TANK CLOSURE PROJECT DECISION MANAGEMENT TOOL FUNCTIONAL DESIGN REQUIREMENTS

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U.S. Department of Energy Contract DE-AC27-99RL14047

EDT/ECN: N/A   UC:
Cost Center: Charge Code:
B&R Code: Total Pages: 12

Key Words: Decision Managment Tool, DMT, vadose, code, software, risk assessment

Abstract: This functional design requirements document describes the design of the preliminary Decision Management Tool application under development to support the CH2M HILL Hanford Group, Inc. single-shell tank closure project.

Janis Aardal 5/18/05
Release Approval   Date

MAY 18 2005
DATE:
STA: 15
HANFORD RELEASE
ID: 65
Release Stamp

Approved For Public Release

RPP-24200
Revision 0

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Date Published
May 2005

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Prepared for the U.S. Department of Energy
Office of River Protection

Contract # DE-AC27-99RL14047, Modification M030

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LIST OF TERMS

CH2M HILL	CH2M HILL Hanford Group, Inc.
DMT	Decision Management Tool
STOMP	Subsurface Transport Over Multiple Phases

1.0 INTRODUCTION

1.1 PURPOSE

This functional design requirements document describes the design of the preliminary Decision Management Tool©[1] (DMT) application under development to support the CH2M HILL Hanford Group, Inc. (CH2M HILL) Tank Closure Project. This document and associated documents were completed in compliance with procedures TFC-BSM-IRM_HS-C-01, "Software Development, Implementation, and Management," and TFC-BSM-IRM_HS-C-03, "Custom Software Development, Implementation, and Management." The DMT is being designed as a graphical user interface that will calculate numerical risk values and groundwater concentrations from user created tank farm closure scenarios. The purposes of this document are: 1) to define the functional requirements of the application, 2) identify desired program attributes, 3) discuss how the DMT will contribute to the Tank Closure Project, and 4) provide guidance to analysts and programmers developing and maintaining the system throughout its lifetime.

2.0 CONCEPT DEFINITION

The DMT is a project specific software application designed to perform risk assessment calculations supporting the Tank Closure Project. Through a graphical interface, the user will be able to evaluate complex tank farm closure scenarios in terms of risk to human health and the environment. Results of the evaluations will support closure decisions and preparation of required closure project documents.

2.1 STATEMENT OF NEED

The single-shell tank farm closure project needs a tool to effectively and rapidly manage and manipulate large amounts of numerical data from various sources to optimize risk assessment calculations. The tool must allow for assessment of complex user defined closure scenarios, repeatedly perform calculations with varying input assumptions to assess sensitivity of risk to various parameters, be able to rapidly respond to input data changes, and provide a means for documenting the source of input data supporting specific risk assessment results.

2.1.1 Overview of Tank Farm Risk Assessment Calculations

CH2M HILL has been tasked with initiating closure activities at the Hanford Site single-shell tank farms. A critical element in the closure process is to perform risk assessments estimating the potential future impacts to human health, groundwater beneath the tank farms and the

[1] Copyright pending.

environment. The following analysis components are included in the current risk assessment modeling effort for the tank farms:

- Identification of contaminant sources
- Contaminant source inventories
- Creation of physical conceptual models of the vadose zone and aquifer beneath individual tank farms
- Source and inventory specific fate and transport simulations
- Development of multiple groundwater and direct contaminant exposure scenario models.

2.1.2 Identification of Contaminant Sources

Source terms considered in the evaluation of risk include residual waste remaining in individual tanks and ancillary equipment, past known unintentional releases of contaminants to the environment, and potential releases to the vadose zone resulting from planned waste retrieval activities. Contaminant sources are identified based on tank farm infrastructure design and process knowledge, along with historical, past sampling, and survey data. Physical dimensions and location within the vadose zone of each source are estimated from the best available information.

2.1.3 Contaminant Source Inventories

For each source identified, the inventories of waste constituents are developed by subject matter experts based on process and historical knowledge, existing sample results, inventory modeling, or other available data.

