CH2M HILL Plateau Remediation Company

ADMINISTRATIVE DOCUMENT PROCESSING AND APPROVAL

DOCUMENT TITLE:	**OWNING ORGANIZATION/FACILITY:**
Technical Approach Description: Automated Quality Assurance Process Design	EP&SP/Risk & Modeling Integration
Document Number: CP-60411	**Revision/Change Number:** 0

DOCUMENT TYPE *(Check Applicable)* [ ] Plan [ ] Report [ ] Study [x] Description Document [ ] Other

DOCUMENT ACTION *(Check One)* [x] New [ ] Revision [ ] Cancellation

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B. Document Number CP-60411 Revision 0

C. Title
Hanford Site Composite Analysis Technical Approach Description: Automated Quality Assurance Process Design

D. Proposed Internet Address

E. Required Information (MANDATORY)

1. Is document potentially Classified? (●) No ( ) Yes

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3. Date of Conference ______
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5. Will Information be Published in Proceedings? (●) No ( ) Yes
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J. Comments

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By Lana Perry at 7:54 am, Jul 31, 2017

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A-6001-401 (REV 5)

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<comments>Due Wednesday June 7, 2017 COB. Please approve "Hanford Site Composite Analysis Technical Approach Description: Automated Quality Assurance Process Design," submitted by Will Nichols for Public release. Thank you, Lana Perry Information Clearance</comments>
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<task name="Add XML" id="1" date-done="20170531T0948" />
<task name="Manager Approval" id="41" date-due="20170605T0948" date-done="20170531T0954" performer="Alaa H Aly" performer-id="141440097" username="h9198318" disposition="Approve" authentication="true" />
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CP-60411
Revision 0

Hanford Site Composite Analysis Technical Approach Description: Automated Quality Assurance Process Design

Prepared for the U.S. Department of Energy
Assistant Secretary for Environmental Management

Contractor for the U.S. Department of Energy
under Contract DE-AC06-08RL14788

P.O. Box 1600
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CP-60411
Revision 0

Hanford Site Composite Analysis Technical Approach Description: Automated Quality Assurance Process Design

Document Type: ENV Program/Project: EP&SP

R. E. Dockter
INTERA, Inc.

Date Published
June 2017

Prepared for the U.S. Department of Energy
Assistant Secretary for Environmental Management

Contractor for the U.S. Department of Energy
under Contract DE-AC06-08RL14788

ch2m℠
P.O. Box 1600
Richland, Washington 99352

APPROVED
By Lana Perry at 7:55 am, Jul 31, 2017

Release Approval Date

Printed in the United States of America

Hanford Site Composite Analysis Technical Approach Description: Automated Quality Assurance Process Design

Randy Dockter

February, 2017

APPROVAL PAGE		
Title:	Hanford Site Composite Analysis Technical Approach Description: Quality Assurance Process Design	
HANFORD SITE COMPOSITE ANALYSIS		
Submitted:	Technical Approach Description Preparer RE Dockter	5-23-17 Date
Approval:	Composite Analysis Project Manager WE Nichols	23 MAY 2017 Date
Approval:	Risk Assessment and Modeling Integration Manager AH Aly	5/30/17 Date

The approval signatures on this page indicate that this technical approach description has been authorized for information release to the public through appropriate channels.

Contents

Figures

Terms

CA	Composite Analysis
CHPRC	CH2M HILL Plateau Remediation Company
DAS	Disposal Authorization Statement
EMDT	electronic modeling data transmittal
ERDF	Environmental Restoration Disposal Facility
HSDB	Hanford Sitewide Disposition Database
ICF	Integrated Computational Framework
IDF	integrated disposal facility
PA	performance assessment
QA	quality assurance
QC	quality control
TSPA	Total System Performance Assessment
WIDS	Waste Information Data System
WMA	waste management area

1 Introduction

The U.S. Department of Energy (DOE) in DOE O 435.1 Chg. 1, *Radioactive Waste Management*, requires the preparation and maintenance of a composite analysis (CA). The primary purpose of the CA is to provide a reasonable expectation that the primary public dose limit is not likely to be exceeded by multiple source terms that may significantly interact with plumes originating at a low-level waste disposal facility. The CA is used to facilitate planning and land use decisions that help assure disposal facility authorization will not result in long-term compliance problems; or, to determine management alternatives, corrective actions, or assessment needs if potential problems are identified.

A CA is not prepared to demonstrate current compliance; rather, its purpose is to model potential future exposure events. In other words, a CA is a DOE planning tool, used to provide a reasonable expectation that DOE public radiation protection requirements will be met over the long-term after the DOE site achieves its projected end state; and, the CA is a prerequisite to acquire and maintain an operational Disposal Authorization Statement (DAS).

