MODFLOW and Related Codes

**SOFTWARE MANAGEMENT PLAN**

**Signature Page**

|  |  |  |  |
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| Software Owner |  | Date |  |
|  | William E. Nichols, Modeling Team Leader  CHPRC |  |  |
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[], 2018

# OVERVIEW AND SCOPE

| Acronym: | MODFLOW | HISI ID: | 2517 | Software Grade: | C |
| --- | --- | --- | --- | --- | --- |
| Acronym: | MT3DMS | HISI ID: | 2518 |
|  | MODPATH |  |  | Software Grade: | C |
|  | Mod-PATH3DU |  |  |  |  |

The purpose of this Software Management Plan (SMP) is to identify how MODFLOW ([McDonald and Harbaugh 2003](#_ENREF_10)) developed and distributed by the U.S. Geological Survey (USGS) and related software identified in this SMP will be managed as acquired software by CH2M HILL Plateau Remediation Company (CHPRC) for use by CHPRC, its subcontractors, and other Hanford contractors as part of CHPRC’s site risk assessment and modeling integration role. The need for and content of this SMP is established in PRC-PRO-IRM-309, *Controlled Software Management* ([CHPRC 2010b](#_ENREF_4)). The intended audience of this SMP includes the software owner, quality engineer, software users, software test team, and management.

The MODFLOW groundwater software has been developed by the USGS and has been continuously upgraded since the first version, MODFLOW88 was released in 1988 ([McDonald and Harbaugh 2003](#_ENREF_10)). MODFLOW-2005 is the newest version currently available. Together, the different versions of MODFLOW have an international user base of over 1000 users. As a groundwater flow and transport simulator, the MODFLOW and related software addressed in this SMP are software suited to the simulation of a wide variety of saturated zone flow and transport problems. DOE has previously mandated use of the MODFLOW software for groundwater modeling at the Hanford Site ([Klein 2006](#_ENREF_9)). Primary reasons for this mandate included the open source, nonproprietary status of this software and the fact that MODFLOW is the most widely used of groundwater flow models.

[This revision: [describe what’s changing]] [add a sentence somewhere that says we’re compliant with NQA-1]

CHPRC-00257, *MODFLOW and Related Codes Functional Requirements Document* (FRD) ([Nichols 2009b](#_ENREF_12)) identifies several software items as related to MODFLOW, but distinguishes between calculational software and support software. The calculational software will be managed with greater rigor due to software classification and grading that is assigned in Section 2.1 than for support software. Support software is covered in this management plan for intended use as support of identified calculational software; other uses of support software are not intended uses managed under this plan. The software items assigned to each category are:

**Calculational Software**

* **MODFLOW-2000, MODFLOW-2000-MST, and MODFLOW-USG** – 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” is used to designate the standard edition issued by the USGS, while “MODFLOW-2000-MST” denotes a variant of MODFLOW that includes source modifications to deal with minimum saturated thickness issues that was developed by S.S. Papadopulos and Associates as part of the 200-ZP-1 Operable Unit groundwater modeling work. CHPRC deems it necessary to qualify both the baseline MODFLOW-2000 and the MODFLOW-2000-MST variant for use of MODFLOW in the Hanford geologic setting. Both will be subject to the same acceptance and installation testing requirements. Hereafter in this SMP, when the term “MODFLOW” is used is refers collectively to both of these software items. The modifications to MODFLOW-2000 prepared by S.S. Papadopulos and Associates are documented in “Documentation for: MODFLOW-2000-SSPA Build 007 Modifications and options added to MODFLOW” provided by the vendor with the source code. These modifications are also described in Bedekar et al. ([2012](#_ENREF_1)). A new version of MODFLOW, called MODFLOW-USG (for UnStructured Grid), was developed to support a wide variety of structured and unstructured grid types, including nested grids and grids based on prismatic triangles, rectangles, hexagons, and other cell shapes. Flexibility in grid design can be used to focus resolution along rivers and around wells, for example, or to sub-discretize individual layers to better represent hydrostratigraphic units. MODFLOW-USG is based on an underlying control volume finite difference (CVFD) formulation in which a cell can be connected to an arbitrary number of adjacent cells. To improve accuracy of the CVFD formulation for irregular grid-cell geometries or nested grids, a generalized Ghost Node Correction (GNC) Package was developed, which uses interpolated heads in the flow calculation between adjacent connected cells. MODFLOW-USG includes a Groundwater Flow (GWF) Process, based on the GWF Process in MODFLOW-2005, as well as a new Connected Linear Network (CLN) Process to simulate the effects of multi-node wells, karst conduits, and tile drains, for example. The CLN Process is tightly coupled with the GWF Process in that the equations from both processes are formulated into one matrix equation and solved simultaneously. This robustness results from using an unstructured grid with unstructured matrix storage and solution schemes. MODFLOW-USG also contains an optional Newton-Raphson formulation, based on the formulation in MODFLOW-NWT, for improving solution convergence and avoiding problems with the drying and rewetting of cells. Because the existing MODFLOW solvers were developed for structured and symmetric matrices, they were replaced with a new Sparse Matrix Solver (SMS) Package developed specifically for MODFLOW-USG. The SMS Package provides several methods for resolving nonlinearities and multiple symmetric and asymmetric linear solution schemes to solve the matrix arising from the flow equations and the Newton-Raphson formulation, respectively. MODFLOW-USG will be tested to the same requirements as MODFLOW-2000 and MODFLOW-2000-MST.
* **MT3DMS** – modular three-dimensional, multi-species transport model for simulation of advection, dispersion, and chemical reactions of contaminants in groundwater systems developed by the University of Alabama’s Hydrogeology Group. The modifications to MT3DMS prepared by S.S. Papadopulos and Associates are documented in “Documentation for: MT3DMS-SSPA Build 007 Modifications and options added to MT3DMS” provided by the vendor with the source code.
* **[modpath]**
* [modpath 3du]

**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)
* **AllocateQwell\_MNW2** – utility code that constructs a MODFLOW well package (“WEL”) file or MNW2 file from well rate and well information files; 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** – custom-developed utility code that determines saturated thickness from MODFLOW layer definitions and calculated heads
* **CalcGradients** – custom-developed utility code that calculates simulated gradient directions and magnitudes from calculated head values
* **CP\_ModelStrat**: custom-developed utility code that translates interpolated HSU surfaces into model layer elevations and assigns HSU zone identification to the individual layer cells (note; a validation and verification package for this support software is provided in Attachment 1)
* **Headtarg\_d** – custom-developed 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
* **Groundwater Vistas™[[2]](#footnote-2)** – acquired software that provides a Windows®[[3]](#footnote-3) graphical user interface for 3-D groundwater flow & transport modeling
* **GSLIB** – acquired geostatistical software library
* **MakeCH** – custom-developed utility code that creates a (“CHD”) file
* **MakeGHB4** – custom-developed utility code that prepares the general head boundary (“GHB”) input file for MODFLOW
* **MakeRecharge5** – custom-developed utility code 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
* **MakeRiver** – custom-developed utility code that creates a river package (.RIV) input file.
* **MODTMR** – acquired software for constructing data sets for local models embedded within regional models constructed with MODFLOW. MODTMR allows construction of local-model data sets that specify perimeter boundary conditions of embedded models, and local-model data sets for most MODFLOW packages. Major features of the program are as follows: (1) MODTMR is self-contained, and will run on a variety of computer types and operating systems. (2) Combinations of flow and head boundary conditions can be specified on the perimeters of local models. (3) Local-model grids can be at any angle to regional-model grids. (4) Local models can include a subset of layers in regional models. (5) Some regional-model layers can be subdivided into multiple layers in local models.
* **NRDWL\_conc** – custom-developed utility code that replaces contaminant concentrations from QuantVar program with specified concentrations at specific cell locations
* **PEST** – acquired software that supports automated model calibration, parameter estimation and predictive uncertainty analysis
* **QUANTILE** – acquired software developed by S.S. Papadopulos and Associates (*User’s Guide for Interpolation using QUANTILE, Version 2* [SSP&A, 2011]) used for spatial interpolation of sampled contaminant concentration data. QUANTILE is based on the USGS Fortran kriging routines of Skrivan and Karlinger (1980). It incorporates routines to conduct the logarithmic, quantile, and categorical data transforms, undertake OK of the transformed values, and complete the necessary back-transformations. It is independent of any specific computer platform, requires only simple ASCII input files, and produces ASCII output files.
* **R** – a language and environment for statistical computing (*R: A Language and Environment for Statistical Computing, R Core Team 2012; R: A Language for Data Analysis and Graphics*, Ihaka & Gentleman, 1996) is included as support software. In this role, use of R is limited to performing data processing tasks, such as tabulation and formatting of data in preparation for analysis using the software program QUANTILE. No calculations with R, nor any of its numeric or computational capabilities, are included in this support software role (as use of these capabilities will require separate qualification of R as approved software rather than support software).
* **Read-lst-budget** – custom-developed 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** – custom-developed 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\_multi\_option\_lahey** – custom-developed 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
* **Surfer®[[4]](#footnote-4)** - acquired software that provides graphical interpolation and display for preparing geostatistical distributions of contaminants to support definition of initial conditions
* **Well-layers** – custom-developed utility code that determines the layers in the model that a well screen of a particular well overlaps
* **ZONEBUDGET** - (USGS Open-File Report 90-392) calculates subregional water budgets from MODFLOW results

**Organizational Structure**

This software will be managed by the CHPRC Environmental Program and Strategic Planning (EP&SP) organization’s Risk and Model Integration Group. Specific personnel assigned to the roles identified in PRC-PRO-IRM-309 are identified in the assignments table below. HISI will be updated to reflect these responsibilities.

|  |  |  |
| --- | --- | --- |
| **Name** | **Organization** | **Project Management Role/Responsibilities** |
| Alaa H. Aly | EP&SP | Responsible Manager |
| William E. Nichols | EP&SP | Software Owner |
| Carl W. Connell | EP&SP | Software Subject Matter Expert (SME) |
| Sunil Mehta | EP&SP | Technical Authority |
| Jose A. Archuleta | EP&SP | Quality Assurance |
| *To be identified in HISI* |  | Software Users |

# FUNCTIONAL REQUIREMENTS

Functional requirements are identified in CHPRC-00257, *MODFLOW and Related Codes Functional Requirements Document* ([Nichols 2009b](#_ENREF_12)).

## Software Safety

The Software Grading Checklist (Appendix A of PRC-PRO-IRM-309) is used to classify and grade the MODFLOW calculational software with respect to the most stringent intended use.

