

26. COMPUTER CODES

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26.1 INTRODUCTION

Computer codes estimate future impacts by using the numerical models that are built on conceptual models (such as those described in [Chapter 16](#)) and that use the parameters described for the various processes (such as those described in Chapters 17 through 23).

Computer codes are widely used to estimate future impacts. This chapter describes the requirements for such codes and the key codes used.

The complexity of the computer code(s) can vary with complexity of the program. Sometimes, the computer codes may be quite simple. An example of a simple calculation (for example, calculations made within popular spreadsheet programs such as EXCEL) is the estimation of the potential impacts of an intruder scenario. Other times, the computer codes may be more complex, and may solve many different types of equations that approximate many different types of processes. An example of a complex calculation is one that integrates the potential impacts to groundwater of many different waste sites.

Many of the computer codes are very sophisticated. For example, a single run of the release of contaminants from a series of glass blocks in a disposal facility can take over 2 weeks on one of the world's fastest supercomputers. The long duration of such a run is driven by solving many (over 100,000) differential equations (representing moisture flow, chemical interactions, and even changes in pore structure) at many points (every inch in a facility 40 feet high) out to and beyond 10,000 years.

The next section outlines some of the key requirements of a computer simulation of a natural system that has been impacted by waste storage and disposal activities, such as at the Hanford Site. [Section 26.3](#) describes the computer codes used in analyzing the groundwater pathway. The final section ([26.4](#)) describes the numerical processes used in analyzing other pathways.

26.2 COMPUTER CODE REQUIREMENTS

Because computer codes are used to develop analytical and numerical models that are ultimately used to make predictions about the future system conditions, it is a requirement that the computer codes are accompanied by documents that support their use for completing such simulations. The documents include the following:

- ◆ Requirements
- ◆ Description of the theory underlying the code
- ◆ User's guide
- ◆ Software testing
- ◆ Configuration management
- ◆ Acceptance testing.

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These requirements are found in U.S. Department of Energy Directives (for example, [DOE G 414.1-2A](#)) and industry standards (for example, [IEEE Std. 730](#), [829](#), [830](#), and [1012](#)). The codes used in the Hanford Tank RCRA Corrective Action Programs meet these standards.

26.3 GROUNDWATER PATHWAY

26.3.1 Role of Computer Codes in Groundwater Pathway Analyses

As seen in [Chapter 16](#), the conceptual model for the groundwater pathway is complex. It is normally modeled in a series of steps:

- ◆ Moisture flow into the source region
- ◆ Release of contaminants and moisture from the source region into the vadose zone
- ◆ Moisture flow and contaminant transport in the vadose zone
- ◆ Water flow and contaminant transport in the groundwater system
- ◆ Water flow and contaminant transport in a surfacewater system ¹
- ◆ Exposure to the contaminants.

The codes used in simulating moisture flow into the source region have similarities to those used for vadose zone simulations and, hence, are described in [Section 26.3.3](#). Since simulations of surfacewater systems (for example, the Columbia River) are not performed by tank farm staff, there is no discussion of these codes.

26.3.2 Moisture Flow into the Source Region

At the Hanford Site, the UNSAT-H computer code ([Fayer 2000](#)), developed by the Hydrology Group of the Pacific Northwest National Laboratory, has been the computer code most often used to establish the amount of moisture that escapes evaporation and transpiration and enters the subsurface. UNSAT-H was selected ([DOE/RL-91-44](#)) in 1992 by the U.S. Department of Energy, U.S. Environmental Protection Agency, and Washington State Department of Ecology as the computer code to be used for such calculations. The UNSAT-H computer code simulates liquid water flow in one dimension, using Richards' Equation, water vapor diffusion using Fick's law, and heat flow using the Fourier equation.

Recently, the STOMP computer code (see [Section 26.3.4](#)) has been modified ([Ward et al. 2005b](#)) to perform similar calculations in two dimensions.