CAs are closely linked with performance assessments for specific disposal facilities, which DOE uses to demonstrate that there is a reasonable expectation that the performance objectives will be met for a given facility. CAs may be documented in a companion report to the performance assessment, or integrated in the same report with a performance assessment (PA). At the Hanford Site, with numerous separate disposal facilities and tank farms, the CA has been developed and maintained as a separate document that includes all facilities contributing to dose at a specific boundary for supporting PAs for several low-level waste disposal facilities at the Hanford Site.

The currently maintained CA for the Hanford Site is documented in PNNL-11800, *Composite Analysis for Low Level Waste Disposal in the 200 Area Plateau of the Hanford Site*, and the subsequent Addendum 1 (PNNL-11800-Addendum-1, *Addendum to Composite Analysis for Low Level Waste Disposal in the 200 Area Plateau of the Hanford Site*). The annual summary report for this CA for fiscal year 2015 reached the determination that an update to the Hanford Site CA is necessary based on information reviewed for fiscal year 2015, as well as information presented in prior annual status reports. DOE has initiated work to develop a revised CA followed a phased approach with planning, scoping, and analysis phases. The scoping phase will culminate in the development of a detailed technical approach for preparing the revised CA. This technical approach description document presents the approach for the Quality Assurance Process Design as one facet of the overall technical approach. This is a companion document to a series of other technical approach description documents for various facets of the revised CA.

2 Background

The Hanford Site CA is being updated to support the significant progress achieved in the recently completed Environmental Restoration Disposal Facility (ERDF) and Waste Management Area C (WMA C) PAs, which are the major achievements in remediation of source areas and groundwater near the Columbia River. The updated CA will also support major PAs being developed for the Integrated Disposal Facility (IDF) and Waste Management Area A-AX (WMA A-AX).

Scoping objectives identified during CA Key Aspects Workshop (May 2016) indicated this analysis should be defined as narrowly as possible to enable a timely completion, but be sufficiently robust to serve as the planning tool envisioned in DOE O 435.1. The Quality Assurance (QA) Process Design presented in this document identifies processes planned to validate data transferred between the various components of the CA. These components include inventory, release, vadose zone transport, groundwater flow, and resultant dose. Figure 2-1 depicts the CA components and data flow between them. This QA Process Design presents the approach to be taken to assure quality is considered at every step.