### Classification

Based on evaluation of the criterion in the Software Grading Checklist, MODFLOW and MT3DMS software are collectively classified as S3, Safety Management and Administrative Controls Software. The basis of this classification is provided in the table below.

| **Checklist Question No.** | **Criterion** | **Response** |
| --- | --- | --- |
| S3 | Is the software Safety Management and Administrative Controls Software? Software that performs a hazard control function in support of nuclear facility or radiological safety management programs or Technical Safety Requirements or other software that performs a control function necessary to provide adequate protection from nuclear facility or radiological hazards. This software supports eliminating, limiting, or mitigating nuclear hazards to workers, the public, or the environment as addressed in 10 CFR 830, 10 CFR 835, and the DEAR ISMS clause. | YES: the express intent is to use this software to calculate transport of radionuclide (and other) contaminants in the groundwater pathway for use in estimating radioactive dose resulting from radioactivity released to the vadose zone at Hanford waste sites – and these estimates therefore constitute safety management and administrative controls software per DOE O 414.1C. |

### Grading

All of the responses to the checklist questions related to establishing software grade in the Software Grading Checklist are negative, except for the criteria listed in the table below along with the basis for an affirmative response to each criterion. The responses were prepared based on the most stringent anticipated uses of calculation products to be produced using this software by the CHPRC.

| **Checklist Question No.** | **Criterion** | **Response** |
| --- | --- | --- |
| 8 | Could software failure cause a potential violation of regulatory permitting requirements? | YES: such errors could result in lawsuits, withdrawn regulatory documents, and related impacts where results from this software are used as a basis for environmental calculations to meet regulatory requirements. |
| 13 | Is the software used in support of a quality assurance program that implements a contractual requirement? | YES: All software used by CHPRC is under contractual requirements for software quality assurance. |
| 14 | Is the software used to support a legal, regulatory, or external milestone? | YES: results generated with the groundwater models based on use of MODFLOW and related codes are expected to be used as a basis for environmental fate and transport calculations that demonstrate compliance with DOE O 435.1, CERCLA, and RCRA. |
| 16 | Is this software used to determine, select, or evaluate remedial actions for cleanup of contaminated sites or facilities? | YES: results generated with the groundwater models based on use of MODFLOW and related codes are expected to be used as a basis for pump and treat designs and selection between groundwater remedial actions. |

No other criteria were found to pertain to the expected purposes of the MODFLOW and related software. Therefore, the use of MODFLOW and related software as controlled by this SMP is graded as Level C and will be managed under this SMP accordingly. Software documentation requirements will follow the graded approach as provided in Appendix B of PRC-PRO-IRM-309.

For support software, none of the checklist questions are answered in the affirmative, and are therefore graded “N/A”.

## Software Procurement and Supplier Management

MODFLOW-2000, MODFLOW-USG, MT3DMS, GSLIB, and MODPATH/MODPATH-PLOT and PEST are freely available as source code from the USGS and others. CHPRC will use either MODFLOW-2000, MODFLOW-2000-MST, or MODFLOW-USG depending upon modeling objectives for each use.

A statement of work (SOW) was not prepared for acquisition of MODFLOW and related software because, at the time of acquisition the controlled software use procedure in effect stated that “In cases when DOE mandates use of a particular software application, a SOW may not be required. However, the remainder of the acquisition process applies.” DOE had mandated use of MODFLOW for groundwater modeling at Hanford ([Klein 2006](#_ENREF_9)), and mandated its use as the simulation code to use in the site-wide groundwater model developed for the Tank Closure and Waste Management Environmental Impact Statement.

Commercially provided software, namely ArcGIS®, Surfer®, and Groundwater Vistas™, were procured by preselected subcontractor INTERA. Licenses to Groundwater Vistas™ were procured by CHPRC for use by selected CHPRC modelers as well.

MODFLOW and related software identified are individually listed in the Hanford Information Systems Inventory (HISI) by CHPRC in accordance with the HISI Software Grading Checklist in Appendix A of PRC-PRO-IRM-309. Each software program will be individually rated and entered into the HISI, but control of calculational software use is collectively addressed in this SMP.

## Project Deliverables

(Not applicable to acquired software.)

# GENERAL SYSTEM REQUIREMENTS

MODFLOW was designed to have a modular structure to facilitate enhancement and increase flexibility for application in a wide range of ground-water flow problems. To facilitate this perspective, the program is divided into pieces (modules) called packages. Each hydrologic capability (such as leakage to rivers, recharge, and evapotranspiration), or solution technique is implemented as a separate package. These packages are often developed, implemented, tested and documented, separately from the basic MODFLOW code development. The test cases developed for each specific package will, necessarily, exercise other capabilities of the code, but, will exercise only a fraction of the capabilities that are available.

MODFLOW, MODFLOW-USG, MT3DMS, GSLIB, MODPATH, mod-PATH3DU, and PEST are written in Fortran and may be implemented in several operating systems. Groundwater Vistas™ and Surfer® are implemented in the Windows® (2000, XP, Vista, or higher) operating system only. ArcGIS® is implemented in several operating systems, including Windows®. The support software identified as utility codes are written in Fortran and may be implemented in several operating systems.

# SOFTWARE DEVELOPMENT

This SMP manages use of acquired software under a graded approach. Certain software development requirements are therefore inapplicable or addressed briefly under the graded approach.

## Assumptions and Constraints

As acquired software, there are no assumptions necessary related to schedule, budget, or resources for software development.

## Deliverables and Controlling Documents

Documentation requirements are identified using the graded approach based on software grading level C as evaluated in Section 2.1. Appendix B of PRC-PRO-IRM-309 specifies the following software documentation requirements for acquired software graded at level C:

| **SQA Document/Product** | **Required** | **Document where Requirement is Met** |
| --- | --- | --- |
| Functional Requirements Document | Graded | CHPRC-00257, *MODFLOW and Related Codes Functional Requirements Document* |
| Alternatives Analysis | Graded |
| Software Management Plan | Graded | CHPRC-00258, *MODFLOW and Related Codes Software Management Plan* |
| Software Configuration Management Plan | Graded |
| Acquisition Documents | Full | N/A (software is not purchased by CHPRC) |
| Software Requirements Specification | Full | CHPRC-00257, *MODFLOW and Related Codes Functional Requirements Document* |
| Software Design Description | N/A | N/A (not custom-developed software) |
| Requirements Traceability Matrix | Full | CHPRC-00260, *MODFLOW and Related Codes Requirements Traceability Matrix* |
| Code Walkthrough | N/A | N/A (not custom-developed software) |
| User Documents | Graded | Vendor documentation is sufficient |
| Unit Testing | N/A | N/A (not custom-developed software) |
| Test Plan and Cases | Graded | CHPRC-00259, *MODFLOW and Related Codes Software Test Plan* |
| Acceptance Test Report | Graded | CHPRC-00261, *MODFLOW and Related Codes Acceptance Test Report* |
| Contingency Plan | Graded | Not required [software is not graded as Key Critical (KC) or Key Essential (KE)] |
| Software Installation Plan | Graded | CHPRC-00258, *MODFLOW and Related Codes Software Management Plan* |
| User Qualification | Graded |
| User Training | Graded |
| Operational (Periodic) Testing | Graded | CHPRC-00259, *MODFLOW and Related Codes Software Test Plan* |
| Change Request / Problem Report | Graded | CHPRC-00258, *MODFLOW and Related Codes Software Management Plan* &  Forms A-6005-149, A-6005-151 |
| Retirement Plan / Checklist | Graded |

The software management documents listed in the table above will be cleared as CHPRC documents and thus stored in the Integrated Document Management System (IDMS). These documents will be reviewed by the Software SME and Quality Assurance as part of the document release process.

Key documents provided by software developers and vendors are listed in Section 6.3.

## Configuration Control

As acquired software, no changes or modifications will be made to the MODFLOW calculational software by the CHPRC under this SMP.

Two variants of MODFLOW 2000 will be maintained until configuration control as current versions available for use: MODFLOW-2000 (baseline) and MODFLOW-2000-MST (the variant with minimum saturation handling). These will be identified as separate “builds” with unique identification and filenames to distinguish between these builds and both are subject to the same software testing requirements. The file name convention for executable files is:

[code]-chprc[build][prec].[ext]

where:

[code] = code identification (mf2k for MODFLOW-2000, mf2k-mst for MODFLOW-2000-MST, or mt3d-mst for MT3DMS-MST)

[build] = build number (e.g., “05” for Build 5)

[prec] = precision for default real variables; “sp” for single precision, “dp” for double precision[ext] = file name extension for executable file (“.exe” for Windows®, “.x” for Linux®)

When any of the vendors of the software items managed in this SMP issue software updates or corrections to calculational software managed under this SMP, these will be adopted if determined necessary, in a controlled manner by the following process:

1. A decision will be made by the software owner whether to adopt the new version. This decision will weigh the following factors:
   1. Will the update corrects errors in coding and whether identified error corrections will matter to models constructed by the CHPRC with the code?
   2. Will the update contains additional features that may be desirable for CHPRC use?
   3. Will the update would be disruptive to work in progress by the CHPRC using the affected software?
2. The decision will be documented and one of these courses of action selected:
3. Adopt the upgrade immediately
4. Defer adoption until a time more suitable with respect to ongoing work
5. Not adopt the upgrade because the changes are unneeded and do not impact calculation results for CHPRC work products
6. If the upgrade is adopted, then the following steps will follow:
   1. The software baseline will be established by the software owner collecting the new source and any associated documentation per requirements of PRC-PRO-IRM-309
   2. The software owner will issue an electronic mail message to the software users alerting them to the forthcoming version and the nature of the change or changes included
   3. The software update will be distributed to the software users, and installation tests repeated and documented. The new baseline will be established, per requirements of PRC-PRO-IRM-309

## Status Reporting

The software owner for the Risk and Model Integration Group maintains a “CHPRC Risk and Model Integration Group Managed Software Inventory” to track the software managed by that group to support environmental calculations [PRO-PRC-EP-40205, *CHPRC Environmental Calculations Preparation and Issue* ([CHPRC 2010a](#_ENREF_3))] and its current quality status. Status of the software managed under this SMP is reported to the responsible manager at least quarterly by means of this tool.

## Software Development Reviews

As acquired software, the codes managed under this SMP do not require all the reviews that would be required for a software development effort. The subsections that follow identify which reviews are deemed not applicable and identify the reviews planned for those that are applicable.

### Peer Reviews and Code Walkthroughs

(Not applicable to acquired software.)

### Software Requirements Review

Approval and release of the FRD will constitute software requirements review for software managed under this SMP.

### Design Review

(Not applicable to acquired software.)

### Audits

(Not applicable to acquired software.)

### Managerial Review

The responsible manager will monitor status reports (Section 4.4) and will conduct management reviews of the software management as needed.

### Software Configuration Management Review

Environmental Quality Assurance provides oversight for compliance by the Risk and Modeling Integration Group’s software activities and implementation of the requirements of PRC-PRO-IRM-309.

### Post-implementation Review

(Not applicable to acquired software.)

## Turnover and Closeout

(Not applicable to acquired software.)

# RISK MANAGEMENT

## Risk Management Techniques

Adherence to the requirements for controlled software use, as detailed in this SMP, provides the primary means of managing risk from use of unqualified software. Adherence to requirements for calculation package preparation and issue provides the primary means of managing risk from use of unverified inputs.

## Risk Management Policies and Procedures

Risk will be managed by managerial oversight to ensure consistent application of the requirements of this SMP and adherence to procedures for calculation package preparation and issue.

## Risk Identification

The primary risk associated with the use of environmental calculation software, including MODFLOW and related codes, are those that arise from errors in calculations. Professional experience and past Hanford examples indicate that the root causes of such errors are most likely to be data input errors.

Another risk is presented by the potential for use of versions of MODFLOW and related software outside the control of this SMP. Because the software managed under this plan is mostly freely available from the internet, it is not possible for the software owner to restrict distribution of this software. Use of unauthorized and unqualified installations of this software would present risk to the quality of the product and reputation of the company and client.

## Risk Avoidance, Mitigation, or Transfer

Risk avoidance for data input errors is achieved through adherence to PRC-PRO-EP-40205, *CHPRC Environmental Calculation Preparation and Issue*, which provides for independent verification of environmental calculations including ensuring use of qualified software and verified inputs.

Risk avoidance for unauthorized and unqualified versions of the software managed by this SMP is achieved at the calculation package stage by managerial oversight. Management, including the software owner and responsible manager, will exercise strong oversight to ensure that all documents that use results obtained with this software cite appropriate environmental calculation packages:

* that are prepared under the requirements of PRC-PRO-EP-40205, *CHPRC Environmental Calculation Preparation and Issue*
* that environmental calculation briefs cite the completed Software Installation and Checkout forms for controlled software

These steps will establish documentary evidence of controlled software use consistent with the requirements of this SMP.

