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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

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Executive Summary

In their assessments of environmental and human health impacts, various Hanford Site projects will have to simulate the movement of moisture and the transport of contaminants through the unsaturated zone between the surface and the groundwater (the region known as the vadose zone). This document provides the mandatory requirements that any such code must have to be suitable for such analyses as well as desirable features that the various projects have identified.

The selection of criteria was based on the needs of the Hanford Site projects and on previous DOE, NRC, and Hanford Site experience. It is expected that based on this information, various projects will select computer codes to perform such modeling. Because different projects have different needs, different projects may choose different codes.

MANDATORY ADMINISTRATIVE CRITERIA

- Technical Documentation
- Code Availability
- Configuration Control
- Input Flexibility
- Real-Time Monitoring/Restart Capabilities

MANDATORY TECHNICAL CRITERIA

- Moisture Flow
- Contaminant Transport
- Boundary Conditions and Initial Conditions
- Source Term
- Hydrologic Properties
- Geochemical Model
- Time-Dependent Hydraulic and Geochemical Values
- Hydraulic, Geologic, and Engineering Structure
- Output
- Interface Between Moisture Flow and Contaminant Transport

DESIRABLE FEATURES

- Ease of Use
- Certification/Verification/Benchmarking
- Reputation Among User Community
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I. INTRODUCTION

A. Overview

Various Hanford Site projects need the ability to simulate the movement of moisture and contaminants through the vadose zone underlying the Central Plateau of the site in order to report on potential impacts of contaminants in the soil. The 200 Area Remediation Program and the Tank Farm Vadose Zone Program will be creating reports to satisfy regulatory commitments. Also, the System Assessment Capability (SAC) activity of the Groundwater / Vadose Zone Integration Project (Integration Project) will be setting requirements for SAC Revision 1 of its simulation tools. In addition, the Science and Technology Activity of the Integration Project will be investigating the need of various capabilities to model moisture movement and contaminant transport in the Hanford Site vadose zone. This effort builds on a similar effort completed by the Immobilized Waste Program (Mann 1998 and Voogd 1999). This document provides a consistent framework across projects in developing code selection criteria, and providing the basis and rationale the individual projects will use in their code selection process.

Following publication of this document,

- potential vendors would be requested to provide an expression of interest in providing the software,
- interested vendors would develop and submit a response to the “requirements” of this document,
- an evaluation board would review the submittals and produce a table illustrating the responses, i.e., develop a check list that summarizes whether a code meets or fails to meet each requirement, and a narrative that summarizes any partial response, and
- existing and future projects would then use the summary that compares alternate codes, and the full application information if necessary, to evaluate and select an analysis package for a specific application.

Information on the history of Hanford Site operations and on our understanding of the vadose zone can be found in *Groundwater/Vadose Zone Integration Project: Background Information and State of Knowledge (DOE/RL 1999).*

B. Participating Activities

1. 200 Area Remediation Program

The 200 Area Remedial Action Project addresses the assessment and remediation of waste sites and associated soil contamination (surface and vadose zone) that resulted from past discharges of wastewater to the ground (via ponds, ditches, and cribs) and the burial of solid waste in the 200 Areas. The 200 Area Remedial Action Project is currently in the first phase of the cleanup process (remedial investigation) which includes soil characterization to (1) establish a sound scientific understanding of the extent, concentration, mobility, and behavior of waste migration in the subsurface; (2) support the evaluation of remedial alternatives; and (3) select a remedy, and support the design of the remedy.

A primary remedial action objective for the project includes the protection of groundwater. As such, the remedial investigations will focus on characterizing subsurface contaminant inventories and distributions through the vadose zone and assess their impact on groundwater. Fate and transport analytical models (computer codes) will be required to facilitate this assessment.

2. Tank Farm Vadose Zone Program

The Tank Farm Vadose Zone Program is responsible for determining the inventory and distribution of contaminants that are present in the vadose zone from leaks and spills that have occurred in the single-shell tank farms. There are 149 single-shell tanks arranged in 12 farms. Each tank is a large facility with most being ~23 meters (75 feet) in diameter and ~14 to 15 meters (40 to 50 feet) tall. There are a variety of wastes in these tanks ranging from dilute water mixtures to sludges and saltcakes having exotic conditions (temperatures above 100 ^{o}C, pH > 14, and specific densities > 1.8).

The Tank Farm Vadose Zone Program is under RCRA (Resource Conservation and Recovery Act) assessment for 8 of the single-shell tank farms. Thus, it will be performing analyses of the environmental and human health impacts of current conditions and of various interim corrective actions. In addition, the project is obtaining information that will determine the impacts of various options for retrieving wastes from the tanks and for final remediation of the tank farms.