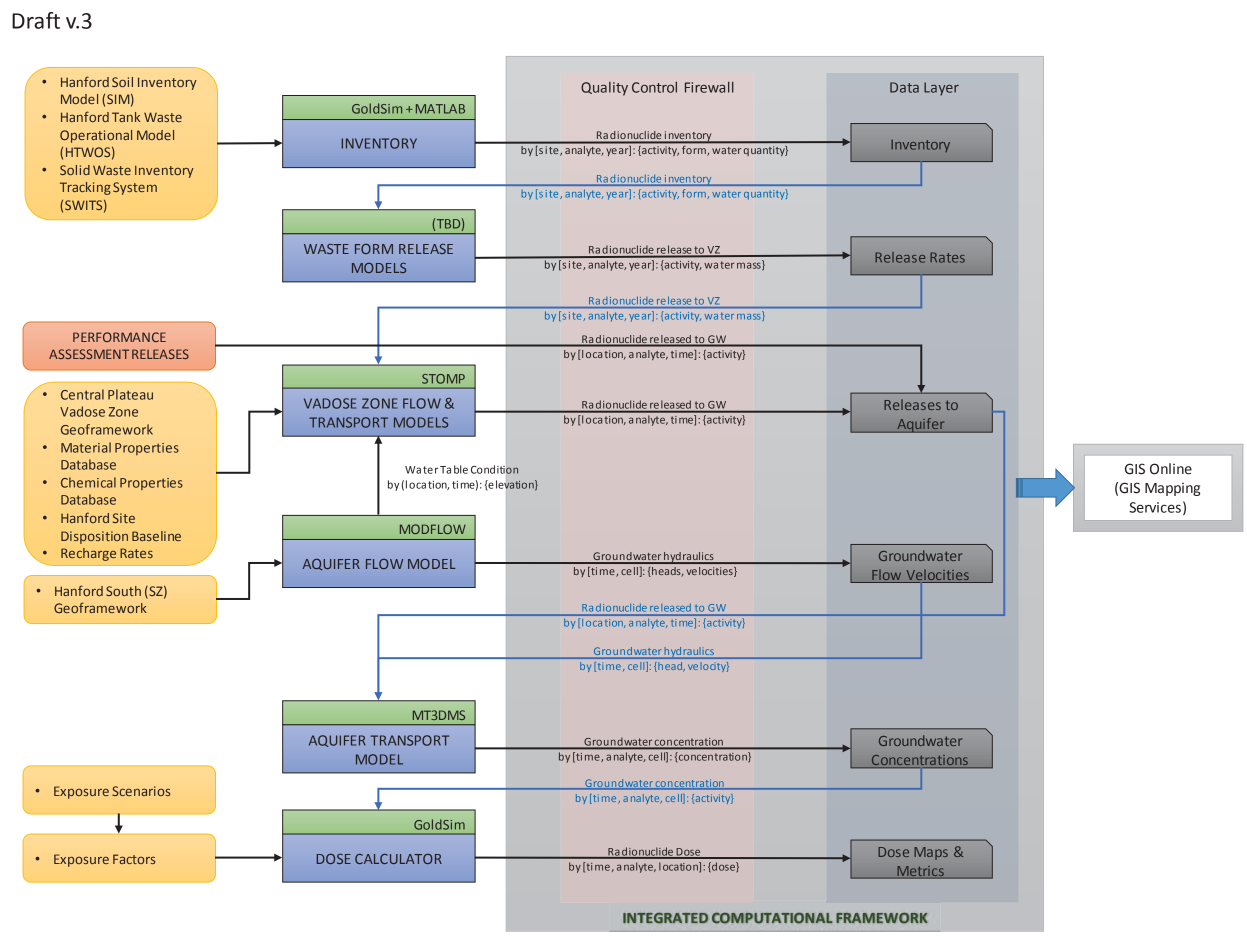

Figure 2-1. Composite Analysis Component Diagram

3 Composite Analysis

The CA technical approach to QA integrates data sources, calculations, modeling, and assessments all under a single umbrella. An integrated computational framework will include necessary data and process checking with a quality control (QC) database and tools used to support data visualization and transfer between components of the CA.

For the purposes of this QA design technical approach, data to be checked and verified have been divided into two categories. "CA Components" are the facets involving modeling or dose calculations. "CA Data Sources" are the databases and sources containing data or geoframework models containing coordinates and dimensions used by the components. Tools built to aid in the automation of data checking, transfer between entities, or to visualize results will be maintained in a CA Toolbox.

The *CA Components* include:

1. Waste form release models
2. Vadose zone flow and transport models
3. Aquifer flow model

4. Aquifer transport model
5. Exposure dose calculations

The *CA Data Sources* include:

1. Inventory Database – with contributions from:
   a. Hanford SIM – Hanford *Soil Inventory Model* with known solid and liquid inventories of chemicals and radionuclides present at locations on the Hanford Site
   b. Hanford Tank Waste Operational Model
   c. Waste Information Data System (WIDS)
2. Hanford Site Stratigraphic Layers Contacts Database – containing the Central Plateau Vadose Zone Geoframework (in development) and Hanford South Geoframework (ECF-HANFORD-12-0029, *Development of the Hanford South Geologic Framework Model, Hanford Site, Washington*) built and edited using Leapfrog®[1] & Kingdom-Geo®[2] software
3. Materials Properties Database – *to be assembled*
4. Chemical Properties Database – *to be assembled*
5. Hanford Sitewide Disposition Database (HSDB) – contains a timeline of surface conditions for sites at the Hanford Site and will be used where needed for vadose zone models

Additional data layer components to be used for automating the QA functions include:

1. QC Database – will contain model run information (logs), parameter checking status, data file MD5 hashes or checksums, and data transfer packages for exchange between CA entities
2. CA Visualization/Tools Toolbox – GitHub repository containing tools to display results for visual checks or presentations and additional software developed to support the various CA components.

3.1 Composite Analysis Components

The major CA components are waste form release models, vadose zone flow and transport models, aquifer flow model, aquifer transport model, and exposure dose calculations.

3.1.1 Waste Form Release Models

Simulates the annual release of contaminants from each site to the vadose zone from various waste types, such as liquid, cementious waste forms, graphite reactor blocks, soil debris, etc. The technical approach for this component is presented in CP-60410, *Hanford Site Composite Analysis Technical Approach Description: Waste Form Release*.

3.1.2 Vadose Zone Flow and Transport Models

Simulates fluid flow and contaminant transport by site in the vadose zone using a model implemented using the *Subsurface Transport Over Multiple Phases* (STOMP©[3]) simulation software. The technical

[1] Leapfrog, Leapfrog Geo, and Leapfrog Viewer are registered trademarks of ARANZ Geo Limited LLC, Christchurch, New Zealand.

[2] IHS™ Kingdom® software and all of its components are trademarks or registered trademarks of IHS Incorporated.

[3] Battelle Memorial Institute (Battelle) retains copyright on all versions, revisions, and operational modes of the Subsurface Transport Over Multiple Phases (STOMP) software simulator, as permitted by the U.S. Department of Energy. STOMP is used here under a limited government use license.

approach for this component is presented in CP-40605, *Hanford Site Composite Analysis Technical Approach Description: Vadose Zone*.