# SOFTWARE OPERATION AND MAINTENANCE

Operation and maintenance of the software managed by this SMP is planned with consideration given to the expert training and prior experience of the small number of software users, the acquired status of the software, and the variety of computers both inside and outside HLAN that will be used to operate this software.

## Responsibilities & Training

Calculational software addressed in this SMP will be managed as acquired software, and therefore code development control is not addressed in this SMP.

Original source code and/or executable code will be preserved in a manner that precludes loss or destruction for traceability purposes. MKS Integrity™ will be used for this purpose.

Because advanced degree work and use of this software is core to the skill set of the software users, no training will be planned or provided in the use of the software itself. A reading assignment will be required to ensure software testers and users understand the software management requirements of this SMP and their responsibilities.

## Operating and Maintaining the Software

Recognizing that the software managed under this plan is acquired and is mostly freely available open-source code that anyone can download from the internet, there is no control that can practically be exerted by the software owner to restrict distribution of this software. Instead, control will be maintained by requiring software users to document in calculation packages that all environmental calculations results obtained using this software were obtained from approved installations this software. All such uses of this software will be logged in HISI, as required by PRC-PRO-IRM-309.

Software configuration management will be by archiving baseline releases of the software in MKS Integrity™. The software installation process will require the user to verify that the version of the software in use matches that archived in MKS Integrity™ and document this in the *Software Installation and Checkout Form*.

There are multiple vendors for the software managed by this SMP; if problems are encountered with any of these software configuration items, the appropriate vendor will be notified by the software user using the mechanisms provided by the vendor, and a copy of the notification provided to the software owner. Upgrades will be addressed using the process specified in Section 4.3.

For MODFLOW calculation software, data consists of inputs and outputs only; integrity is managed by adherence to PRC-PRO-EP-40205, *CHPRC Environmental Calculation Preparation and Issue*.

The software installation plan is as follows:

1. Authorized users will obtain the version of the software that has received approval for use from the software owner (who will obtain it from the baseline archived in MKS Integrity™), or verify that the installed software is the same version as the baseline maintained in MKS Integrity™.
2. Perform installation testing per CHPRC-00259, *MODFLOW and Related Codes Software Test Plan* (STP) ([Nichols and Clemo 2009](#_ENREF_15)) and document results in the *Software Installation and Checkout Form* (Form A-6005-149), except that the signature of the Software SME on this form is not required to complete the installation and checkout process for this software.
3. Return a PDF version the completed *Software Installation and Checkout Form* to the software owner for archival in MKS Integrity™.

For work in process with this software, each user is required to perform daily backup to external media is required for model inputs and output files to minimize risk of data loss during development. At the completion of model runs, the inputs and outputs will be electronically preserved according the Records Inventory and Disposal Schedule (RIDS) requirements. Software preservation is accomplished by maintaining the baseline version in MKS Integrity™. Because there is no software development for this software, incremental backup of code and executables is not required.

## Software Documentation and Records

The following existing documentation for the (MODFLOW) code has been reviewed by CHPRC Risk and Model Integration Group staff:

* *MODFLOW-2000, The U.S. Geological Survey Modular Ground-Water Model-User Guide to Modularization Concepts and the Ground-Water Flow Process* ([Harbaugh et al. 2000](#_ENREF_7))
* *MODFLOW-2000, The U.S. Geological Survey Modular Ground-Water Model - User Guide to the Observation, Sensitivity, and Parameter-Estimation Processes and Three Postprocessing Programs* ([Hill et al. 2000](#_ENREF_8))
* *MT3DMS: A Modular Three-Dimensional Multispecies Transport Model for Simulation of Advection, Dispersion, and Chemical Reactions of Contaminants in Groundwater Systems; Documentation and User’s Guide* ([Zheng and Wang 1999](#_ENREF_18))
* *MT3DMS v5.2 A Modular Three-Dimensional Multispecies Transport Model for Simulation of Advection, Dispersion and Chemical Reactions of Contaminants in Groundwater Systems Supplemental User’s Guide* ([Zheng 2006](#_ENREF_16))
* MODFLOW-2000, *The U.S. Geological Survey Modular Ground-water Model-User Guide to the LMT6 Package, the Linkage with MT3DMS for Multi-species Mass Transport Modeling* ([Zheng et al. 2001](#_ENREF_17))

Based upon review of the above documents, the software owner has determined that the software requirements specification, software design document, and software user manual documentation requirements are met by existing documentation.

Section 4.2 identifies controlling documents required for CHPRC use of this software:

* CHPRC-00257, *MODFLOW and Related Codes Functional Requirements Document* ([Nichols 2009b](#_ENREF_12)) specifies functional requirements with respect to the CHPRC’s intended uses and provides the alternatives analysis.
* CHPRC-00258, *MODFLOW and Related Codes Software Management Plan* ([Nichols 2009d](#_ENREF_14)) - this document that identifies how the software will be managed for controlled use, configuration management requirements, software installation plan, user qualification and training, and retirement plan.
* CHPRC-00259, *MODFLOW and Related Codes Software Test Plan (*[*Nichols and Clemo 2009*](#_ENREF_15)*)* specifies acceptance tests to validate the software for CHPRC intended uses and installation tests to ensure correct code operation.
* CHPRC-00260, *MODFLOW and related Codes Requirements Traceability Matrix* ([Nichols 2009c](#_ENREF_13)) tracks software requirements and status.
* CHPRC-00261, *MODFLOW and Related Codes Acceptance Test Report* ([Nichols 2009a](#_ENREF_11)) documents results of acceptance testing.

The above software documents generated by software developers and vendors will be archived with the software in MKS Integrity™.

In accordance with PRC-PRO-IRM-309, documentation required by this SMP (including this SMP itself) will comply with requirements as applicable in the following procedures:

* PRC-PRO-IRM-232, *Project Files Management* ([CHPRC 2009](#_ENREF_2))
* PRC-PRO-IRM-8310, *Document Control Processes* ([CHPRC 2010c](#_ENREF_5))
* PRC-PRO-IRM-10588, *Records Management Processes* ([CHPRC 2010d](#_ENREF_6))

# SOFTWARE RETIREMENT

The software owner will determine when the software managed under this plan is no longer needed with the concurrence of the responsible manager. This determination will reflect projected modeling needs as well as required support for past and current modeling work. Once determination that retirement is appropriate is reached, the procedure specified in Section 3.9 of PRC-PRO-IRM-309 for retirement of software will be followed.

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**Acronyms, Abbreviations, and Definitions**

| Acronym or Term | 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 |
| CHPRC | CH2M HILL Plateau Remediation Company |
| finite difference | Numerical method for approximating the solutions to differential equations using finite difference equations to approximate derivatives |
| FRD | Functional Requirements Document |
| GSLIB | Geostatistical Software LIBrary (software) |
| HISI | Hanford Information Systems Inventory |
| IDMS | Integrated Document Management System |
| MKS Integrity™ | Hanford Site’s software configuration management software and repository |
| MODFLOW | MODular three-dimensional finite-difference ground-water FLOW model (software) |
| MODFLOW-USG | MODFLOW UnStructured Grids (software) |
| MODPATH | particle-tracking post processing code for MODFLOW (software) |
| MT3DMS | modular three-dimensional, multi-species transport model for simulation of advection, dispersion, and chemical reactions of contaminants in groundwater systems (software) |
| PEST | model-independent Parameter ESTimation (software) |
| SIP | Software Implementation Plan |
| SMP | Software Management Plan |
| SME | Subject Matter Expert |
| SSP&A | S.S. Papadopoulos & Associates |
| STP | Software Test Plan |
| USGS | U.S. Geological Survey |

# ATTACHMENTS

**Attachment 1** - Support Software Validation and Verification Package CP\_ModelStratV6

**Attachment 2** – Support Software Validation and Verification Package KT3D

Attachment 1

Support Software Validation and Verification Package

CP\_ModelStratV6

**Support Software Validation & Verification Package: CP\_ModelStratV6**

|  |  |  |  |
| --- | --- | --- | --- |
| Support Software Identifier: | CP\_ModelStratV6 | Software Version / Software Build Numbers: | Version 6 |

This document provides a validation and verification (V&V) package for custom-developed support software used to support mf2k-mst-chprc06dp.

INTRODUCTION

The Central Plateau Ground Water (CPGWM) Model Stratigraphy code constructs a model discretization suitable for MODFLOW-2000 from surface grids of the Hanford South Geologic Model. Each surface grid is a discretized representation of bottom of the five hydrostratigraphic units defined in the Hanford South Geologic Model. The surface grids use the same regular 100x100 m cell size map view grid as the CPGWM. The stratigraphy code’s job is to define the size and composition of the stack of volumetric cells, of varying thickness, representing the volume of the model for each cell of the map view grid. The code is essentially a large decision tree coded in Fortran.

The code creates a seven layer discretization so that each map view grid cell has seven discretization cells. The seven-layer model, with a 100x100 m grid, is a compromise between simulation time efficiency and the amount of geometric detail that can be represented in the model. Ideally, the seven layers would be horizontal so that the discretization grid would match theory used to develop the finite-difference MODFLOW code. In practice, a model with only seven horizontal layers would be unable represent the large spatial variation in hydrostratigraphic units or the larger variation in the elevation of the lower bounding surface of the model. We treat the top of basalt below the sedimentary beds of the Central Plateau as an impermeable lower bound. MODFLOW is designed so that layers need not be horizontal, they do not need to be even contiguous. Not having horizontal layers means the model is a coarser approximation to reality than with horizontal layers. But as with the finite-difference approach its self, the approximation due to non-horizontal grid structure is relatively small compared to other modeling assumptions.

SUPPORT SOFTWARE REQUIREMENTS & DESIGN

The following design goals were identified for the stratigraphy code:

* Create a seven-layer MODFLOW discretization
* An exact replication of the hydrographic unit structure below the maximum historic water table
  + Exact replication refers to the input grid files.
* An exact replication of the basalt surface boundary at the bottom of the model
* Treat basalt as impermeable
* Minimize number of cells with thickness less than 1 m
* No cell thickness less than a foot (0.3 m)
* Minimization of layer discontinuities
* Focus detail where transport is to be simulated; below the current (2009) water table
* Focus detail in higher conductivity units
* Enforce continuity of the low permeability mud unit
* Identify western fine-grained Hanford unit as a separate unit from the higher permeability Hanford formation
* Extend top of the model to land surface without regard to units above the maximum historic water table
* Generate all MODFLOW input files that contain discretization information
* Generate all MT3DMS input files that contain discretization information
* Generate all the support code input files that contain discretization information

This software is required to contain and report a unique version number (corresponding to its release) to the screen, which can be redirected to a log file, and to output files, where practicable.

The software owner will designate the unique version number for each build of this software released for use.

Some of these goals are contradictory such as an exact replication of the hydrographic unit structure contradicts the goal of no cells less than a foot thick for units that are less than a foot thick. Minimum cell thickness wins here.

The exact representation of hydrographic unit structure is ill defined without some assumptions because the surfaces have values everywhere; even where the units do not exist. First, it is assumed that the hydrostratigraphic units (HSU) always occur in the following top to bottom stratigraphic sequence;

|  |  |  |
| --- | --- | --- |
| Unit | HSU | Name |
| 1 | 1 | Hanford formation or 2 Hanford fines |
| 2 | 3 | Cold Creek unit |
| 3 | 5 | Ringold E |
| 4 | 9 | Ringold mud unit |
| 5 | 9 | Ringold A |
|  | | |

Next, it is assumed that a unit extends from the bottom surface to the bottom of a unit above. If the bottom of a unit above is lower than the bottom of a particular unit then the unit does not exist in that grid cell. The bottom of Ringold A, or any unit extending below Ringold A, is defined by the top of basalt because the top of basalt is described with more reliability.