3. System Assessment Capability

The System Assessment Capability (SAC) is the capability needed to assess the cumulative impacts of radioactive and chemical waste at the Hanford Site on water resources, living systems, cultures, and regional economics. The SAC consists of a suite of tools and databases that are evolving and maturing as new data and knowledge are gained. Results from SAC assessments will allow site-specific cleanup decisions and disposal authorizations to be made in the context of the overall impact of the Hanford Site on the region, including the Columbia River.

There are nearly 2600 individual waste sites in the Hanford Site record, and a recent analysis of waste disposal sites in the central plateau evaluated the impacts from nearly 300 sites for which inventory estimates were available. While the SAC may initially aggregate sites and consider relatively few contaminated soil columns in the vadose zone, it will need to eventually examine individual site releases. The initial SAC assessment (i.e., Rev. 0) will examine a 1000-year period following Hanford Site closure, but future assessments (i.e. Rev. 1, 2,...) will consider the long-term migration and fate of highly sorbed but long-lived hazards for a period of up to one million years. Thus, the vadose zone component of the SAC needs to efficiently represent the large-scale and long-term aspects of the cumulative release, migration and fate of contaminants. Highly simplified approaches may be necessary to achieve the simulation. Science and Technology, and Hanford Site project studies will be relied upon to establish the defensibility of simplifications employed in the SAC.

4. Science and Technology

The role of the Science and Technology (S&T) component of the Groundwater / Vadose Zone Integration Project is to provide the data, tools, and understanding to make progress on open scientific issues that are critical to waste management decisions on the site. In coordination with research sponsored by the Environmental Management Science Program (EMSP) and S&T, high-end modeling analyses will be performed by S&T using some of the most detailed and comprehensive models of subsurface processes, and the most advanced computational and simulation technologies. While the S&T modeling approach will not be subject to the code selection criteria for "off-the-shelf" engineering simulators in this document, the modeling analyses performed by S&T will provide the scientific basis for some of the simplifying assumptions reflected in the criteria. Furthermore, elements of the S&T modeling approach could eventually become requirements for future engineering simulators used by the site projects.

5. Immobilized Waste Program

The Immobilized Waste Program is responsible for the disposal of immobilized low-activity tank waste (ILAW). ILAW is tank waste that will be separated to the maximum extent economically and technically practicable and that has been vitrified. This immobilized low-activity waste will be disposed of in large underground vaults or trenches. Although large inventories of contaminants will be present in the waste form, because of the expected slow release rate, relatively little contaminants are present outside of the disposal facility.

To support this disposal action, the project performs analyses of the long-term environmental and human health of the disposal of this immobilized low-activity waste. An important component of the analyses is the transport of contaminants through the vadose zone.

C. Background

1. Types of Analyses Covered

Contamination events in the vadose zone at the Hanford Site span the range of simple to complex physicochemical settings. The structural features that can influence the movement of waste fluids and water, and the transport of contaminants range from thin lenses (e.g., centimeters) of fine silts and clays, to large-scale geohydrologic units (e.g., 10s of meters). The processes of interest span the range from complex multicomponent reactive geochemistry transport models, to the linear sorption isotherm model; from the migration of a DNAPL (carbon tetrachloride) in a multiphase setting to the migration of tritium – a molecule indistinguishable from water in terms of its migration and fate. It is envisioned there will be a complete hierarchy of modeling capabilities necessary to conduct and defend a defensible analysis of risks and impacts resulting from the permanent disposal of Hanford Site wastes. Science and technology efforts will focus initially on the finer scale spatial and temporal events to create a better understanding of contaminant migration within the vadose zone. In the longer term those initial studies will be extended to provide defensible simplifications that can be used efficiently in larger scale studies. These larger scale analyses will in most cases be performed by the Hanford Site projects that are interested in estimating the long-term release of contaminants from the vadose zone into the unconfined aquifer. The System Assessment Capability represents an even larger scale assessment of all releases at the Hanford Site.