3.1.3 Aquifer Flow Model (MODFLOW)

Simulates sitewide fluid flow in the unconfined aquifer that underlies the Hanford Site using a calibrated groundwater model that has incorporates the structural basis provided in the Hanford South Geoframework (ECF-HANFORD-13-0029), and implemented using MODFLOW software. The technical approach for this component is presented in CP-60406, *Hanford Site Composite Analysis Technical Approach Description: Groundwater*.

3.1.4 Aquifer Transport Model (MT3DMS)

Simulates contaminant transport at plume scale in the unconfined aquifer that underlies the Hanford Site using a transport based on flow predicted by the aquifer flow model and implemented in the MT3DMS software. The technical approach for this component is presented in CP-60406, *Hanford Site Composite Analysis Technical Approach Description: Groundwater*.

3.1.5 Exposure Dose Calculations

Calculates the dose at which a reasonably maximally exposed individual would be exposed as a function of time. The technical approach for this component is presented in CP-60409, *Hanford Site Composite Analysis Technical Approach Description: Groundwater Pathway Dose Calculation*.

3.2 Composite Analysis Data Sources

The CA data sources include the inventory database, the stratigraphic layers database, the materials properties database, the chemical properties database, and the HSDB.

3.2.1 Inventory Database

This database provides an inventory of specific waste disposal and storage locations for the period 1944 to Hanford Site closure based on disposal records, process knowledge, and planned disposals and remedial actions. The technical approach for assembling this data source is described in CP-60195, *Hanford Site Composite Analysis Technical Approach Description: Radionuclide Inventory and Waste Site Selection Process.*

3.2.2 Stratigraphic Layers Database

Used for the structural basis of vadose zone models implemented using the STOMP simulation software, this database contains geoframeworks that represent the three-dimensional structure of various hydrostratigraphic layers in which the vadose zone and unconfined aquifer occur beneath the Hanford Site. These geoframeworks were developed to support a number of numerical fate and transport models and modeling applications. These geoframeworks contain dimensions and descriptions of the hydrostratigraphic units that can be displayed visually using Kingdom or Leapfrog software. Where needed for vadose zone or groundwater modeling, these frameworks will be exported in a format (grids) compatible with the numerical fate and transport modeling software (STOMP, MODFLOW, MT3DMS).

3.2.3 Materials Properties Database

Materials and their properties common to any or all components of the CA will be stored in a materials properties database to ensure the same values are used across the CA. All entry into the database, including updates and changes, will be logged indicating the date and user that made the changes. Versioning of the database will be defined by "snapshots" of the data values at specific dates, and references to parameters in this database will be made by version number. All models that use parameters from this table must query the database for values to use prior to running a model.

3.2.4 Chemical Properties Database

Physical and chemical properties common to any or all components of the CA will be stored in a chemical properties database to ensure the same values are used across the CA. All entry into the database, including updates and changes, will be logged indicating the date and user that made the changes. Versioning of the database will be defined by "snapshots" of the data values at specific dates, and references to parameters in this database will be made by version number. All models that use parameters from this table must query the database for values to use prior to running a model.

3.2.5 Hanford Sitewide Disposition Database (HSDB)

The HSDB currently contains a timeline of soil surface conditions for waste sites and facilities throughout the Hanford Site and, as updates are needed, will be versioned through periodic maintenance. Additional software that queries this database may be developed to generate permeability coefficients for constituents being modeled in the vadose zone. It is expected that additional software will become part of the CA Toolbox.

3.3 Other Composite Analysis Databases

3.3.1 QC Database

This database or workbook will contain model run information (logs), parameter checking status, data file MD5 hashes or checksums, and data transfer packages for exchange between CA components.

3.3.2 CA Visualization/Tools Database

All software automation and checking tools developed to support the various components' data exchanges will be place in a GitHub repository for access by all. This repository will also be used to store tools used to display results for visual checks or presentations and additional software developed to support the various CA components.

3.4 Integrated Computational Framework

The Integrated Computational Framework (CP-) at the heart of data verification and exchange can be thought of as a multi-layer framework as depicted in Figure 3-1. The data layer contains the databases and files with data values and metadata. The Server Layer contains the host or automation software that serves the data to the Application Layer, where the Visualization Tools, Firewall, and Data Utilities run.