SUPPORT SOFTWARE MANAGEMENT

Classification and Grading: This software works in conjunction with, and in support of, software classified as S3 Safety Software and graded level C. Management of this software is through the software management plan for the software supported.

* Responsibilities: Organization is CHPRC Risk and Model Integration Group; Responsible Manager Alaa Aly; Software Owner Will Nichols; Quality Assurance Jose Archuleta; SME Carl Connell.
* Configuration Management: The source for this software will be archived in the Hanford Site’s MKS Integrity™ software configuration-management system following acceptance testing in the archive devoted to the software supported. All qualified installations will be traceable to the archived copy. The Software Owner will notify all approved users of baseline changes to this software.

IMPLEMENTATION

The first task is to define the active region of the model. An external file defines regions outside the model region such as north of the western and Gable Gap boundaries and south of the Dry Creek boundary. This in used to set all layers of the indicated grid cells inactive. In addition, all map view grid cells that have a top of basalt above the historically high water table are made inactive. Finally a small region of the western Cold Creek drainage is made inactive because dumping the Cold Creek flow directly on to the Ringold mud, which is at the water table here, caused stability problems.

Next each active grid cell is tested to see which units exists there. An array is used to indicate if a unit exists in an active grid cell. If the unit exits only above the maximum water table it is marked as non-existent in the array. Similarly, if a unit above in the stratigraphic sequence has a bottom surface below the top of basalt it is marked as non-existent. Finally, if an existing unit is less than 0.3 m thick it is removed. The space becomes filled by the unit below. The definition of existing units is followed by adjusting the bottom of the lowest existing unit in a cell to the top of basalt.

At this point, the thicknesses and elevations of the units in each active grid cell have been defined. The code is ready to begin the discretization process. It starts by defining which unit hosts the water table. Water table elevations for 2009 are defined by an input file.

In order to ensure continuity of the lower mud, if the mud exists in a grid cell’s sequence it is assigned to layer 6. If Ringold A exists below the mud, the entire thickness of Ringold A is assigned to layer 7. If not, the mud is split between layers 6 and 7. At this point a complication arises that occurs frequently. If the mud is less than two meters thick then layers 6 and 7 would be assigned to be less than a meter thick in violation of the design goals. The solution in this case is to leave the entire thickness of the mud in layer 6 and make layer 7 a meter of inactive basalt set below the top of basalt. The bottom of layer 7 is set to a meter below top of basalt. Throughout the descriptions that follow, trying to maintain a minimum 1-meter thickness is a complication that always exits but is rarely worth mentioning. If the mud does not exist but Ringold A does then Ringold A is split between layers 6 and 7. If there is no mud or Ringold A in the grid cell, a flag (nomud) is set indicating that layers 6 and 7 have been made inactive. Making layers 6 and 7 inactive prevents the situation where pinch-out of the mud and Ringold A against the basalt could lead to an erroneous window through the mud to Ringold A via populated layers 6 and 7. Ringold A will be in contact with a unit higher in the stratigraphic sequence than the mud only where indicated in the input surface files.

The code then moves on to defining layers 1-5. It starts by counting the number of hydrostratigraphic units to be distributed above layer 6. The logic varies based on the number counted. If there is only one unit then all layers 1-5 are composed of this unit, The only choice is how big to make the layers. Setting the bottom of layer 1 to just above the 2009 water table accomplishes the goal of concentrating detail where transport is to occur. Throughout most of the model domain, the bottom of layer 1 is set 0.4 m above the water table to allow for some mismatch between simulated and historic water tables. In high conductivity region well connected to the eastern boundary this offset is only 0.1 m because the simulated heads are more accurate in this region. A 2009 water table of 123 m above sea level or less is used to define the region with only a 0.1 m offset. If the portion of the unit below the water table unit is thick enough then it is equally divided between layers 1-4. If it is not thick enough to create four layers greater than a meter thick, then adjustments have to be made.

If there are two or three units to be represented in layers 1-5, the logic is similar to that described in the last two paragraphs, with the additional possibility of needing to represent more than layer above the 2009 water table. Each unit above the water table is represented with a single layer. When there is enough leeway to subdivide units below the water table the preference is to subdivide the upper unit in the sequence since the upper units are more permeable and hence be likely to have more influence on transport.

In some cases, the current water table is in the Ringold mud or in Ringold A. If possible, the mud is represented in layers 1-6 with Ringold A filling layer 7 if present. To ensure one-meter thicknesses, more than one layer can be positioned above the current water table.

After the original discretization process is done. Some post-processing is performed to see if it can be improved with small adjustments. One aspect is to identify neighboring grid cells that have more than one additional (or fewer) layers of the same hydrostratigraphic unit. If this is the case, the program tries to subdivide another unit to eliminate multiple increases in layer numbers for any unit. The routine is only successful about 7 percent of the time.

OUTPUT - MODFLOW, MT3DMS, and Support Code Input Files

In order to minimize the editing of files that could lead to input errors the attempt is made to completely generate the input files through the use of support codes. All files that are usually independent of changes made during automated calibration are written by *CP\_ModelStratV6.* These files contain more information about the CP model than simply the discretization created by *CP\_ModelStratV6.* This extra information is provided by a series of separate input files. Some of the support codes that are executed during calibration combine discretization information with new parameter proposals from PEST™[[5]](#footnote-5). *CP\_ModelStratV6* provides input files for these codes or provides PEST™ template (.tpl) files that PEST then uses to convey new parameter values to the support codes or in some cases to make MODFLOW input files directly.

The following MODFLOW input files are created:

* CPModel\_historic\_ID.dis
* CPModel\_historic\_ID.bas
* CPModel\_historic\_ID.zone
* CPModel\_predictive\_ID.dis

Where ID is a model identifier used to ensure quality control. Part of the ID is defaulted in the code and part is supplied in file *CP\_ModelStrat.in*. The model ID tag is V3\_G2\_B1\_I1\_F\_00\_XXXX\_1 where

* V3 is the CHPRC MODFLOW-2000 build version number
* G2 is the grid number
* B1 is the boundary condition number
* I1 is iteration number for further identification of minor changes
* F or T for flow or transport
* 00 identifies the contaminant for MT3D runs
* XXXX identifies the computer used
* 1 is a run iteration number

\_F\_00\_XXXX\_1 is defaulted in the code and the equivalent of “V3\_G2\_B1\_I1” is supplied on line 2 of *CP\_ModelStrat.in.* There is a support utility called *run-setup* that updates the ID in the file names and within files that refer to file names, such as the MODFLOW name file, for specific runs.

Creation of the .dis files requires stress period information. Stress period information is supplied in input file *historic\_stress.in* for the historic run and *predictive\_stress.in* for the predictive run. See the section titled Input File Instructions for the format of these files.

A file call *lpf.tpl* is created that is a template file for PEST. PEST inserts parameter values for hydraulic conductivity and specific yield into this file to create *CPModel\_historic\_ID.lpf*.

The output file *GHB.tpl* is a PEST template file used to make *GHB.in* for the *makeGHB4* support code to create the general head boundary condition input file, *CPModel\_historic\_ID.ghb*. File *CHDhistoric.in* is the input file used by the *Create\_CHD\_V6* support code to make the specified head boundary condition input file *CPModel\_historic\_ID.chd*.

The program also creates a set of input files for MT3DMS. These are *CPModel\_predictive\_ID.btn* that applies to all contaminants and a *CPModel\_predictive\_ID.rct* file for each contaminant listed in *MT3DMS\_rct.in*. Two other input files are needed to create the .btn file. *MT3DMS\_porosity.in* provides the porosity to be simulated for each HSU and *MT3DReport.in* is used to control the reporting of the simulation results. Details of these input files are provided in Section Input File Instructions.

OUTPUT - Error Checking and Review

There are a large number of information files that can be created to help assess the quality of the grid structure that has been created. Generally this section is only of interest for those who using the program and want to know why it discretizes as it does or those who want to improve how it works. Those wanting a general overview should skip this section. The creation of some files is controlled from the instruction file, *CP\_ModelStrat.in*. Others are always created. The most useful, for understanding the program, is created by a process called watch cell. This follows the discretization of a single specified map view grid cell. It reports the status of the grid cell, to file called *cell\_info* in directory *checking*, as it works through different processes of the code. While extremely useful for identifying where in the decision tree a problem might be occurring it rarely provides enough detail to track the exact location. Additional output is almost always helpful. Addition information can be obtained by either adding a line “CALL cell\_watch(cell\_unit ,1,j,i)” or adding a write statement to the code using the following if statement; “IF( i .EQ. irow .AND. j .EQ. jcol)” and then recompiling the code.

A call to cell\_watch generates the following information;

* An indication of where in the code cell\_watch was called
* The column and row number of the grid cell being reported
* The elevation of the 2009 water table for the grid cell
* Top - The maximum water table elevation (top of active region) follow by the bottom of each layer
* Bot - The bottom of each unit
* Thk – the thickness of each layer
* Ibd – the HSU of each layer
* Iunit – the existence flag: 1 (exists) or 0 for each unit

For the final two reports this information is repeated for adjacent previously defined grid cells. For most reports not all of these data have been determined yet.

Other informational files are created that can be used to assess the process and quality of the discretization. These are:

* warnings
* extents
* basalt\_surface\_adjustments
* Ibound\_check
* layer\_fixes
* layer\_jumps\_1
* layer\_jumps\_2
* minthk\_test
* no\_flow\_cells
* Optionally
  + layer\_continuity
  + Unit\_continuity

*Warning* is written during the discretization process. It provides notice of; when the maximum water table elevation is pushed up to allow for one meter thick cells, when a no flow cell is created below the basalt for the same reason, flags each instance of where a cell is less than one meter thick because a unit is less than a meter thick, and resetting the bottom of a unit to the top of basalt.

If a unit is removed because an upper unit has a bottom below the unit’s bottom, then a message is written to the file *extents*. *Extents* is also the file where a notification is written when units are removed because they are thinner than 0.3 meters.

*Basalt\_surface\_adjustments* is written during the discretization process. It lists all instances where a layer cell is set below the top of basalt. The first data listed is a code that flags the reason for the action;

1. No longer used
2. No longer used
3. Mud too thin to fill both layers 6 and 7 to one meter thickness
4. Mud is less than one meter thick but needed for layers 6 and 7
5. Ringold A too thin to fill both layers 6 and 7
6. Mud or Ringold A absent and bottom unit too thin – layer 7 set to basalt
7. Mud and Ringold A absent – layers 6 and 7 set to basalt

*Ibound\_check* gets written too only if the internal ibound array has a residual negative number after discretization is complete. This is a fatal error condition that causes to program to abort. *Ibound\_check* points to where the error occurs. The watch cell process can then be used to determine why the error occurred.

*Layer\_fixes* is written too if a post-discretzation check indicates that a unit can be subdivided to fill a cell that had previously set to basalt. The file uses watch cell format to indicate both the pre and post-adjustment discretization.

*layer\_jumps\_1* and *layer\_jumps\_2* provide a list of where there are increases or decreases of more than one layer for any unit that exists in two adjacent grid cells. *layer\_jumps\_1* is the state before application of the layer smoothing routine and *layer\_jumps\_2* is afterward.

*Minthk\_test* provides a list in watch cell format of where layers are less than one meter thick.

*no\_flow\_cells* provides a list in watch cell format of cells than have been set to no flow. It does not include where the entire grid cell is inactive. If other than layers 6 and 7 are inactive output in watch cell format is made.

*layer\_continuity* is an optional file that is created if ilayer\_continuity is set non-zero in file *CP\_ModelStrat.in*. The file lists all instances where layers do not connect horizontally. It can be a large file. In the current Central Plateau model slightly less than 10% of the grid cells have layers that do not connect horizontally to all adjacent layers. Some primary causes are where basalt transitions above the current water table, large changes to basalt surface elevations, and where entire units do not connect due to steep elevation changes.