For example, an S&T effort may reconcile the filtration, sorption, or precipitation of a specific contaminant that has been observed on the scale of a silt/clay lens beneath a disposal facility. Knowledge gained during the S&T effort would yield an understanding of why the contamination is retained in the environment and under what conditions it could be mobilized in the future. A related project would be interested in producing an estimate of the long-term (e.g., 1000 to 10,000 year) release of that contaminant to the water table, so its analysis could be multidimensional in order to account for geologic and hydraulic complexities of interest in fully understanding the problem. Finally, the Groundwater/Vadose Zone Integration Project will conduct a system assessment that will treat the aggregate problem of all waste disposals at the Hanford Site. Thus, multiple sites (i.e., tens to hundreds) will be examined and the models applied must be very efficient to conduct the necessary long-term analyses. Simplifications made to the simulation from S&T to project to SAC must be consistent with the conceptual model of vadose zone and the contaminants. The higher resolution S&T effort must support the scale of model applied at the site-specific scale of the projects, and the medium resolution project effort must support the scale of model applied at the site-wide scale of the SAC effort.

This document is designed to support the selection of vadose zone codes for Core Project and SAC (Rev. 1 and later) applications. As such, it should support the selection of codes for modeling one-, two-, and three-dimensional simulations. It should also support the selection of codes providing a complete spectrum of physicochemical processes, (e.g., multiphase DNAPLs to dilute contaminants in water, from reactive geochemistry and transport needed to address tank leaks to the linear sorption isotherm model for application in the long-term system assessment.

2. Analyses Not Covered by This Document

The types of analyses covered by this document are those that need computer simulations of moisture flow and contaminant transport in the vadose zone, that is, in the sediments between the ground surface and the top of the water table. The Field Manager of DOE Richland Operations (Wagoner 1996) has set up a separate program to select computer codes to simulate groundwater flow and contaminant movement in the groundwater. The code selected, CFEST 96, can only simulate saturated conditions and cannot be used for vadose zone simulations.

3. Standardization of Data Used in Assessments

This document does not address the selection of data or methods of scaling data for use in model applications at a variety of scales. It deals solely with the criteria used to evaluate and select software for the simulation of fluid flow and contaminant transport problems in the vadose zone. It is recognized that use of consistent data at all scales of analysis is paramount to achieve consistent results, but data assembly, data interpretation, and data upscaling for use in less resolved and more highly integrated models will be addressed during the individual application following software selection.

The Integration Project has set up a task (named "Characterization of Systems") whose goal is to standardize conceptual models and associated data.

4. Compatibility among Projects

An effort is underway at the Hanford Site to produce consistent results when conducting analyses of the environment, risk and impact. Consistency is an issue because of the variety of analyses conducted, the independent efforts of DOE contractors, and the number of independent analysts. In recent years, the DOE has been required to develop an understanding of the composite impacts of all waste disposals following the Hanford Site closure. This is being done to support decisions on the disposal of wastes and the closure of waste sites. However, the requirement that a composite analysis be performed has brought the realization that the analysis of individual sites should yield output in consistent formats for use in the site-wide composite assessment. Thus, while vadose zone codes may differ, they should produce consistent results in consistent formats for general use.

Although there is a desire to minimize the number of different computer codes used, it is recognized that the various projects do have different needs that may lead to different codes being selected. However, the projects wish to minimize incompatibilities among themselves, as they are modeling similar (if not the same) system. Moreover, the output of these vadose zone codes must interface with the Hanford Site groundwater code. Such compatibility is not meant to mean to preclude different codes or approaches, but it does mean that compatibility becomes an important "ease of use" criteria (see Section IV.A).

5. Revisiting Criteria

The projects realize that more is becoming known about moisture flow and contaminant transport in the vadose zone, particularly the vadose zone as complex and as impacted as the one underneath the Hanford Site. Therefore, it is likely that these criteria may be revisited in a few years. It is unlikely that any of the current mandatory requirements will change, but it is likely that some desirable features may become mandatory and some unlisted features will become important.

D. Sources for Code Selection Criteria

These code selection criteria are based on the information from the low-level waste programs of the U.S. Department of Energy [DOE] (Case 1988) and of the U.S. Nuclear Regulatory Commission (Kozak 1989a) as well as experience gained in the DOE Complex [Mann 1998, WSRC 1992] in applying these criteria. The efforts of the U.S. Department of Energy, the U.S. Environmental Protection Agency, and the Washington Department of Ecology in the early 90's (DOE/RL 1991) to determine suitable codes for Hanford Site simulations was also used. Appendix A provides in the form of tables a comparison between the criteria in these documents and those used here.

Because several projects choose these criteria, the mandatory requirements presented in this document are those criteria in which all of the projects agree are necessary for the successful modeling of their project. The criteria identified under desirable features are those criteria that would enhance the probability of success for one or more projects . Thus, whereas a listed desirable feature may be very important (even a requirement) for one project, that feature may not be of any interest to other Hanford Site projects. Also, even if each project views a feature as desirable, such a feature may not be deemed mandatory because some of the projects may be willing to sacrifice the feature for another one.