2.1.4 Conceptual Model Creation

A physical conceptual model of the vadose zone and aquifer underlying the specific tank farm is created as the basis for the fate and transport simulations. Geologic information gathered from existing boreholes is used to identify the prominent material units. Hydraulic properties of each unit are estimated from textural analysis of collected samples (i.e., grain size) and other existing information.

2.1.5 Contaminant Fate and Transport Modeling

Potential impact to groundwater from identified contaminant sources is simulated using Subsurface Transport Over Multiple Phases (STOMP)[2] modeling software developed by Pacific Northwest National Laboratory. The STOMP program solves complex saturated and unsaturated flow equations to predict contaminant movement through the vadose zone over time.

2.1.6 Exposure Scenarios for Calculating Estimated Risk

Complex exposure scenarios over multiple pathways are developed to assess potential impacts to human health and the environment. Exposure scenarios make assumptions of how future residents may use the land and groundwater potentially impacted and estimate the risk to human health based on predicted contaminant concentrations. Conversion factors are developed for each exposure scenario to calculate risk and or dose values from predicted groundwater or solid waste concentrations.

2.1.7 Summary of Risk Assessment Calculations

In general, groundwater risk calculations include dividing the STOMP simulation contaminant mass flux by the water volume flux across a specified plane, correcting for radioactive or organic decay of each constituent, selecting a simulated distribution coefficient surrogate value for each constituent, multiplying by the constituent inventory to derive the resulting groundwater concentration, and finally multiplying the groundwater concentration by the appropriate risk conversion factor. This series of computations must be performed for each constituent for each type of source selected in the closure scenario and for each time step in the simulation. In addition, multiple STOMP simulations may be generated for the same source differing in assumed infiltration rates or waste release mechanisms. Complex closure scenarios involve several sources of different types, unique inventory estimates for each source, and multiple STOMP simulations to be compiled into a cumulative sum for evaluation.

2.2 SCOPE OF NEED

Traditionally, tank closure risk assessment calculations have been completed using a standard spreadsheet application (i.e., Microsoft Excel[3]), a time-consuming, error prone process that is difficult to control from a configuration management standpoint. Evaluation of complex closure scenarios and performing input sensitivity analysis is difficult using spreadsheet calculations due to the sheer volume of data to be processed. Difficulties in effectively completing the required analyses using spreadsheet based systems prompted the Tank Closure Project to initiate design of

[2] Subsurface Transport Over Multiple Phases (STOMP) is copyrighted by Battelle Memorial Institute, 1996.
[3] Microsoft and Excel are either registered trademarks or trademarks of Microsoft Corporation in the United States and/or other countries.

the DMT: a comprehensive problem-specific, software-based system focused on the specific analysis needs of tank closure.

DMT development requires qualified software programmers to work with Tank Closure Project personnel to ensure the final application performs as desired. Until the DMT is functional, risk assessment calculations with be performed using the traditional spreadsheet methods to support discussion of risk assessment results in project documents.

2.3 SOLUTION OBJECTIVES

The DMT will perform the defined risk assessment calculations more efficiently and will allow for greater sensitivity analyses to be performed than previously possible using spreadsheet calculations. The DMT will provide critical data management capabilities, will be able to respond quickly to changes in input data, and the correctness of calculated results will be ensured through verification testing performed under an approved quality assurance program accompanying the development of this software. The development of the DMT will provide a consistent structure to the calculation method used to generate risk assessment results and will be expandable to accommodate risk assessments of any contaminated site for which the appropriate input data is available (i.e., fate and transport modeling results).

The DMT is required to have the following functions:

- Data import and management: Input data files for source inventories and STOMP simulation results must be read and imported into the DMT from their native formats.
- User Defined Closure Scenarios: The software must allow for user defined closure scenarios. Users will be able to select individual contaminant sources, inventories, and STOMP simulations. Additionally, users will be able to manually input individual contaminant inventories and distribution coefficients.
- Perform groundwater concentration and risk calculations as currently required by tank closure risk assessment methodology.
- Display defined risk assessment results and groundwater concentration results both numerically and graphically over the entire simulation modeling period (e.g., 10,000 years).
- Calculate individual and cumulative results.
- Include documentation and configuration management information for each DMT or data revision.