For each failure to connect the column and row of the grid cell is listed. The next row lists layer elevation values starting with the top of the maximum water table and follow by the bottom elevation of each layer. Unit bottom elevations are listed next. A value of zero is reported if the unit does not exist in the grid cell. The same information is the provided for the adjacent cell where the failure to connect occurs. To avoid duplication of effort, only adjacent grid cells with lessor column or row numbers are tested.

Unit\_continuity is an optional file that is created if iUnit\_continuity is set non-zero in file *CP\_ModelStrat.in*. It list instances where units do not connect horizontally and where they overlap by less than the fraction Unit\_overlap\_criteria. Unit\_overlap\_criteria is set in *CP\_ModelStrat.in.* Lack of unit continuity is not something that the program is designed to address since one of the design goals is to maintain the unit distributions provided by the input grid files. This output file can be used to focus inspection of the transport results for these cells and possibly to modify the discretization by hand to overcome problems introduced by the scale of the grid size where unit contact dips are steep.

If there is a lack of continuity then a message “Column Continuity” or “Row Continuity" is written followed by the unit id. Next the grid column and row numbers are written followed by the units bottom elevations for both the grid cell and the adjacent cell. A value of zero is reported for bottom elevation if the unit does not exist in the grid cell. Below this for columns of numbers are written describing the discretization of the grid cells the columns are layer units and layer elevations for each of the two grid cells.

If units overlap by less than the fraction Unit\_overlap\_criteria a message "Column Overlap" or "Row Overlap" is written, followed by the unit id and the fraction of overlap. Next the grid column and row numbers are written followed by the units bottom elevations for both the grid cell and the adjacent cell.

OUTPUT - Layer Information Maps

A series of information files will be written when ilayer\_output is set non-zero in the *CP\_ModelStrat.in* input file. The files are written in .asc format to subdirectory layer\_info. They are usually intended to be graphics files that can be used to inspect the discretization. The files are:

* *aquifer\_2009\_thickness.asc*
* *WT\_unit.asc*
* *layerX.asc* where X becomes one of the 7 possible layers
* *layerX\_bottom.asc*
* *layerX\_center.asc*
* *layerX\_thick.asc*
* *conflictX.asc* where X represents one of the HSUs

*aquifer\_2009\_thickness.asc* is the thickness of the region between the 2009 water table and the basalt surface.

*WT\_unit.asc* displays what HSU has the water table in it. Both the Hanford formation and the Hanford fine HSU are assigned to HSU 1 in this file.

*Layer1.asc* displays the HSU represented in each grid cell of layer 1.

*layerX\_bottom.asc* displays the bottom elevation of the indicated layer.

*layerX\_center.asc* displays the node (center) elevation of the indicated layer. This file has been used in the past to aid in assigning initial contaminant concentrations.

*layerX\_thick.asc* displays the thickness of the indicated layer which could be used to look for potential transport trouble spots.

*conflictX.asc* displays a code indicating why the indicated unit is not represented in a grid cell. The following code id used:

* -2 thickness less than 0.3 meters
* -1 not in extent files. This is no longer used.
* 0 used in model
* 1-5 identifies unit above that has a lower bottom elevation. Does not use HSU numbering.
* 8 unit above water table
* 9 unit below basalt
* 10 outside active model
* 11 outside model and basalt above elevation

OUTPUT - Groundwater Vista™[[6]](#footnote-6) Helper Files

The following files make it easier to use Groundwater Vistas™’ graphic capabilities to inspect changes to a model discretization without having to go through the complete model import process. *computed\_zone.ibd* provides the zone information. This file is useful to originally set up Goundwater Vistas™ as well as to update the model. It sets to zone ids to match our HSU unit numbers. Before this file is imported make sure that the number of zones has been set to at least ten. The ibound information is not updated to match the new zone information. The file no\_flow\_ibound.ibd is needed to update the ibound information. *computed\_tops.top* and *computed\_bottoms.bot* are used to update the discretization. These files are written to directory GWV\_files.

Input File Instructions

CP\_ModelStrat.in – Program Control

*CP\_ModelStratV6* requires a large amount of input data, but here is very limited control over its operation. The only options are to the amount of review information provided. These are control by line 1 of *CP\_ModelStrat.in* or the file name used as an inline argument in the *CP\_ModelStratV6* calling statement. Line 1 must provide a series of 4 ones and zeros. A one turns an option on; a zero turns if off. The option are, in order; 1) to watch the progression of discretization for a selected cell, 2) report grid cell layers that do not connect horizontally, 3) report hydrostratigraphic units that do not connect horizontally, 4) output the layer information maps described above.

The second line must contain the run ID as described in Section OUTPUT - MODFLOW, MT3DMS, and Support Code Input Files. An example of a run ID is N6\_G8\_B3\_I0 which codes for CHPRC Build 6, Grid discretization 8, boundary condition 3, with minor modification 0.

A third line is required only if options 1 or 3 are turned on. If option 1 is on, then line 3 should list the column number and then row number if the grid cell to monitor. Specifying column or row 1 will generate an error message. No cells of column or row 1 will ever be active in the central plateau model. If option 3 is turned on then the code will read a line that specifies the maximum overlap that will generate a listing in file *Unit\_continuity*. I have been using 0.1 for this value.

basalt\_m.ibd – active domain

basalt\_m.ibd is used to make the regions outside the domain boundaries inactive. The file has been used, unchanged, since the original development of the model. It is a series of 0 (inactive) and 1 (active) in MODFLOW’s integer array format. For each row, all the columns are reported. Each number uses 5 spaces with 100 space lines. This generates 13 lines per row with only 16 entries in the last line for the central plateau model’s 256 columns.

land\_surface.in – Final Top Elevation of Layer 1

land\_surface.in is used to make set the final top elevation of the model for esthetic display purposes only. The file has been used, unchanged, since the original development of the model. It is a series real numbers in scientific notation in MODFLOW’s Real array format. For each row, all the columns are reported. Each number uses 12 spaces with 120 space lines. This generates 26 lines per row with only 6 entries in the last line for the central plateau model’s 256 columns.

Surfer®[[7]](#footnote-7) style grid files (.grd)

Surfer® style grid files have the letters DSAA on line 1. Line 2 lists the number of columns (256) and rows (134) of the grid. Line 3 contains the coordinates of the west and east coordinates of the model grid. These are 555700 581200. Line 4 has the south and north boundary coordinates; 129900 143200. Line 5 contains two numbers; the minimum and maximum values in the data set. The data field starts on line 6.

The data field has ten numbers per line in free format listed for each row. The last row is empty. This yield 27 lines per row with only 6 entries in the second to last line for the central plateau model’s 256 columns. The rows are listed south to north which is opposite of MODFLOW’s row numbering. Thus, the first data field has information for row 134 of the MODFLOW grid.

ASC style grid files (.asc)

ASC style grid files start with the text ncols in line 1 with the number of columns beginning in column 11. Line 2 has the text nrows plus the number of rows starting in column 11. The next line is the Easting coordinate of lower left corner of the grid (text xllcorner) which must be 555700. 0 (a real number). This is the center of the cell in the lower left corner not the lower left corner of the MODFLOW domain which is one-half a grid cell lower. The next line is the Northing coordinate of the lower left corner (xllcorner 129900.0). Line 6 is text cellsize and 100.0. Line 7 has the text NODATA\_value followed by a number starting in column 11. The text in lines1-7 is not needed but the numbers must start in column 11. The number of columns and rows must be integer values. ASC format uses only one line per row with the values for all columns listed in free format. . The rows are listed south to north which is opposite of MODFLOW’s row numbering. Thus, the first data field has information for row 134 of the MODFLOW grid.

max\_WL\_m.grd – Top of Active Region

max\_WL\_m.grd defines the surface that the maximum water table reached with some additional room for larger simulated heads. This surface is used as the top elevation of the model during the discretization process. It is replaced with the land surface after the discretization process is complete. It is a Surfer® grid (.grd) formatted file.

WT09asc.grd – Current Water Table

WT09asc.grd defines the elevation used to define the water table that serves as a guide to setting layer 2 as the upper boundary for transport simulations. As the name implies, it has been extracted from an ASC file of the 2009 water table map for the Hanford site from PNNL. It is a Surfer® grid (.grd) formatted file.

TOB.asc - Top of Basalt

*TOB.asc* is the definition of the basalt surface for the central plateau model domain extracted from the Hanford south geologic model and digitized to a square 100 m grid.

HSU\_btm.asc - Bottom of Hydrostratigraphic Units

HSU\_btm.asc is generic term for the bottom surface of each HSU of the central plateau model domain extracted from the Hanford south geologic model and digitized to a square 100 m grid. The actual file names are; *Hf\_btm.asc*, *CCU\_btm.asc*, *RgE\_btm.asc*, and *RgLM\_btm.asc*. *TOB.asc* is used for the bottom of Ringold A.

historic\_stress.in and predictive\_stress.in - Simulation Stress Period Information

historic\_stress.in lists the information for each stress period in almost identical format to free-format MODFLOW-2000. It can easily be constructed using cut and paste from an existing .dis file. The only difference is that line 1 must contain the number of stress periods enter in the .dis file. One line for each stress period should contain the length of the period in days, the number of time steps in the period, the time step expansion factor, and TR for transient period or possibly SS, if a steady state calculation is to be performed for the first stress period. The format for predictive\_stress.in is identical. Both files must be supplied.

CHD.dat Gable Gap Specified Heads – Well-60-60

CHD.dat provides data for the specified head boundary conditions for the Gable Gap and the western gap. The structure of the data input was revised for *CP\_ModelStratV6*. The change was introduced to make a transition to monthly stress periods easier to accommodate. The file can begin with an arbitrary number of comment lines. These lines must have a # symbol in column 1. The first data line must contain a code; 1 specifies the older format is used and 2 indicates the new format follows. Older input files can be used with the addition of this code. The western gap boundary condition has been treated as a constant value. This value follows the format code. The next line indicates the number of data lines to follow. Prior to *CP\_ModelStratV6* ,a year and both the starting and ending head of each stress period were listed for Gable Gap. These were directly tied to the stress periods. For the new format a time and a head value are listed for each entry. This provides a time series that is almost independent of the stress periods. The second entry is tied to the beginning of stress period two which is assumed to be 1944. Values in the time series are interpolated to get the starting and ending values for each stress period. Times are entered in decimal years. Thus, 1944 is Jan 1, 1944 and 1944.08 is February 1, 1944.

GHB\_info –General Head Boundary Condition Setup

Treatment of general head boundary condition has gone through substantial revision during the development of the central plateau model. Much of the information supplied in *GHB.info* is has been redundant and no long used. The general head boundary is broken into three segments along the eastern boundary. The file can begin with an arbitrary number of comment lines. The first line of the data identifies the row numbers of the segment endpoints. Next is a fixed size list of data for the southern boundary this list contains a line for each grid cell on the boundary starting with column 162 and continuing to column 255. Each line should contain three indices of a node on the boundary (needed but these are not used). The three indices are followed by a distance in meters to the reference head and a value for the head in the cell. Using the head supplied in *GHB.info* has been replaced by reading the head value from a previous simulation. The head is no long used. After the list for the south boundary is a list for the east boundary using the same format. This list begins at row 37 and continues to row 134.

MT3DMS\_porosity.in

MT3DMS\_porosity.in supplies the porosity for MT3DMS. The file can begin with an arbitrary number of comment lines. These lines must have a # symbol in column 1. The file contains a single porosity value per line for each of the HSUs in this order: Hanford formation, Hanford fine, Cold Creek, Ringold E, Ringold Lower Mud, Ringold A.