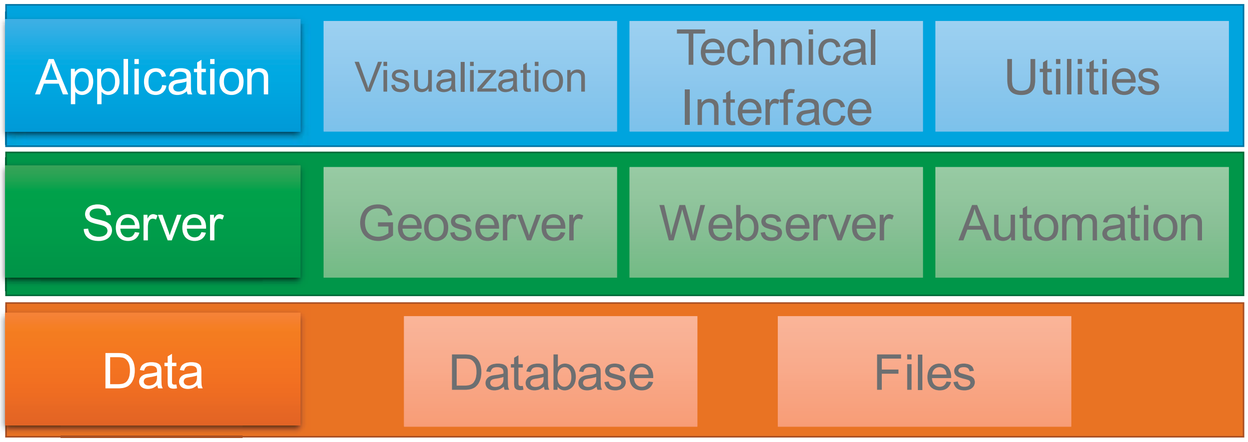

Figure 3-1. Layers of the Integrated Computational Framework

4 Methodology

Data packages will be defined identifying any data transferred into or out of a CA component. These data packages will be used to maintain control over parameter values transferred from one CA component to another, and to ensure consistency that the same parameter values are used in each of the various components. Input parameters may be cascaded from one CA component to another as long as the version being used is identified and every version of a parameter is stored in the original source.

Data packages will contain as much information about each parameter as needed for QC verification and traceability. Each data item will contain the following information:

- Parameter Name – 25 character or less string identifying the parameter
- Data Type – binary floating point (single or double precision), integer (32-bit, 64-bit), string, single value or N-dimensional array, probabilistic or cumulative distribution, reference pointer (file location), etc.
- File Name and Path – if data type is reference pointer
- Data Structure – how data are arranged: arrays, lists (linked, ordered, random), stacks (fifo), trees, etc.
- Special meanings – how special values are to be interpreted (nulls, zeros, negatives, zero-length strings, end-of-line, end-of-record, etc.)
- Units – units of the parameter
- Source – where the parameter originated in the source CA component (table, calculation, variable, etc.)
- Destination – which CA components will use the data item
- Other – other pertinent information

5 Quality Assurance and Quality Control

5.1 Project Quality Assurance Plan

The CH2M HILL Plateau Remediation Company's (CHPRC's) plan PRC-MP-EP-53107, *Hanford Composite Analysis Project Management Plan*, Appendix B ("Hanford Site Composite Analysis Quality Assurance Plan") specifies the QA/QC requirements for the CA update, noting the importance of QA/QC to this project:

> "A critical aspect of preparation of the revised Hanford Site Composite Analysis is quality assurance and quality control (QA/QC). This Project-Specific Quality Assurance Plan documents the plan for QA/QC for the project that is consistent with CHPRC plans and procedures that implement DOE requirements, EPA guidance, and adds additional project-specific requirements deemed necessary to facilitate delivery of a successful product."

Guiding principles are provided in the project QA plan (Section 1.2 of Appendix B), including that QA/QC controls will address three key areas:

1. Software quality and control – to ensure use of only software that meets DOE requirements for use under a graded approach.
2. Data quality and control – to promote fully traceable development of model input parameters from traceable and qualified data.
3. Application quality and control – to promote fully traceable calculations using numerical software in which inputs are traceable to data (basis information), code use is traceable to inputs, and outputs are traceable to code use.

Software quality and control are to be addressed through the application of procedure PRC-PRO-IRM-309, Controlled Software Management, which implements requirements of DOE O 414.1, Quality Assurance, for software used for modeling and calculations in the CA.

Data quality and control are addressed through provisions of the project QA plan, including the designation of a data configuration manager for the CA update project, maintenance of data configuration control, and requirements for the use of electronic modeling data transmittal (EMDT) forms to document submittal and review of all data configuration items utilized in the updated CA.

Definition of application quality and control was deferred in the project QA plan until completion of scoping. A key function of this technical approach description document is to identify the approach for application quality and control will be managed within the integrated computational framework. The project QA plan will be revised to include this approach at the conclusion of the scoping phase of the project.

5.2 Firewall for the Integrated Computational Framework

To facilitate integration into the CA computational QA framework, individual technical approach documents will identify data inputs and outputs as specified in Section 4 of this document. This will provide the necessary information for building QC checking automation and visualization tools that help ensure data integrity and meaningful calculation results.