26.3.3 Waste Form Release

As seen from Section 16.3 of [Chapter 16](#) and from [Chapter 19](#), the conceptual models for release vary from contaminants being instantly available to moving moisture (for example, from debris) to a complicated system involving various physical and chemical processes that vary over time

¹ Surfacewater transport (for example, transport down the Columbia River) is not part of the tank farm scenarios.

and space. The choice of which code(s) to use depends upon the waste form and the sophistication of the conceptual model. In practice, one of the codes is used to generate inputs to the vadose zone computer codes that represent the release of contaminants from the various waste forms:

- ◆ No explicit code, input is created directly for the vadose zone code (for example, debris),
- ◆ Vadose zone code – STOMP (for waste forms modeled as simply porous media, for example, grouts and cements),
- ◆ STORM code (for waste forms where the changing chemically and physical interactions over time and space is important, for example, glass waste forms).

The first choice, no explicit code, is usually simple (for example, the contaminants all release in a year) and self-explanatory. The second choice, the vadose zone code, is described in the next section. This section will describe STORM, an extremely sophisticated code involving spatial- and time-dependent physical and chemical processes.

The Subsurface Transport Over Reactive Multiphases (STORM) code ([Bacon et al. 2004](#)) calculates the time-dependent flux of radionuclides released from the waste form and the subsequent transport of contaminants in the man-made facility, given the inputted assumptions and data. STORM is based on basic principles of physics, chemistry, and thermodynamics that provide the calculated contaminant release over the spatial and time periods of interest. Also, the computer model for the facility can be coupled with a model for radionuclide release, thus providing the ability to couple the effects of facility design with waste form performance.

Using chemical reaction rates (including glass corrosion rates) and defined recharge rate into the facility, STORM provides the source term for the vadose zone calculations. STORM calculates the following:

- ◆ The flow of moisture in the disposal facility
- ◆ The degradation of the waste form with corresponding release of radionuclides
- ◆ The chemical reactions that depend on time and space (including the formation of secondary mineral phases and the consumption of water)
- ◆ The transport of the water and contaminants through the facility.

The STORM code calculates the total mass flux of radionuclides leaving the disposal facility by solving a coupled set of equations. The set describes the radionuclide release from the waste form and the mass transport of the radionuclides from the waste form through the facility, constrained by chemical reactions. This coupled set of equations is commonly known as the reaction-transport equation. More detailed documentation of the design and models used in the STORM code is found in the STORM user's guide ([Bacon et al. 2004](#)).

The selection of STORM for the Immobilized Low-Activity Waste/Integrated Disposal Facility (ILAW/IDF) performance assessments was selected ([McGrail and Bacon 1998](#)) because it best met the criteria and requirements for the Integrated Disposal Facility (then ILAW) disposal system release model and the general code requirements. The needed capabilities were identified

from an analysis of the important physical and chemical processes expected to affect LAW glass corrosion and the mobility of radionuclides.

The verification studies for STORM are documented in Chapter 8 of the SORM user's guide ([Bacon et al. 2004](#)). STORM has been used in the more recent assessments analyzing the disposal of treated tank waste ([Mann et al. 2001](#) and [Mann et al. 2003](#)).

26.3.4 Vadose Zone

A number of codes (STOMP, VAM3D-CG, PORFLOW, MEPAS, RESRAD) have been used to calculate moisture flow and contaminant transport through the Hanford Site vadose zone. Recently, the DOE Offices at Hanford ([Klein 2006](#), [Schepens 2006](#)) have directed that Hanford Site contractors use STOMP for vadose zone simulations, though RESRAD can be used for screening calculations.

The *Subsurface Transport Over Multiphases* (STOMP) code ([White and Oostrom 2003](#)) calculates the time-dependent thermal flow, moisture flow, and contaminant transport (including the aqueous and vapor phases) in variably saturated media, including groundwater. The code can be run in one, two, or three dimensions. The design goals for the code are the following:

- ◆ Be accessible and exploitable to scientists and engineers familiar with subsurface environmental phenomena, but not necessarily with numerical modeling techniques
- ◆ Have enough general applicability to recruit a user group that is capable of supporting training, maintenance, and enhancement activities
- ◆ Be verified by comparison to analytical solutions and benchmarked against existing simulators
- ◆ Be validated against germane laboratory and field experiments
- ◆ Have controlled configuration and documentation under an appropriate quality assurance program.