MT3DReport.in – Concentration Reporting Times

*MT3DReport.in* provides the desired concentration output times for MT3DMS*. MT3DReport.in* can begin with an arbitrary number of comment lines. These lines must have a # symbol in column 1. The first data line in the file is the number of times supplied. Starting on the next line is the list of times in units of days after the beginning of the simulation.

MT3DMS\_rct.in – Reactive Transport Parameters

The file can begin with an arbitrary number of comment lines. These lines must have a # symbol in column 1. The first data line in the file is the number of contaminants to be listed. Next is the grain density for each of the HSUs (one per line) in the same order as for *porosity.in*. For each contaminant, a name is provided and then the contaminant’s code on the same line. The name should be limited to 20 characters and the code to 4. The code becomes part of the .rct file name (See Section OUTPUT - MODFLOW, MT3DMS, and Support Code Input Files). After the names, the Kd, MT3DMS RC1 parameter, and RC2 parameter are listed for each HSU in the same order as in the *porosity.in* file.

Attachment 2

Support Software Validation and Verification Package

KT3D

**Support Software Validation & Verification Package: kt3d**

|  |  |  |  |
| --- | --- | --- | --- |
| Support Software Identifier: | kt3d | Software Version & Build Numbers: | GSLIB Version 2.0 |

This document provides a validation and verification (V&V) package for the support software kt3d used to perform kriging for points or blocks.

Software Requirements & Design

The program kt3d is a three-dimensional kriging program for points or grid nodes by simple kriging, ordinary kriging, or kriging with a trend. The software is a subroutine of the geostatistical software library GSLIB assembled and compiled by Deutsch and Journel (1998).

This software is required to contain and report a unique version number corresponding to its release to screen, log file, or output file as appropriate to enable traceability and support configuration management. The software owner will designate the unique version number for each build of this software released for use.

Support Software Management

Classification and Grading: This software works in conjunction with, and in support of, software classified as S3 Safety Software and graded level C. Management of this software is through the software management plan for the software supported.

Responsibilities: Organization is CHPRC Risk and Model Integration Group; Responsible Manager Alaa Aly; Software Owner Will Nichols; Quality Assurance Joe Archuleta; SME Carl Connell; Software Users will be listed in the Hanford Information Systems Inventory (HISI).

Configuration Management: The source for this software will be archived in the Hanford Site’s MKS Integrity™ software configuration-management system following acceptance testing in the archive devoted to the software supported. All qualified installations will be traceable to the archived copy. The Software Owner will notify all approved users of baseline changes to this software.

Changes in the software after issuance of approval for use will constitute a new version that must be qualified by updating and issuing a revision to this V&V package. The software owner is responsible for such revisions.

Support Software User Instructions

Kt3d is one of the subroutines in GSLIB, which are written to adhere as closely as possible to ANSI standard FORTRAN 77. In order to perform the validation and verification of the program kt3d, a compiled executable version is used, which invokes from the command line.

To run the executable file, an input parameter file and a dataset file are needed. The parameter file identifies the location and name of dataset file, and assigns certain parameters to perform the kriging, such as selection of kriging method, grid block discretization, number of data points to use for kriging, etc. The dataset file contains the original data which are used for kriging. Furthermore, an external file with “jackknife” data points is needed if the regular grid specified in the input file is not used.

An output data file will be generated by the executable file, which contains the estimated values and variances at the points or grid nodes.

Support Software Test Plan

The test case problem consists of estimating the 100 reference values from the sparse sample of 20 known data. The output file will include the estimated value and variance at the 100 nodes. The x coordinate is from 1 to 10, as well as the y coordinate. The known data are shown in Table 1.

Kriging is a minimum error-variance estimation algorithm. Kt3d can perform simple kriging, ordinary kriging, or kriging with a trend. There are five variogram model types in GSLIB, including the exponential model, spherical model, Gaussian model, power law variogram model, and cosine hole effect model. For this test, ordinary kriging and the exponential model are used. Simple kriging assumes the dataset mean is constant throughout the domain and may be considered a special case of ordinary kriging.

| **Table 1. The known dataset** | | |
| --- | --- | --- |
| **X** | **Y** | **Value** |
| 1 | 1 | 120 |
| 1 | 9 | 200 |
| 2 | 3 | 250 |
| 2 | 6 | 110 |
| 3 | 2 | 320 |
| 3 | 8 | 350 |
| 4 | 5 | 130 |
| 4 | 9 | 130 |
| 5 | 2 | 480 |
| 5 | 5 | 250 |
| 6 | 3 | 240 |
| 6 | 7 | 160 |
| 7 | 6 | 520 |
| 7 | 9 | 300 |
| 8 | 3 | 230 |
| 8 | 8 | 290 |
| 9 | 1 | 140 |
| 9 | 4 | 500 |
| 10 | 6 | 260 |
| 10 | 10 | 380 |

**Ordinary Kriging**

The ordinary kriging system can be expressed in the matrix below:



where *Cij*is the covariance between two sample points *i* and *j* (here point *0* is the point to be predicted), *ωi* is the weight for sample point *i*, and *λ* is a Lagrange multiplier that constrains .

For the exponential variogram model, the covariance function is:

where *C0* is nugget effect, *C0*+ *C1* is sill, *a* is range of the variogram, and |*h*| is the distance between two sample points. For this test, *C0* is equal to 0, *C1* is equal to 100, and *a* is equal to 10.

The covariance values between two sample points are calculated using the above exponential variogram model. Then, the matrix of the ordinary kriging system can be solved, and the weight for each sample point *ωi* and Lagrange multiplier *λ* are determined.

The estimate at point 0 (*V0*) is:

where *ωi* is the weight for sample point *i*, and *Vi* is the value at sample point *i*.

The error variance at point 0 () is:

where is the sill (=*C0*+ *C1*), *ωi* is the weight for sample point *i*, *Ci0* is the covariance between the sample point *i* and point to be predicted *0*, and *λ* is a Lagrange multiplier.

**Simple Kriging**

The simple kriging system can be expressed in the matrix below:

where *Cij*is the covariance between two sample points *i* and *j* (here point *0* is the point to be predicted), and *ωi* is the weight for sample point *i*. The difference between the simple kriging and ordinary kriging is that there is no Lagrange multiplier *λ* which constrains .

The exponential variogram model is used as well. The estimate at point 0 (*V0*) is:

where *ωi* is the weight for sample point *i* and *Vi* is the value at sample point *i*.

The error variance at point 0 () is:

where is the sill (=*C0*+ *C1*), *ωi* is the weight for sample point *i*, and *Ci0* is the covariance between the sample point *i* and point to be predicted 0.

The above equations are used to determine the estimated value and error variance at the 100 points: (x=1, y=1), (x=1, y=2), ······, (x=10, y=10). These calculations are performed in Microsoft Excel to determine 100 reference values from the published model equations. The kt3d output is verified against the reference values using a spreadsheet to calculate the percent error at each of the 100 points. To accept use of the software, the error at each point should be less than 1%.

**KT3D Setup**

The executable and parameter files are obtained from GSLIB user’s guide. Specifically, the executable file is KT3D.exe and the input parameter file is KT3D.PAR. The parameter file (KT3D.par) is revised to address the parameters used in this test case. The dataset file (data.dat) includes the information in Table 1. The parameter file (KT3D.PAR) has the location information (folder and path in the computer) of the dataset file. For this test, the dataset file, parameter file, and KT3D executable file are put in the same folder.

The revised KT3D.PAR file for ordinary kriging is shown as below:

Parameters for KT3D

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

START OF PARAMETERS:

data.dat \file with data

1 2 0 3 0 \columns for X, Y, Z, var, sec var

-1.0e21 1.0e21 \trimming limits

0 \option: 0=grid, 1=cross, 2=jackknife

xvk.dat \file with jackknife data

1 2 0 3 0 \columns for X,Y,Z,vr and sec var

1 \debugging level: 0,1,2,3

kt3d.dbg \file for debugging output

kt3d.out \file for kriged output

10 1 1.0 \nx,xmn,xsiz

10 1 1.0 \ny,ymn,ysiz

1 1 1 \nz,zmn,zsiz

1 1 1 \x,y and z block discretization

10 40 \min, max data for kriging

0 \max per octant (0-> not used)

100 100 100 \maximum search radii

0.0 0.0 0.0 \angles for search ellipsoid

1 0 \0=SK,1=OK,2=non-st SK,3=exdrift

0 0 0 0 0 0 0 0 0 \drift: x,y,z,xx,yy,zz,xy,xz,zy

0 \0, variable; 1, estimate trend

ydata.dat \gridded file with drift/mean

3 \column number in gridded file

1 0.0 \nst, nugget effect

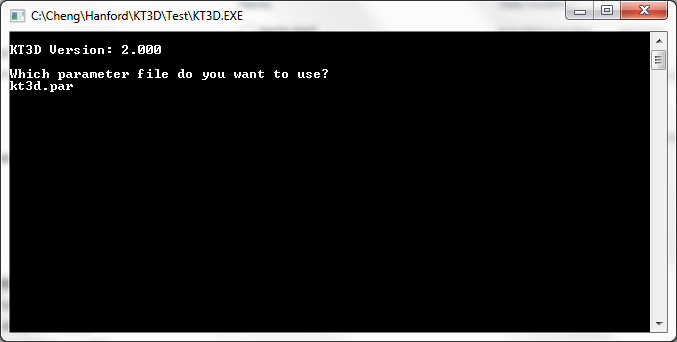
2 100.0 0.0 0.0 0.0 \it,cc,ang1,ang2,ang3

10.0 10.0 10.0 \a\_hmax, a\_hmin, a\_vert

For simple kriging, all lines in the \*.par file are the same as those of the ordinary kriging except for the following line:

0 0 \0=SK,1=OK,2=non-st SK,3=exdrift

When running the KT3D executable file, the parameter file needs to be identified as shown in the figure below. After running the KT3D executable file, a KT3D.out file is generated, which includes the information of estimated value and error variance at each point.



Support Software Acceptance for Use

The estimated values and error variances at the 100 points based on ordinary kriging are shown in Table 2, and based on simple kriging are shown in Table 3.

KT3D generates the same estimated values (±0.0003%) and error variances (±0.002%) as the spreadsheet calculations for both ordinary and simple kriging at all 100 points. Most of the differences occur beyond the 6th digit of precision for the estimate values or the 5th digit of precision for the variance values. Note that only the exponential model is tested. Consequently, KT3D with exponential model provides a reasonable and accurate estimation for ordinary and simple kriging.