Additionally, the QC firewall should contain a mechanism for tracking parameters, versions of parameter sets used, reference sources for each parameter, and the status of parameter checking. An example of this approach is the Total System Performance Analysis (TSPA) parameter database (as used in the Yucca

Mountain Project) that contained the forms shown below (Figure 5-1, Figure 5-2, Figure 5-3, and Figure 5-4), although only a subset of the fields would be needed for the CA. Alternately, if time does not permit the creation of a parameter database or it is deemed more complicated than necessary, the same information could be tracked in a controlled MS-Excel®[4] workbook.

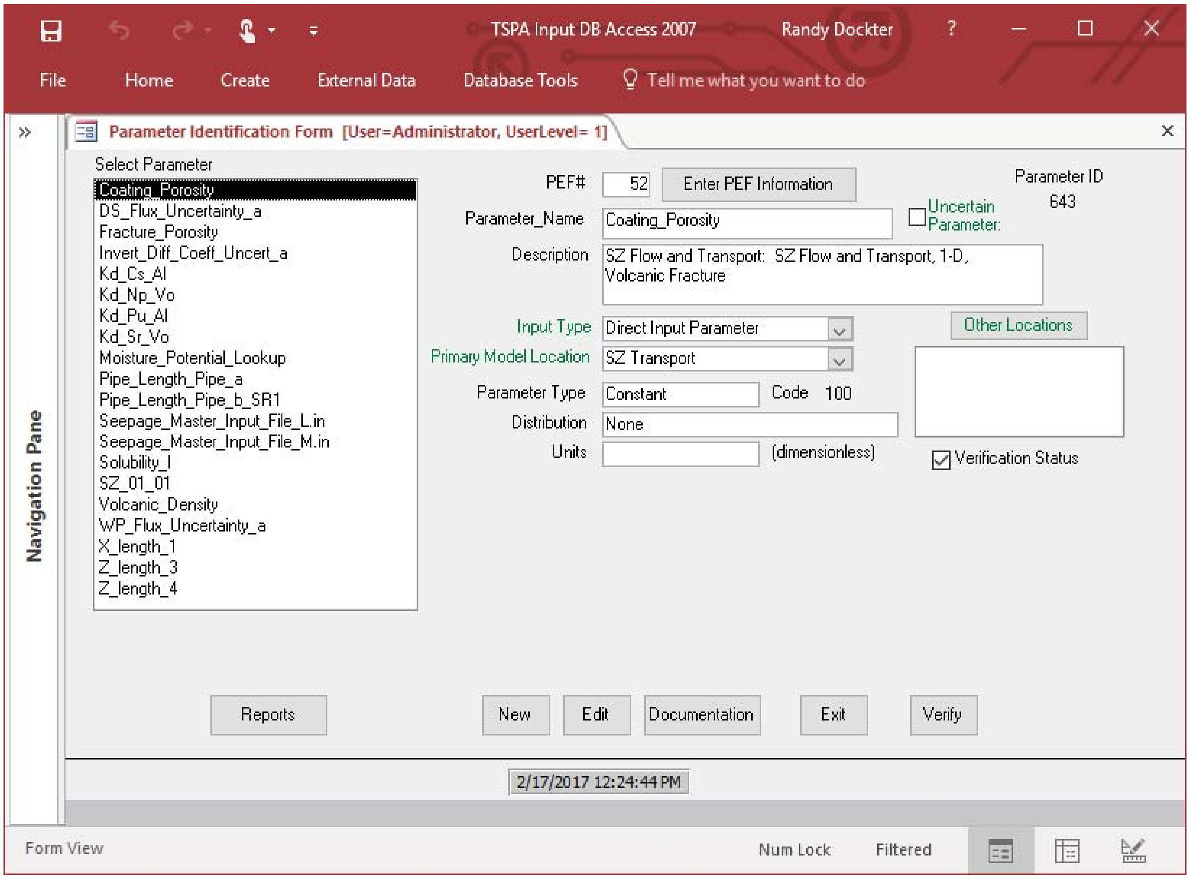

Figure 5-1. Parameter ID Form with Parameter Name, Description, Data Type, Units, etc.

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[4] Microsoft Excel is a registered trademark of Microsoft Corporation in the United States and in other countries.