E. Future Steps

This document will be made available to organizations that may wish to supply computer codes that simulate moisture flow and contaminant transport in the Hanford Site vadose zone. The responses from these organizations will be formally compared against the criteria in this document. It is expected that based on this information various projects will select computer codes to perform such modeling. Because different projects have different needs, different projects may choose different codes.

F. Organization of this Report

The code selection criteria are listed in three chapters

- Chapter II - Mandatory Administrative Criteria: those criteria dealing with how the code is created, maintained, and used.
- Chapter III - Mandatory Technical Criteria: the technical features which the code must have, and
- Chapter IV - Desirable Features: those features which the code should have, but the absence of which will not disqualify a code.

Each code selection criterion will not only be presented but it will also be justified.

II. MANDATORY ADMINISTRATIVE CRITERIA

These criteria deal with how the code is created, maintained, and used.

A. Technical Documentation

1. **Criterion.** Documentation describing

   - model theory, governing equations, and assumptions,
   - computational techniques and algorithms,
   - code verification,
   - user input, and
   - example applications

   must be available not only to DOE and its contractors but also to the regulatory agencies and other interested parties..

2. **Requirements.** The proponent of the code shall submit the documentation that describes the items listed above along with a notation describing the location of each required item. The proponent shall commit that all such documentation is publicly available.

   It is recognized that the current version of the code may not have all the documentation at the time of code selection. If this is the case, the proponent shall supply documentation for the latest version of the code for which documentation exists along with a schedule of the expected availability of documentation for the current code version.

3. **Reason.** Environmental analyses performed on the Hanford Site receive regulatory and public scrutiny. Therefore, it is important that the underlying principles of the codes be available to anyone interested. For some analyses, regulators or others may want to repeat calculations.

   Codes are regularly improved. The Hanford Site projects do not want to penalize a code because required documentation (although available by the time of code use) is not published at the time of code selection.

B. Code Availability

1. **Criterion.** The executable version of the code shall be available to any interested party for computers likely to be used by analysts performing Hanford Site environmental studies. Codes that execute only on large parallel systems (having more than 4 processors) will not be considered.

2. **Requirements.** The proponent of the code shall document the availability of the executable version of the code and list those computers (and operating systems) on which it will run.

   Satisfactory computer hardware is Intel-compatible processors using the Windows or NT operating system or Sun/SGI/HP computers using the UNIX operating system.

3. **Reason.** Hanford Site projects want to select a computer code that executes on standard computer hardware and is available to interested parties. Such interested parties may wish to repeat calculations.

C. Configuration Control

1. **Criterion.** The code shall be maintained under a software quality management program that assures that modifications and updates are traceable, auditable, and documented. Audits may occur.

2. **Requirement.** The proponent of the code must submit the software quality management program plan for the code.

3. **Reason.** Different versions of computer codes may give different results. It is crucial that the causes of any such differences are known. Configuration control of a software product is essential for traceability of results from analyses conducted over a multi-year period.

D. Input Flexibility

1. **Criterion.** The code shall allow the use of site- and facility-specific data/standard/guidelines as appropriate. For example, the ability to use site-specific vadose zone parameters is required rather than parameters from a generic soil type.

2. **Requirements.** The proponent of the code must show that the code can accept input that is site- and facility-specific.

3. **Reason.** The Hanford Site has many different sites and facilities that must be analyzed. Generic values are not sufficient.

E. Real-Time Monitoring/Restart Capabilities

1. **Criterion.** The code must contain real-time monitoring capability during actual run-time. A restart option must be provided.

2. **Requirements.** The proponent of the code shall document the real-time diagnostic and restart capability of the code. The monitoring activity can be satisfied by timestamps written to a file.

3. **Reason.** Because of the complexity of the models, simulations may take many days. In addition, in some analyses, parameters may need to be changed during a simulation to represent changes in the source term or degradation of engineered structures and waste forms. Therefore, it is important that the analyst be able to determine progress, update the simulation, and be able to restart the run.

III. MANDATORY TECHNICAL CRITERIA

These criteria are the technical features that the code must have. In general, the theoretical framework of the code shall be based on appropriate scientific principles (for example, conservation of mass, momentum, and energy) and well established engineering equations (for example, Darcy's law, Fick's law).

A. Moisture Flow

1. **Criterion.** The code shall be capable of simulating one-, two-, and three-dimensional unsaturated flow of water of a constant density in an isothermal setting under both steady state and transient flow-field conditions, particularly under conditions expected at the Hanford Site.