The independent software testing was performed by Cheng Cheng of INTERA, Inc., Austin, Texas, under contract to Washington River Protection Solutions, Richland, Washington.

| **Table 2. Estimate and error variance at each point from two calculation methods of ordinary kriging** | | | | | | | |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **Location** | | **Spreadsheet** | | **KT3D** | | **Error (%)** | |
| **X** | **Y** | **Estimate** | **Variance** | **Estimate** | **Variance** | **Estimate** | **Variance** |
| 1 | 1 | 120.000 | 0.000 | 120.000 | 0.000 | 0.0000 | 0.000 |
| 2 | 1 | 213.959 | 34.710 | 213.959 | 34.710 | 0.0000 | 0.001 |
| 3 | 1 | 294.970 | 39.755 | 294.970 | 39.755 | 0.0001 | 0.001 |
| 4 | 1 | 358.581 | 44.090 | 358.581 | 44.090 | 0.0000 | 0.001 |
| 5 | 1 | 383.432 | 42.742 | 383.432 | 42.742 | 0.0001 | 0.000 |
| 6 | 1 | 326.060 | 50.421 | 326.060 | 50.421 | 0.0000 | 0.000 |
| 7 | 1 | 252.768 | 52.706 | 252.768 | 52.706 | 0.0000 | 0.000 |
| 8 | 1 | 194.349 | 39.425 | 194.349 | 39.425 | -0.0001 | -0.001 |
| 9 | 1 | 140.000 | 0.000 | 140.000 | 0.000 | 0.0000 | 0.000 |
| 10 | 1 | 189.394 | 45.102 | 189.394 | 45.102 | -0.0001 | 0.001 |
| 1 | 2 | 176.805 | 34.742 | 176.805 | 34.742 | -0.0002 | 0.000 |
| 2 | 2 | 238.433 | 27.961 | 238.433 | 27.961 | -0.0002 | 0.002 |
| 3 | 2 | 320.000 | 0.000 | 320.000 | 0.000 | 0.0000 | 0.000 |
| 4 | 2 | 382.946 | 28.954 | 382.946 | 28.954 | -0.0001 | 0.001 |
| 5 | 2 | 480.000 | 0.000 | 480.000 | 0.000 | 0.0000 | 0.000 |
| 6 | 2 | 328.141 | 31.755 | 328.141 | 31.755 | 0.0001 | 0.001 |
| 7 | 2 | 249.355 | 39.729 | 249.355 | 39.729 | 0.0000 | 0.001 |
| 8 | 2 | 211.679 | 33.612 | 211.679 | 33.612 | 0.0002 | -0.001 |
| 9 | 2 | 217.247 | 33.675 | 217.247 | 33.675 | -0.0001 | 0.001 |
| 10 | 2 | 238.994 | 49.873 | 238.994 | 49.873 | 0.0001 | 0.000 |
| 1 | 3 | 197.935 | 40.499 | 197.935 | 40.499 | -0.0002 | 0.000 |
| 2 | 3 | 250.000 | 0.000 | 250.000 | 0.000 | 0.0000 | 0.000 |
| 3 | 3 | 279.035 | 30.183 | 279.035 | 30.183 | 0.0001 | -0.001 |
| 4 | 3 | 319.091 | 36.738 | 319.091 | 36.738 | 0.0000 | 0.000 |
| 5 | 3 | 331.812 | 29.747 | 331.812 | 29.747 | 0.0000 | 0.001 |
| 6 | 3 | 240.000 | 0.000 | 240.000 | 0.000 | 0.0000 | 0.000 |
| 7 | 3 | 254.301 | 28.850 | 254.301 | 28.850 | -0.0001 | 0.000 |
| 8 | 3 | 230.000 | 0.000 | 230.000 | 0.000 | 0.0000 | 0.000 |
| 9 | 3 | 320.899 | 30.958 | 320.899 | 30.958 | 0.0001 | 0.001 |
| 10 | 3 | 318.501 | 49.116 | 318.501 | 49.116 | -0.0001 | 0.001 |
| 1 | 4 | 183.584 | 49.513 | 183.584 | 49.513 | 0.0002 | 0.000 |
| 2 | 4 | 196.914 | 36.467 | 196.914 | 36.467 | 0.0000 | -0.001 |
| 3 | 4 | 208.561 | 37.453 | 208.561 | 37.453 | 0.0000 | 0.000 |
| 4 | 4 | 228.292 | 34.299 | 228.292 | 34.299 | -0.0002 | 0.001 |
| 5 | 4 | 266.565 | 31.883 | 266.565 | 31.883 | 0.0002 | -0.001 |
| 6 | 4 | 290.640 | 32.575 | 290.640 | 32.575 | 0.0001 | 0.000 |
| 7 | 4 | 328.660 | 36.910 | 328.660 | 36.910 | 0.0001 | 0.000 |
| 8 | 4 | 381.975 | 30.190 | 381.975 | 30.190 | 0.0000 | -0.001 |
| 9 | 4 | 500.000 | 0.000 | 500.000 | 0.000 | 0.0000 | 0.000 |
| 10 | 4 | 380.599 | 40.546 | 380.599 | 40.546 | 0.0000 | -0.001 |
| 1 | 5 | 158.586 | 49.887 | 158.586 | 49.887 | -0.0001 | -0.001 |
| 2 | 5 | 147.325 | 36.157 | 147.325 | 36.157 | 0.0001 | 0.001 |
| 3 | 5 | 148.342 | 32.774 | 148.342 | 32.774 | -0.0003 | -0.001 |
| 4 | 5 | 130.000 | 0.000 | 130.000 | 0.000 | 0.0000 | 0.000 |
| 5 | 5 | 250.000 | 0.000 | 250.000 | 0.000 | 0.0000 | 0.000 |
| 6 | 5 | 330.996 | 32.193 | 330.996 | 32.193 | -0.0001 | -0.001 |
| 7 | 5 | 417.849 | 34.784 | 417.849 | 34.784 | -0.0001 | 0.001 |
| 8 | 5 | 439.328 | 37.401 | 439.328 | 37.401 | 0.0000 | -0.001 |
| 9 | 5 | 420.403 | 32.743 | 420.403 | 32.743 | 0.0000 | 0.001 |
| 10 | 5 | 348.469 | 34.900 | 348.469 | 34.900 | 0.0001 | -0.001 |
| 1 | 6 | 151.954 | 42.766 | 151.954 | 42.766 | -0.0001 | 0.000 |
| 2 | 6 | 110.000 | 0.000 | 110.000 | 0.000 | 0.0000 | 0.000 |
| 3 | 6 | 154.032 | 32.503 | 154.032 | 32.503 | 0.0001 | -0.001 |
| 4 | 6 | 170.729 | 34.371 | 170.729 | 34.371 | 0.0003 | 0.001 |
| 5 | 6 | 215.532 | 32.084 | 215.532 | 32.084 | 0.0000 | 0.001 |
| 6 | 6 | 311.536 | 27.887 | 311.536 | 27.887 | 0.0001 | 0.001 |
| 7 | 6 | 520.000 | 0.000 | 520.000 | 0.000 | 0.0000 | 0.000 |
| 8 | 6 | 433.181 | 34.704 | 433.181 | 34.704 | 0.0001 | 0.000 |
| 9 | 6 | 359.452 | 34.725 | 359.452 | 34.725 | 0.0000 | 0.001 |
| 10 | 6 | 260.000 | 0.000 | 260.000 | 0.000 | 0.0000 | 0.000 |
| 1 | 7 | 183.127 | 46.251 | 183.127 | 46.251 | 0.0002 | 0.000 |
| 2 | 7 | 200.223 | 33.200 | 200.223 | 33.200 | -0.0001 | 0.000 |
| 3 | 7 | 229.840 | 32.832 | 229.840 | 32.832 | -0.0001 | 0.001 |
| 4 | 7 | 206.840 | 39.717 | 206.840 | 39.717 | 0.0002 | -0.001 |
| 5 | 7 | 182.669 | 35.186 | 182.669 | 35.186 | 0.0000 | -0.001 |
| 6 | 7 | 160.000 | 0.000 | 160.000 | 0.000 | 0.0000 | 0.000 |
| 7 | 7 | 329.802 | 27.708 | 329.802 | 27.708 | 0.0000 | 0.001 |
| 8 | 7 | 356.368 | 32.585 | 356.368 | 32.585 | -0.0001 | 0.001 |
| 9 | 7 | 324.820 | 38.363 | 324.820 | 38.363 | -0.0001 | 0.000 |
| 10 | 7 | 288.316 | 38.977 | 288.316 | 38.977 | 0.0001 | 0.000 |
| 1 | 8 | 208.591 | 38.018 | 208.591 | 38.018 | 0.0000 | -0.001 |
| 2 | 8 | 255.559 | 32.710 | 255.559 | 32.710 | 0.0001 | -0.001 |
| 3 | 8 | 350.000 | 0.000 | 350.000 | 0.000 | 0.0000 | 0.000 |
| 4 | 8 | 217.261 | 30.448 | 217.261 | 30.448 | 0.0000 | 0.001 |
| 5 | 8 | 178.860 | 37.554 | 178.860 | 37.554 | 0.0002 | 0.001 |
| 6 | 8 | 203.633 | 32.620 | 203.633 | 32.620 | 0.0002 | 0.001 |
| 7 | 8 | 272.684 | 27.721 | 272.684 | 27.721 | 0.0001 | -0.001 |
| 8 | 8 | 290.000 | 0.000 | 290.000 | 0.000 | 0.0000 | 0.000 |
| 9 | 8 | 312.123 | 37.012 | 312.123 | 37.012 | -0.0001 | 0.000 |
| 10 | 8 | 309.432 | 48.936 | 309.432 | 48.936 | -0.0001 | 0.001 |
| 1 | 9 | 200.000 | 0.000 | 200.000 | 0.000 | 0.0000 | 0.000 |
| 2 | 9 | 234.937 | 33.675 | 234.937 | 33.675 | 0.0001 | 0.000 |
| 3 | 9 | 232.080 | 30.993 | 232.080 | 30.993 | -0.0001 | -0.001 |
| 4 | 9 | 130.000 | 0.000 | 130.000 | 0.000 | 0.0000 | 0.000 |
| 5 | 9 | 175.469 | 36.478 | 175.469 | 36.478 | 0.0000 | -0.001 |
| 6 | 9 | 227.945 | 36.184 | 227.945 | 36.184 | -0.0001 | -0.001 |
| 7 | 9 | 300.000 | 0.000 | 300.000 | 0.000 | 0.0000 | 0.000 |
| 8 | 9 | 307.673 | 30.880 | 307.673 | 30.880 | -0.0001 | -0.001 |
| 9 | 9 | 326.782 | 38.674 | 326.782 | 38.674 | 0.0000 | 0.001 |
| 10 | 9 | 338.583 | 38.989 | 338.583 | 38.989 | -0.0001 | 0.000 |
| 1 | 10 | 208.209 | 45.214 | 208.209 | 45.214 | 0.0000 | 0.001 |
| 2 | 10 | 213.011 | 50.147 | 213.011 | 50.147 | 0.0002 | 0.001 |
| 3 | 10 | 200.094 | 49.902 | 200.094 | 49.902 | -0.0002 | 0.000 |
| 4 | 10 | 175.911 | 43.785 | 175.911 | 43.785 | 0.0001 | 0.001 |
| 5 | 10 | 193.589 | 50.322 | 193.589 | 50.322 | 0.0000 | 0.001 |
| 6 | 10 | 237.216 | 50.146 | 237.216 | 50.146 | 0.0000 | -0.001 |
| 7 | 10 | 282.236 | 42.880 | 282.236 | 42.880 | 0.0000 | 0.000 |
| 8 | 10 | 311.400 | 46.365 | 311.400 | 46.365 | 0.0000 | -0.001 |
| 9 | 10 | 340.392 | 38.483 | 340.392 | 38.483 | 0.0000 | 0.000 |
| 10 | 10 | 380.000 | 0.000 | 380.000 | 0.000 | 0.0000 | 0.000 |