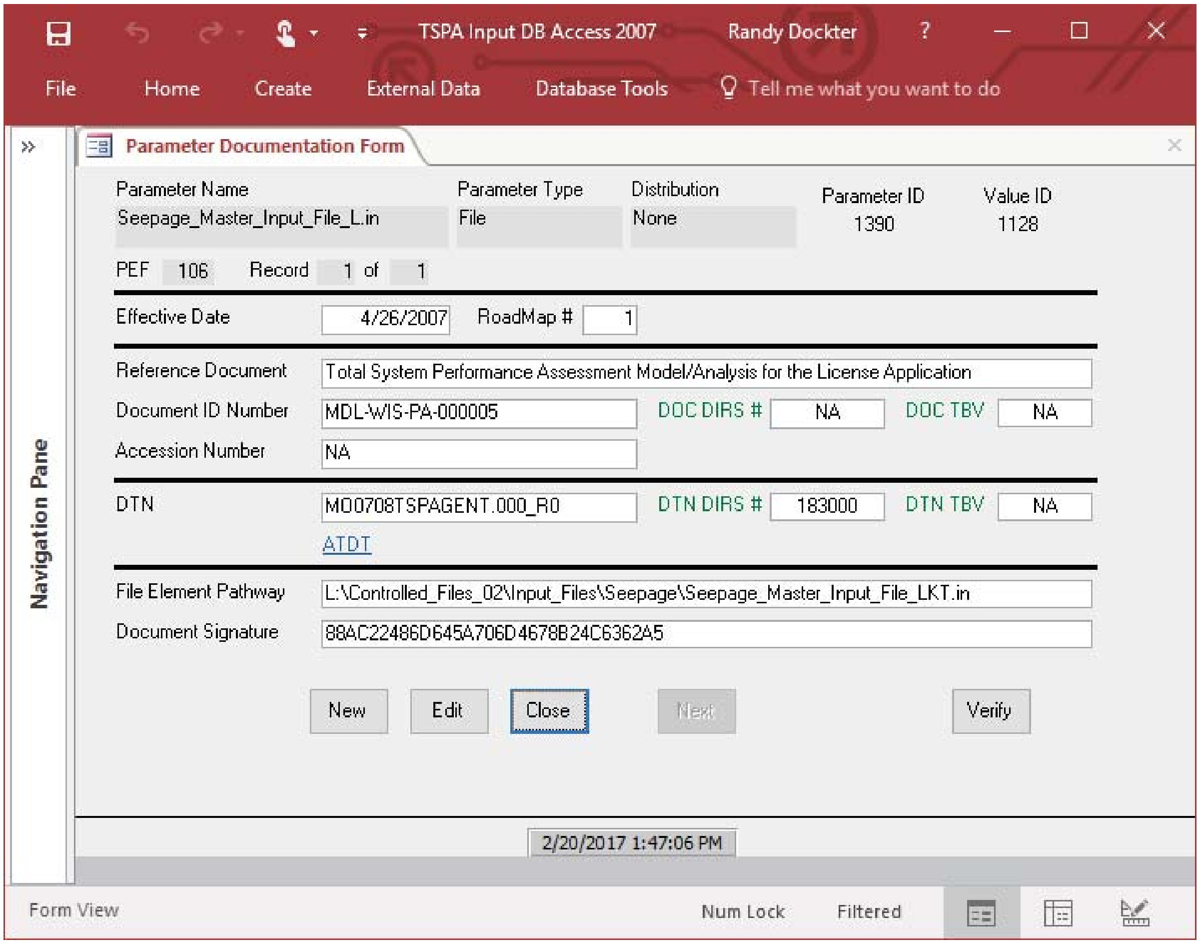

Figure 5-2. Parameter Documentation Form with Reference, File Location, Digital Signature, etc.