To anticipate future functional and design changes, the software will be designed to be as modular as possible with formal interfaces established allowing changes to one module without affecting others. Several design principles guide the development in order to implement these objectives. These design principles include:

1. System Configuration External to Executable Code to the Extent Possible

   The computer program implementing the DMT will be a single executable, "DMT.exe", and will be designed to run in an arbitrary directory on a hard drive, compact disc, or flash memory card. The data required for DMT operation shall be organized into a standardized directory structure.

2. Creation of an Object Oriented Engine to Organize Data and Requirements

   The DMT shall provide a configuration screen at startup allowing the user to determine which data to load. The configuration screen shall consist of trees that mirror the data directory structure. After the data to be used in the session are selected, the program shall load the data into an object data structure containing all of the information required for the DMT to perform all of its functions.

3. Use of Object Oriented Components to Establish Interfaces

   The object data structure containing loaded data shall be a single object with a specified interface containing all of the information necessary for the DMT to function. Programmers will be able to modify the methods of the object without changing the interface, facilitating system enhancement and maintenance. This modular technique will be used throughout the DMT program.

4. Full Display and Traceability of All Input Data

   The DMT shall provide pages to numerically display all data imported from the data directory structure. Displayed data can then be compared to configuration-managed source data to ensure that the source data has been properly imported. Each numerical display can be copied to the operating system's clipboard for insertion into a spreadsheet or other off-the-shelf software to facilitate comparison of the imported data with the original source data.

5. Calculation Functions Separate from the Data Engine

   The object data structure will be accessible from all calculation modules in the DMT and will not depend on any calculation module. This will allow developers to add new calculation modules as required without impacting previously existing modules.

6. Full Export of All Input Data, Intermediate Results, and Final Results in a Format Suitable for Use in Other Software

   Where numeric data are displayed in the DMT, a range of the data can be selected and copied to the operating system's clipboard. This makes the data range available for any other analyses that the user might need. Further, many data displays provide direct export to Microsoft Excel or to a format suitable for import into Tecplot[4]. Additionally, a configuration page is provided to batch export graphical results to Tecplot.

[4] Tecplot is a registered trademark or trademark of Tecplot, Inc.

7. Operation on Standard Computer Platforms

   The DMT will run on Microsoft Windows 2000 and Windows XP[5] platforms.

3.0 PROGRAMMATIC SUMMARY

3.1 SPONSORING ORGANIZATIONS

CH2M HILL is sponsoring the development of the DMT as a tool to support the Tank Closure Project risk assessment activities.

3.2 STRATEGIC DIRECTION

The DMT is a key component of the strategic plan of the Tank Closure Project. It is envisioned that future risk analyses supporting tank closure decisions will be performed using the DMT.

Development of the DMT will streamline the risk assessment calculation process, provide greater technical analysis by allowing for rapid, complex closure scenario comparisons, create a standard interface and database that can be distributed to multiple users, respond rapidly to changes in input data, and create a visualization tool that can be used to present risk assessment results to regulators and other stakeholders. The DMT is a graphical and numerical summary of the entire risk assessment process. As stand alone software, configuration management is simplified and correct calculation of results can be verified as part of a quality assurance plan.

The DMT contributes to the strategic direction of the Tank Closure Project, and CH2M HILL as whole, by increasing calculation efficiency, enhancing the quality of risk assessment discussion by providing a means to quickly perform detailed sensitivity analyses (limited only by the input STOMP simulations), creating an elegant visualization tool to present complex closure scenarios to regulators and stakeholders, responding rapidly to changes in data, creating a platform that provides complete traceability of input data and assumptions, and providing a means to distribute the risk assessment data and results to multiple end users with better confidence in the accuracy of the results. The ability to rapidly respond to new or altered input data will significantly aid in the preparation of closure documents, and will support the accelerated schedule of the closure activities.