The STOMP code calculates the contaminant flux by solving a coupled set of equations, commonly known as the reactive-transport equations.

The Tank Farm Vadose Zone Program selected STOMP as its vadose zone computer code in 2000 as part of an open procurement process. The program determined that STOMP met all of the requirements of the *Computer Code Selection Criteria for Flow and Transport Code(s) to be Used in Vadose Zone Calculations for Environmental Analyses in the Hanford Site's Central Plateau* ([Mann et al. 1999](#)). STOMP is also used by the Hanford Groundwater Remediation Project as well as by the team preparing the Tank Closure and Waste Management Environmental Impact Statement.

The VAM and PORFLOW codes were the two vadose zone codes selected ([DOE/RL-91-44](#)) in 1992 by the U.S. Department of Energy, the U.S. Environmental Protection Agency, and the Washington State Department of Ecology). The VAM family of codes has been used in a variety of analyses, the most significant being the assessments of the disposal of treated tank waste

([Mann et 1998](#), [Mann et al. 2001](#), and [Mann et al. 2003](#)). The use of PORFLOW at the Hanford Site diminished in the late 1990s.

The RESRAD ([Yu et al. 2001](#)) and MEPAS ([Buck et al. 1995](#)) codes are one-dimensional codes used in screening analyses. They have not been used in the last 15 years to analyze the impacts of tank waste.

26.3.5 Groundwater

The DOE Offices at Hanford ([Klein 2006](#), [Schepens 2006](#)) have directed that Hanford Site contractors use MODFLOW ([McDonald and Harbaugh 1988](#), [Harbaugh et al. 2000](#), and [Hill et al. 2000](#)) for groundwater simulations. MODFLOW is a three-dimensional finite-difference groundwater model that was first published in 1984 by the U.S. Geological Survey. It has a modular structure that allows it to be easily modified to adapt the code for a particular application. Many new capabilities have been added to the original model.

The staff preparing the Tank Closure and Waste Management Environmental Impact Statement will develop the official Hanford Site Groundwater numerical model using MODFLOW. Future risk analyses will use and build on this effort.

26.3.6 Exposure

Radionuclides taken into the body by inhalation or ingestion may be distributed among different organs and retained for various times. In addition, long-lived radionuclides deposited on the ground become possible sources for long-term external exposure and uptake by agricultural products. Dietary and exposure parameters were applied to calculate radionuclide intakes and radiation doses to the public. Standardized computer programs were used to perform the calculations. These programs contain internally consistent mathematical models that use site-specific dispersion and uptake parameters. These programs are incorporated in a master code, GENII ([Napier et al. 1988](#)), which employs the dosimetry methodology described in International Commission on Radiological Protection (ICRP) Reports.

