurance issues (Triay and Gilbertson 2006).
* The Finite Element Heat and Mass Transfer (FEHM) code (Dash 2006) is another finite-element numerical simulation code for subsurface transport processes. It simulates three-dimensional, time-dependent, multiphase, multi-component, nonisothermal, reactive flow through porous and fractured media. Like CFEST, it can accurately represent complex three-dimensional geologic media and structures and their effects on subsurface flow and transport. FEHM has been used to simulate groundwater and contaminant flow and transport in deep and shallow, fractured and un-fractured porous media throughout the US DOE complex.
* Subsurface Transport Over Multiple Phases (STOMP) (Nichols et al. 1997, White and Oostrom 2000, White and Oostrom 2006) and TOUGH2 (Pruess et al. 1999) are extremely capable open-source finite-difference codes developed at DOE national laboratories. While these variable-saturation multiphase codes are fully capable of simulating saturated conditions, they carry high overhead in saturated zone applications due to their multiphase capabilities and limited geometrical capabilities for simulation of extensive complex aquifers at this time.
* Various analytical models – are suitable only for the simplest of groundwater model applications, and are insufficient for most simulation needs in the complex Hanford Site subsurface environment.

The key benefits of the MODFLOW and related software for CHPRC use in saturated zone flow and transport modeling are:

* Acceptance and mandate by the DOE (Klein 2006) for use in saturated zone modeling at Hanford
* Open source distribution of MODFLOW and related utilities promotes transparency
* Exceptionally wide application of these software packages nationally and internationally
* Available expertise in use of this software at the CHPRC (specifically in the CHPRC’s preselected subcontractor, Intera).

In view of DOE’s standing directives concerning permissible codes for use to simulate subsurface flow and transport at Hanford as well as the desire to use open source products to promote model transparency, the available expertise with MODFLOW within the CHPRC, the use of MODFLOW as the basis for the site-wide groundwater model in the forthcoming Tank Closure and Waste Management Environmental Impact Statement (TC&WM EIS), plus MODFLOW’s status as the most widely used groundwater model in the world, this software is deemed the best available alternative for CHPRC intended use in modeling groundwater at the Hanford Site.

# CONCEPT DEFINITION

## Statement of Need

Support to Operable Unit work at the Hanford Site will be highly reliant upon successful management and use of this software. Achievement of site-wide model and risk integration aspects of the Plateau Remediation Contract by CHPRC will require successful management and use of the software listed in Section 1. Data sources will be primarily those available in site-wide environmental databases managed by the CHPRC as well as other documented and qualified data sources and documents for environmental information.

## Scope of Need

MODFLOW is used for several operable unit-scale and larger groundwater modeling tasks.

## Solution Objectives

The major performance objective for the use of the MODFLOW and related software is to calculate subsurface fluid flow and contaminant transport solutions for saturated conditions to support *Resource Conservation and Recovery Act of 1976* (RCRA), *Comprehensive Environmental Response, Compensation, and Liability Act of 1980* (CERCLA), DOE O 435.1, *Radioactive Waste Management*, and other environmental calculations for regulatory and administrative purposes. The goals met by using this software are completion of traceable, reproducible, transparent, and defensible flow and transport simulations.

Requirements for MODFLOW will include a demonstrated accurate solution of a simple groundwater flow model domain using features and properties representative of Hanford geological media as judged by comparison to an analytical solution or other acceptable comparison.

Requirements for MT3DMS will include a demonstrated accurate solution of contaminant transport in a simple groundwater model using numerical features and properties representative of Hanford geological media as judged by comparison to an analytical solution or other acceptable comparison.

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# EXECUTIVE SUMMARY

## Sponsoring Organizations

This FRD documents functional requirements for use of the MODFLOW and related codes by the CHPRC and its preselected subcontractors. Specific responsibility assignments are made in the SMP.

MODFLOW and related codes are primarily intended for use for modeling of subsurface flow and transport by the Integration and Assessments Group in the Environmental Programs and Regulatory Management organization. This group is migrating to central management of model and risk software to ensure consistent software quality assurance of software used for environmental calculations.