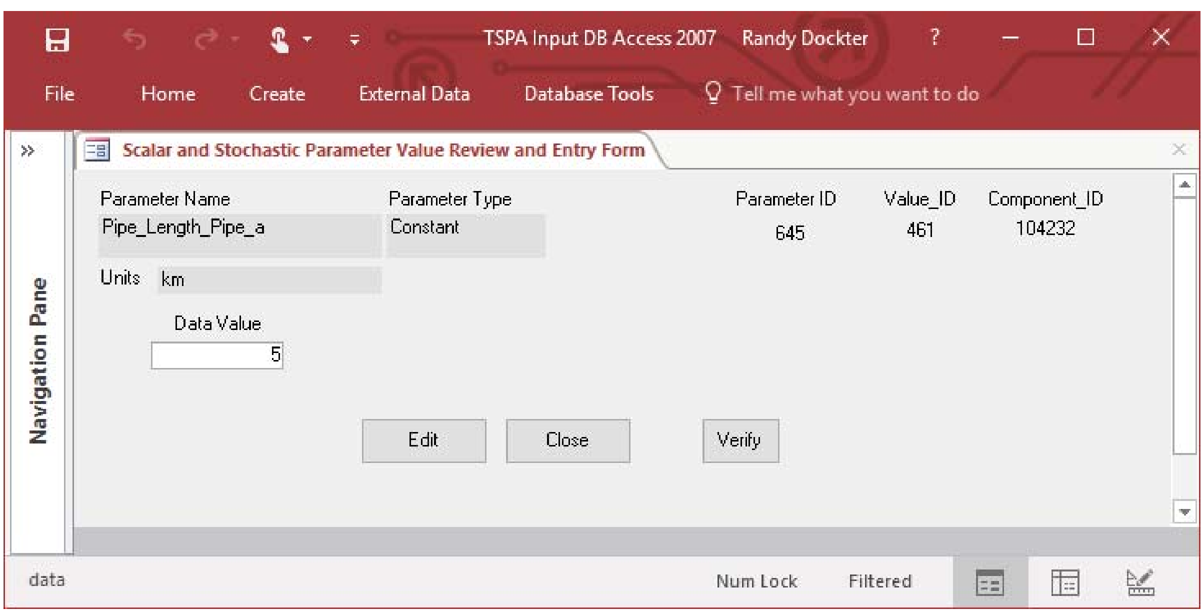

Figure 5-3. Parameter Value Form with Data Value(s) & Units

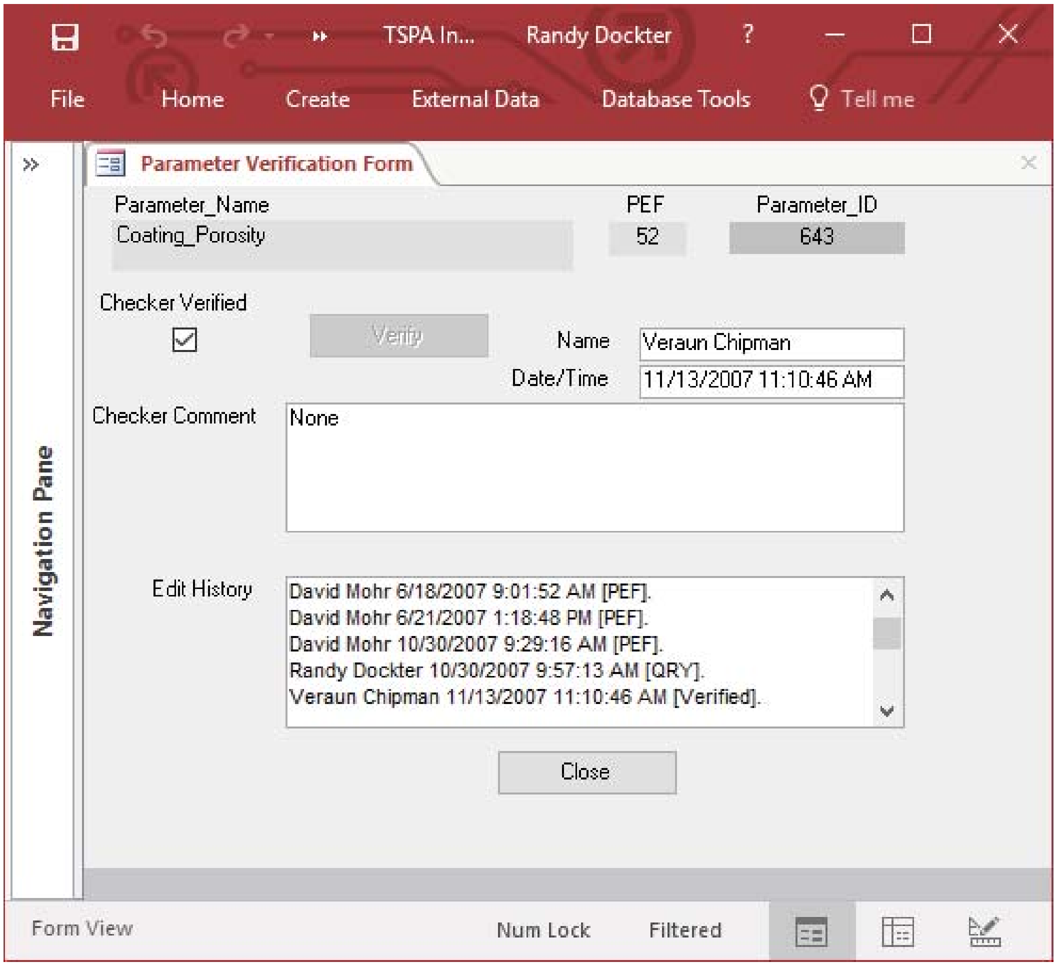

Figure 5-4. Parameter Verification Form with Verification Status

A versioning mechanism should be maintained that correlates parameter versions to actual model runs in the event a value is changed or different values are used for different scenarios. This can be accomplished by incorporating revision metadata into the parameter database, or through a separate controlled MS-Excel workbook.

Controlled folders containing CA data files will have sufficient security to assure files are not changed inadvertently or by unauthorized users. Additionally, the controlled data folders must be backed up routinely (daily or weekly incremental, weekly or monthly full) to mitigate possibilities of file corruption or loss.

6 Conclusions

It is expected that the QA guidelines presented in this document will result in an exchange of data input and output expectations for each of the CA components. This exchange will provide the basis for developing manual and automated QA tools.

7 References

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