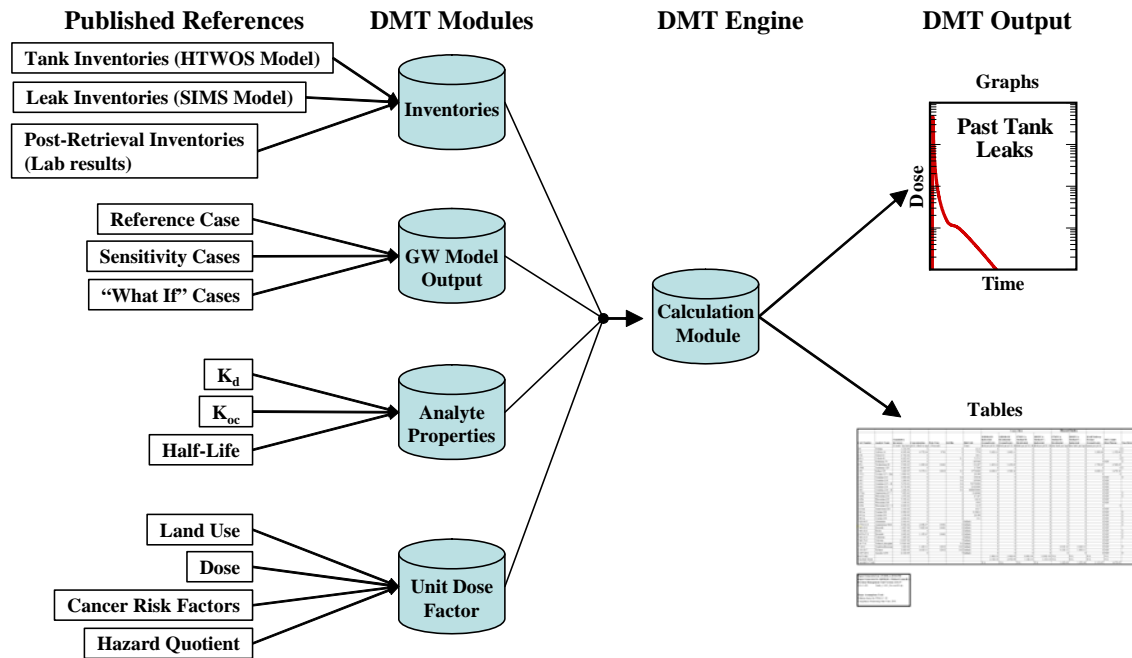
Most risk analyses involving tank waste, however, have used spreadsheets to calculate the relevant exposure parameters (see [Chapter 25](#)).

26.3.7 Integration

The wide variety of computer codes used for modeling different groundwater pathway parameters produce large volumes of data in a variety of electronic formats. Results from different models must often be integrated to draw meaningful conclusions about the entire groundwater system. Among the variety of ways to integrate these model results, an integrating computer code is most efficient. The *Initial Single-Shell Tank Performance Assessment for the Hanford Site* ([DOE/ORP-2005-01](#)) and other risk assessments have used the Decision Management Tool (DMT [[Watson 2005](#)]) to integrate groundwater-modeling results and estimate a wide variety of human-health risk metrics.

The DMT was developed to streamline the risk assessment process by managing the vast amount of data available from Hanford Site databases and models and efficiently using these data to estimate human-health risk presented by tank farm source terms. Before DMT development, the wide variance in data formats and the number of data sources resulted in a lengthy period of data gathering and pre-processing prior to calculating risks. The DMT quickly imports and formats the required data and organizes them into several distinct modules, which can then be accessed by the DMT calculation engine for a variety of risk assessment calculations (Figure 26-1).

Figure 26-1. Schematic of Decision Management Tool Data Sources, Data Integration and Calculation Output



By serving as the integrator for risk assessment data, DMT eliminates the need for hand or spreadsheet calculation of risks. Historically, data format differences required time-intensive hand-calculation of risks, which typically left little time for performing very many sensitivity analyses. The DMT’s calculation engine and graphic user interface allow analysts to quickly define numerous tank closure sequence permutations, tank closure and model timeframes, and regulatory performance objectives to produce detailed analyses of human-health risks based on the data managed in the DMT data modules. The speed and efficiency of the code typically produces results in under a minute, giving analysts the flexibility to examine the effects from several different tank closure sequences or to perform numerous sensitivity analyses. The DMT can output results in several user-defined formats, including graphic, text, and Microsoft Excel.

INTEG (Mann 1996), a less sophisticated integration tool, was used in the Immobilized Low-Activity performance assessments.

26.4 ANALYSES OF OTHER PATHWAYS

Because air pathway and inadvertent intrusion analyses involve simpler models (i.e., diffusion and decay), the computer models used in these analyses are usually spreadsheets.

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