## Strategic Direction

DOE has mandated the use of MODFLOW for groundwater modeling at the Hanford Site (Klein 2006). Qualification and use of MODFLOW and related codes is therefore fully supportive of the strategy for the Hanford Site.

## Risk Analysis

Primary identified risks to the use of this software are those that emerge from evaluating software grade and classification, which are discussed in the SMP. To summarize, those risks are that

* software failure could cause a potential violation of regulatory permitting requirements
* software is used to support a legal, regulatory, and other external milestones and therefore software failures could damage DOE and CHPRC reputation and withdrawal of documents or other undesirable outcomes

Adherence to quality assurance procedures for management of software provides the primary mitigation to these identified risks.

Past experience strongly suggests, however, that the greatest risk associated with the use of environmental calculation software arises not from problems that could be present in the software itself, but rather in use of unverified or erroneous inputs. This risk is minimized by ensuring strong adherence to quality assurance procedures for calculation package preparation and issue.

# PROBLEM DEFINITION

The problems to be solved through use of MODFLOW and related codes, the software users, dependencies, limitations and constraints of use, applicable regulations and orders, and process for acceptance of this software are outlined below.

## Business Process

In view of DOE’s standing directives concerning codes to use for subsurface simulation at Hanford as well as the desire to use open source products to promote model transparency, the available expertise with MODFLOW within the CHPRC, the use of MODFLOW as the basis for the site-wide model in the forthcoming TC&WM EIS, plus MODFLOW’s status as the most widely used groundwater model in the world, this software is deemed the best available alternative for CHPRC intended uses in modeling groundwater flow and transport at the Hanford Site.

## System Users

Users of MODFLOW and related codes must possess these characteristics;

* + - Advanced training, and preferably graduate level study, in hydrology, geology, soil physics, or water resources engineering including numerical simulation techniques
    - Training and/or experience in using MODFLOW and related codes

## Dependencies, Limitations, and Constraints

As a general simulator, the MODFLOW and related codes are suitable to application of a wide variety of conceptual models that incorporate relevant features, events and processes involving mass and momentum conservation of water and contaminants in saturated porous media. It is not possible to enumerate all the possible conceptual models for which this software will be used to implement numerical models.

The MODFLOW software is highly portable, as it is distributed as Fortran source code that can be compiled and linked on a number of different computer platforms using a variety of operating systems. The Fortran language is one of the fastest and most efficient of the computer languages available for scientific computing.

The availability of source code would also permit CHPRC to modify or extend MODFLOW capabilities easily, though there are no plans to do this at this time and the SMP will exclude such modifications from the software management scope.

Hardware failures will only result in the need to repeat the simulation that was not finished at the time of failure. Regular backup of model input and output files, as directed by the SMP, will mitigate this risk.

## Regulations, Procedures, and Policies

Primary regulations and orders that give rise to the need for the calculations that will be performed using the MODFLOW are RCRA, the CERCLA, and DOE O 435.1.

As software used for evaluation of radioactive contaminants at a DOE site, the quality requirements of NQA-1 are imposed on CHPRC’s use of MODFLOW software by DOE O 414.1C.

## Acceptance Criteria

The calculation software (MODFLOW-2000, MODFLOW-2000-MST, and MT3DMS) will require demonstration of accurate solution to a groundwater flow and transport problem or problems representative of Hanford geologic conditions and for which a known solution (analytical is preferred) is available. The specific problem(s) and acceptance criteria are identified in CHPRC-00259, *MODFLOW and Related Codes Software Test Plan* (STP) (Nichols and Clemo 2009) and requirements are be traced in CHPRC-00260, *MODFLOW and Related Codes Requirements Traceability Matrix* (RTM) (Nichols 2009a).

Supporting software will not be used to generate decision making basis calculations, but rather support the development and visualization of the solutions. Therefore separate testing beyond installation testing will not be required for supporting software.