| **Table 3. Estimate and error variance at each point from two calculation methods of simple kriging** | | | | | | | |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **Location** | | **Spreadsheet** | | **KT3D** | | **Error (%)** | |
| **X** | **Y** | **Estimate** | **Variance** | **Estimate** | **Variance** | **Estimate** | **Variance** |
| 1 | 1 | 120.000 | 0.000 | 120.000 | 0.000 | 0.0000 | 0.000 |
| 2 | 1 | 198.250 | 34.608 | 198.250 | 34.608 | -0.0002 | -0.001 |
| 3 | 1 | 271.093 | 39.518 | 271.093 | 39.518 | -0.0001 | 0.001 |
| 4 | 1 | 329.787 | 43.746 | 329.787 | 43.746 | 0.0001 | 0.000 |
| 5 | 1 | 352.758 | 42.351 | 352.758 | 42.351 | 0.0001 | 0.000 |
| 6 | 1 | 292.867 | 49.963 | 292.867 | 49.963 | 0.0001 | 0.000 |
| 7 | 1 | 221.855 | 52.309 | 221.855 | 52.309 | 0.0001 | 0.000 |
| 8 | 1 | 174.132 | 39.255 | 174.132 | 39.255 | 0.0002 | -0.001 |
| 9 | 1 | 140.000 | 0.000 | 140.000 | 0.000 | 0.0000 | 0.000 |
| 10 | 1 | 140.694 | 44.117 | 140.694 | 44.116 | 0.0002 | 0.001 |
| 1 | 2 | 160.690 | 34.634 | 160.690 | 34.634 | -0.0001 | 0.001 |
| 2 | 2 | 235.065 | 27.957 | 235.065 | 27.957 | 0.0001 | -0.001 |
| 3 | 2 | 320.000 | 0.000 | 320.000 | 0.000 | 0.0000 | 0.000 |
| 4 | 2 | 377.142 | 28.940 | 377.142 | 28.940 | 0.0000 | 0.001 |
| 5 | 2 | 480.000 | 0.000 | 480.000 | 0.000 | 0.0000 | 0.000 |
| 6 | 2 | 317.628 | 31.709 | 317.628 | 31.709 | 0.0000 | 0.001 |
| 7 | 2 | 237.568 | 39.672 | 237.568 | 39.672 | -0.0001 | -0.001 |
| 8 | 2 | 204.440 | 33.590 | 204.440 | 33.590 | -0.0002 | 0.000 |
| 9 | 2 | 206.220 | 33.625 | 206.220 | 33.625 | -0.0001 | 0.000 |
| 10 | 2 | 199.410 | 49.222 | 199.410 | 49.222 | 0.0001 | 0.000 |
| 1 | 3 | 172.601 | 40.232 | 172.601 | 40.232 | 0.0002 | 0.001 |
| 2 | 3 | 250.000 | 0.000 | 250.000 | 0.000 | 0.0000 | 0.000 |
| 3 | 3 | 279.905 | 30.182 | 279.905 | 30.182 | -0.0001 | 0.002 |
| 4 | 3 | 319.307 | 36.738 | 319.307 | 36.738 | -0.0001 | 0.000 |
| 5 | 3 | 332.448 | 29.747 | 332.448 | 29.747 | -0.0001 | 0.001 |
| 6 | 3 | 240.000 | 0.000 | 240.000 | 0.000 | 0.0000 | 0.000 |
| 7 | 3 | 251.784 | 28.847 | 251.784 | 28.847 | 0.0001 | 0.002 |
| 8 | 3 | 230.000 | 0.000 | 230.000 | 0.000 | 0.0000 | 0.000 |
| 9 | 3 | 310.714 | 30.915 | 310.714 | 30.915 | -0.0002 | 0.001 |
| 10 | 3 | 283.326 | 48.602 | 283.326 | 48.602 | 0.0000 | 0.000 |
| 1 | 4 | 151.101 | 49.074 | 151.101 | 49.074 | -0.0001 | 0.001 |
| 2 | 4 | 185.893 | 36.416 | 185.893 | 36.416 | 0.0000 | 0.001 |
| 3 | 4 | 206.001 | 37.450 | 206.001 | 37.450 | 0.0000 | 0.001 |
| 4 | 4 | 227.753 | 34.299 | 227.753 | 34.299 | 0.0001 | 0.001 |
| 5 | 4 | 266.250 | 31.883 | 266.250 | 31.883 | -0.0001 | -0.001 |
| 6 | 4 | 289.797 | 32.575 | 289.797 | 32.575 | 0.0001 | -0.001 |
| 7 | 4 | 327.888 | 36.910 | 327.888 | 36.910 | 0.0001 | -0.001 |
| 8 | 4 | 382.611 | 30.189 | 382.611 | 30.189 | -0.0001 | 0.001 |
| 9 | 4 | 500.000 | 0.000 | 500.000 | 0.000 | 0.0000 | 0.000 |
| 10 | 4 | 353.018 | 40.229 | 353.018 | 40.229 | 0.0001 | 0.001 |
| 1 | 5 | 124.845 | 49.413 | 124.845 | 49.413 | 0.0002 | 0.001 |
| 2 | 5 | 135.941 | 36.104 | 135.941 | 36.104 | 0.0000 | -0.001 |
| 3 | 5 | 145.493 | 32.770 | 145.493 | 32.770 | 0.0002 | 0.001 |
| 4 | 5 | 130.000 | 0.000 | 130.000 | 0.000 | 0.0000 | 0.000 |
| 5 | 5 | 250.000 | 0.000 | 250.000 | 0.000 | 0.0000 | 0.000 |
| 6 | 5 | 329.520 | 32.192 | 329.520 | 32.192 | 0.0001 | -0.001 |
| 7 | 5 | 416.830 | 34.784 | 416.830 | 34.784 | 0.0000 | 0.000 |
| 8 | 5 | 439.296 | 37.401 | 439.296 | 37.401 | -0.0001 | -0.001 |
| 9 | 5 | 418.034 | 32.741 | 418.034 | 32.741 | -0.0001 | 0.000 |
| 10 | 5 | 330.421 | 34.764 | 330.421 | 34.764 | 0.0001 | 0.000 |
| 1 | 6 | 121.926 | 42.391 | 121.926 | 42.391 | -0.0001 | 0.000 |
| 2 | 6 | 110.000 | 0.000 | 110.000 | 0.000 | 0.0000 | 0.000 |
| 3 | 6 | 153.605 | 32.503 | 153.605 | 32.503 | -0.0002 | -0.001 |
| 4 | 6 | 169.764 | 34.371 | 169.764 | 34.371 | -0.0001 | 0.000 |
| 5 | 6 | 214.065 | 32.084 | 214.065 | 32.084 | -0.0002 | -0.002 |
| 6 | 6 | 310.223 | 27.887 | 310.223 | 27.887 | -0.0001 | -0.002 |
| 7 | 6 | 520.000 | 0.000 | 520.000 | 0.000 | 0.0000 | 0.000 |
| 8 | 6 | 432.797 | 34.704 | 432.798 | 34.704 | -0.0001 | 0.000 |
| 9 | 6 | 359.034 | 34.725 | 359.034 | 34.725 | -0.0001 | 0.001 |
| 10 | 6 | 260.000 | 0.000 | 260.000 | 0.000 | 0.0000 | 0.000 |
| 1 | 7 | 156.442 | 45.955 | 156.442 | 45.955 | 0.0002 | 0.000 |
| 2 | 7 | 193.784 | 33.183 | 193.784 | 33.183 | 0.0001 | -0.001 |
| 3 | 7 | 229.414 | 32.832 | 229.414 | 32.832 | -0.0002 | 0.001 |
| 4 | 7 | 206.226 | 39.717 | 206.226 | 39.717 | 0.0000 | -0.001 |
| 5 | 7 | 181.158 | 35.185 | 181.157 | 35.185 | 0.0003 | -0.001 |
| 6 | 7 | 160.000 | 0.000 | 160.000 | 0.000 | 0.0000 | 0.000 |
| 7 | 7 | 329.619 | 27.708 | 329.619 | 27.708 | 0.0001 | 0.001 |
| 8 | 7 | 355.531 | 32.585 | 355.531 | 32.585 | -0.0001 | 0.000 |
| 9 | 7 | 320.344 | 38.355 | 320.344 | 38.355 | 0.0001 | -0.001 |
| 10 | 7 | 271.544 | 38.860 | 271.544 | 38.860 | 0.0001 | 0.000 |
| 1 | 8 | 190.570 | 37.883 | 190.570 | 37.883 | 0.0001 | -0.001 |
| 2 | 8 | 250.322 | 32.698 | 250.322 | 32.698 | 0.0001 | 0.001 |
| 3 | 8 | 350.000 | 0.000 | 350.000 | 0.000 | 0.0000 | 0.000 |
| 4 | 8 | 217.501 | 30.448 | 217.501 | 30.448 | 0.0002 | 0.001 |
| 5 | 8 | 175.875 | 37.551 | 175.875 | 37.551 | 0.0001 | -0.001 |
| 6 | 8 | 200.814 | 32.617 | 200.814 | 32.617 | -0.0002 | 0.000 |
| 7 | 8 | 272.916 | 27.721 | 272.916 | 27.721 | 0.0001 | -0.001 |
| 8 | 8 | 290.000 | 0.000 | 290.000 | 0.000 | 0.0000 | 0.000 |
| 9 | 8 | 304.547 | 36.988 | 304.547 | 36.988 | -0.0001 | 0.000 |
| 10 | 8 | 287.561 | 48.738 | 287.561 | 48.738 | 0.0001 | -0.001 |
| 1 | 9 | 200.000 | 0.000 | 200.000 | 0.000 | 0.0000 | 0.000 |
| 2 | 9 | 223.608 | 33.622 | 223.608 | 33.622 | -0.0001 | -0.001 |
| 3 | 9 | 221.089 | 30.942 | 221.089 | 30.942 | 0.0002 | 0.001 |
| 4 | 9 | 130.000 | 0.000 | 130.000 | 0.000 | 0.0000 | 0.000 |
| 5 | 9 | 162.905 | 36.412 | 162.905 | 36.412 | 0.0000 | 0.000 |
| 6 | 9 | 215.551 | 36.120 | 215.551 | 36.120 | -0.0001 | -0.001 |
| 7 | 9 | 300.000 | 0.000 | 300.000 | 0.000 | 0.0000 | 0.000 |
| 8 | 9 | 300.168 | 30.856 | 300.168 | 30.856 | 0.0001 | 0.001 |
| 9 | 9 | 317.865 | 38.641 | 317.865 | 38.641 | -0.0001 | 0.000 |
| 10 | 9 | 322.021 | 38.875 | 322.021 | 38.875 | 0.0000 | 0.000 |
| 1 | 10 | 158.076 | 44.170 | 158.076 | 44.170 | 0.0001 | -0.001 |
| 2 | 10 | 170.911 | 49.411 | 170.911 | 49.411 | 0.0001 | -0.001 |
| 3 | 10 | 160.441 | 49.248 | 160.441 | 49.248 | 0.0000 | 0.001 |
| 4 | 10 | 139.037 | 43.220 | 139.037 | 43.220 | -0.0002 | 0.001 |
| 5 | 10 | 155.134 | 49.708 | 155.134 | 49.708 | -0.0001 | -0.001 |
| 6 | 10 | 200.137 | 49.574 | 200.137 | 49.574 | 0.0002 | 0.000 |
| 7 | 10 | 250.417 | 42.459 | 250.417 | 42.459 | 0.0002 | 0.001 |
| 8 | 10 | 283.384 | 46.038 | 283.384 | 46.038 | 0.0000 | 0.001 |
| 9 | 10 | 321.151 | 38.329 | 321.151 | 38.329 | -0.0001 | 0.000 |
| 10 | 10 | 380.000 | 0.000 | 380.000 | 0.000 | 0.0000 | 0.000 |

Support Software Approval for Use

According to above test, the KT3D executable from GSLIB can be used to perform ordinary and simple kriging with an exponential variogram model. Other options within kt3d have not been validated at this time.

Support Software Check-Out and Installation Procedure

The procedure to check out and install this software is: 1) request copy from Software Owner, who will furnish a copy from the MKS Integrity™ archive and add the user and machine to the list of approved users; 2) install the software on the target computer; 3) repeat the software test identified for acceptance testing and verify the same results were obtained as reported above. If the installation test fails, the user will make reasonable efforts to identify and correct the source of the problem. If the problem cannot be resolved, the software user will report the difficulty to the software owner. The software owner will take appropriate steps upon receipt of this form to evaluate the problem and correct; corrected code will require issuance of a new build.

Reference

Deutsch, C.V. and Journel, A.G. 1998. Geostatistical Software Library and User’s Guide (second edition). Oxford University Press.

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