3.3 RISK ANALYSIS

Development of the planned DMT software does provide some programmatic risk. The identified risks include:

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[5] Microsoft, Windows 2000, and Windows XP are either registered trademarks or trademarks of Microsoft Corporation in the United States and/or other countries.

- The software might not be completed in time to support project needs.

  Resources have been provided to develop the software in a timely manner. Further, development of the DMT is based on similar earlier projects successfully completed by CH2M HILL, Inc. companies. Many of the same personnel who worked on the earlier projects are members of the DMT development team.

- Incorrect input data might be used.

  Data to be used by the DMT are supplied from external sources and validation will be performed by these suppliers. The DMT will provide complete traceability to the validated data.

- The required calculations might not be performed accurately.

  Verification and validation of calculations will be performed prior to release of the DMT. Standard verification input files will be utilized by DMT users during installation of the software to verify correct installation of the DMT. A test plan will be developed for the DMT in accordance with the procedure, "Custom Software Development, Implementation, and Management" (TFC-BSM-IRM_HS-C-03).

4.0 PROBLEM DEFINITION

Risk assessment methodology supporting the Tank Closure Project requires manipulation of large amounts of numerical data. Traditionally, tank closure risk assessment calculations have been completed using a standard spreadsheet application (i.e., Microsoft Excel), a time-consuming, error prone process that is difficult to control from a configuration management standpoint. Spreadsheet calculations become even more unwieldy as the complexity of closure scenarios increases. Limitations of spreadsheet calculations curtail the degree of sensitivity analysis performed on the defined closure scenarios. The DMT is designed to efficiently manage large amounts of data required to evaluate complex closure scenarios. The modular nature of the DMT allows multiple tank farms to be evaluated from a single application.

4.1 CONSTRAINTS

4.1.1 Risk Assessment Methodology and Simulations

Design and flexibility of the DMT is limited by the defined risk assessment methodology, defined contaminant sources, and source fate and transport modeling results. The DMT structure is intended to be flexible and accommodate future upgrades. The total number of closure scenarios that can be evaluated with the DMT is limited by the number of STOMP fate and transport simulations run for each defined source type. The validity of the numerical results is dependent upon the assumptions supporting the fate and transport modeling and source inventories. The DMT is strictly a post-processing data management tool. The weight of validity rests solely on the assumptions supporting the simulations and inventory input data.

4.1.2 Document Schedule

The DMT is envisioned to provide selected numerical risk values to be included in Tank Closure Project documents and to support recommended closure decisions. Therefore, the DMT must be completed, tested, and verified for correctness of calculations, and approved before it can be used to support final project documents.

4.1.3 Input Data Structure

The DMT is designed to import currently identified input files according to their unique file formats. Input data in different formats may require the import routine to be modified to accept the new format.

4.1.4 Regulations, Procedures, and Policies

The DMT is envisioned as tool expanding upon existing tank farm closure risk assessment technique. Regulatory requirements, procedures, and policies applicable to single-shell tank closure have been incorporated in the risk assessment methodology to the extent they are known or defined. The DMT is intended to be upgraded to meet evolving risk assessment needs whether these are from regulatory requirements or are technical modifications. In short, regulatory drivers affecting the needs of the user will be addressed at the project level, the risk assessment methodology will be modified accordingly, and then the DMT will revised to perform the desired calculations.

4.1.5 Acceptance Criteria

Data must be imported into the DMT correctly and all calculations must be performed accurately. A test plan will be developed for the DMT in accordance with TFC-BSM-IRM_HS-C-03.

5.0 REFERENCES

TFC-BSM-IRM_HS-C-01, "Software Development, Implementation, and Management," Rev. A-8, CH2M HILL Hanford Group, Inc., Richland, Washington.

TFC-BSM-IRM_HS-C-03, "Custom Software Development, Implementation, and Management," Rev. A-2, CH2M HILL Hanford Group, Inc., Richland, Washington.