In addition to acceptance and installation testing designed to confirm correct operation of the calculational software, modeling work using the MODFLOW software will be subject to evaluation of specific models developed using this simulator. This may include history matching (demonstration that the model reproduces historical data), comparison to flow cell data, or other means to validate the specific model (which includes the combination of the conceptual model, the software, the input parameters and data, and the numerical implementation). Such model validation work will be documented in calculation packages.

# FUNCTIONAL DESIGN

## Structure

(Not applicable; acquired software.)

## Data Design and Control

(Not applicable; acquired software.)

## Human-Machine Interface Design

(Not applicable; acquired software.)

## System Interface Design

(Not applicable; acquired software.)

## Security Structure

(Not applicable; security functions are not part of this software.)

## Implementation

Groundwater Vistas™ will primarily be used for visualization purposes. This software is a sophisticated Windows® graphical user interface for three-dimensional groundwater flow & transport modeling. It couples a powerful model design system with comprehensive graphical analysis tools. It is a model-independent graphical design system for MODFLOW/MODPATH (both steady-state and transient versions), MT3DMS, MODFLOW-2000, and the model-independent calibration software PEST (Parameter ESTimation for any model). The combination of PEST and Groundwater Vistas™ automatic sensitivity analysis provides a powerful calibration tool.

Because the MODFLOW software itself and related modules are written in ANSI Standard Fortran, these can be compiled and operated on any computer platform for which a Fortran compiler is available. This includes Linux®, Windows® and other desktops and workstations, as well as various supercomputer systems and clusters. There is no particular minimum hardware configuration; rather, the maximum size of problem that can be solved using MODFLOW is a function of the computer memory of the host computer.

A suitable operating system (Linux®, Windows®, and others) along with an ANSI-standard Fortran compiler is required to prepare MODFLOW and related executables from source code distributed by the USGS and run the resulting executables. The commercial interface code Groundwater Vistas is distributed as an executable and is restricted to use on a Windows® computer and provides a graphical user interface.

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**Acronyms, Abbreviations, and Definitions**

| Acronym | Description |
| --- | --- |
| ATR | Acceptance Test Report |
| calibration | Modification of model parameters to improve the fit of the model to measured data; for example, systematically changing the transmissivities in a flow model until the difference between predicted and measured hydraulic heads at well locations is minimized |
| CBAS | CERCLA Baseline Assessment Strategy |
| CERCLA | *Comprehensive Environmental Response, Compensation, and Liability Act of 1980* |
| CFEST | Coupled Fluid, Energy, and Solute Transport (software) |
| CHPRC | CH2M HILL Plateau Remediation Company |
| COTS | Commercial Off-The-Shelf (software category) |
| FEHM | Finite Element Heat and Mass Transfer Code |
| finite difference | Numerical method for approximating the solutions to differential equations using finite difference equations to approximate derivatives |
| finite element | Numerical technique for finding approximate solutions of partial differential equations as well as of integral equations. The solution approach is based either on eliminating the differential equation completely (steady state problems), or rendering the partial differential equations into an approximating system of ordinary differential equations, which are then numerically integrated using standard techniques such as Euler's method, Runge-Kutta, etc. |
| FRD | Functional Requirements Document |
| MODFLOW | MODular finite-difference FLOW model |
| PEST | Parameter EStimation for any Model |
| RCRA | *Resource Conservation and Recovery Act of 1976* |
| SMP | Software Management Plan |
| STOMP | Subsurface Transport Over Multiple Phases (software) |
| STP | Software Test Plan |
| TC&WM EIS | Tank Closure and Waste Management EIS |
| TOUGH | Transport Of Unsaturated Groundwater and Heat (software) |
| USGS | U.S. Geological Survey |

# ATTACHMENTS

None.

1. ArcGIS is a trademark, registered trademarks, or service marks of ESRI in the United States, the European Community, or certain other jurisdictions [↑](#footnote-ref-1)
2. Groundwater Vistas™ is a trademark of Scientific Software Group, Sandy, Utah. [↑](#footnote-ref-2)
3. Windows® is a registered trademark of Microsoft Corporation in the United States and/or other countries. [↑](#footnote-ref-3)
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