2. **Requirements.** The proponent of the code shall document that the code can perform one-, two-, and three-dimensional modeling of unsaturated, constant density moisture flow in an isothermal setting, both under steady state and transient conditions. The code proponent shall supply the names of authors, titles, and document identifiers of some published papers or reports that document the underlying scientific principles and use of the code to model moisture flow.

3. **Reason.** The technical basis is that contaminant transport modeling follows that for moisture flow. Because of the complexity of the facilities to be simulated, both two- and three-dimensionality are required for many analyses. However, for analyses that cover an extremely large spatial area, computation resources may require only a one-dimensional analysis of many individual sources. Although some projects may require nonconstant fluid densities, not all projects will. Similarly, for most projects, there will not be a significant temperature gradient in the situations where these codes will be employed. Because of man-caused disturbances of the vadose zone infiltration rate and because of facility degradation, transient calculations will be needed in many cases.

B. Contaminant Transport

1. **Criterion.** The code shall be capable of simulating contaminant fluxes in one, two-, and three-dimensions as a function of driving hydrologic processes and mass transport phenomena, including advection, hydrodynamic dispersion, molecular diffusion, and geochemical reactions.

2. **Requirements.** The proponent of the code shall document that the code can simulate contaminant transport in one-, two-, and three dimensions as a function of hydrologic conditions established by the moisture flow subsystem and by the listed mass transport processes. The code proponent shall supply the names of authors, titles, and document numbers of some published papers or reports that document the underlying scientific principles and use of the code to model contaminant transport.

3. **Reason.** The ability to simulate contaminant transport driven by hydrologic processes is the main technical reason for the code. Because of the complexity of the facilities to be simulated, both two- and three-dimensionality is required for many analyses. However, for analyses that cover an extremely large spatial area, computation resources may require only a one-dimensional analysis of many individual sources. Previous Hanford Site performance assessments, environmental impact studies, and composite analysis have shown that the mass transport phenomena listed are the dominant processes for contaminant transport.

C. Boundary Conditions and Initial Conditions

1. **Criterion.** The code shall be capable of incorporating time-dependent upper boundary conditions (e.g., a variable infiltration rate). The code shall be capable of simulating homogeneous and non-homogeneous Dirichlet and Neumann boundary conditions. It shall be possible to configure the boundary conditions to simulate either upward (i.e., evaporation driven) or downward (i.e., infiltration driven) migration and fate of contaminants.

   The user shall be able to specify initial conditions for key variables at all nodes.

2. **Requirements.** The proponent of the code shall document the code's ability to simulate moisture flow for an infiltration rate that varies with time. The proponent shall also document that the code satisfies the other boundary condition criteria. The proponent shall document the code's abilities to handle initial conditions at all node points.

3. **Reason.** Because of man-caused changes of surface conditions and of natural climatic changes, the amount of water entering the vadose zone may have to be modeled in a time-dependent manner. The other boundary condition criteria are needed to provide flexibility in modeling. Because of various past human-initiated activities, the value of key variables (e.g., moisture content, contaminant concentrations) must be able to be set at each node.

D. Source Term

1. **Criterion.** The code shall be able to accept a specified time-dependent release rate from one or more volume sources and from disconnected surface sources and then simulate the release until the inventory is depleted.

2. **Requirements.** The proponent of the code shall document the code can handle the source term criterion.

3. **Reason.** The source term will be time-dependent in many simulations (for example, small tank leaks and releases from waste forms). The source term will also differ among the various projects.

E. Hydrologic Properties

1. **Criterion.** The code shall be able to use standard relationships to represent moisture retention and unsaturated conductivity functions (e.g. van Genutchen-Mualem or Brooks & Corey). Such values could be different in the various geohydrologic zones or structural zones of the simulation. The parameters need not be a function of time-varying environmental conditions (e.g. temperature, pH, or concentration of contaminations).

2. **Requirements.** The proponent of the code shall document that the code has the capability to use such functions in the simulation of moisture movement and that the code has the ability to have different values in each user chosen zone.

3. **Reason.** Most of the Hanford Site moisture/conductivity data have been fitted to van Genutchen - Mualem relationships. The hydraulic properties of the Hanford Site vadose zone are location dependent.

F. Geochemical Model

1. **Criterion.** The code shall be able to represent geochemical retardation using the linear sorption isotherm or K_d model where the value for K_d depends only on the contaminant and on zonal spatial position.

2. **Requirements.** The proponent of the code shall document that the code can simulate geochemical retardation using the linear sorption isotherm model where K_d only depends on the contaminant and the spatial position.

3. **Reason.** In most model simulations, geochemical retardation can be modeled using the linear sorption isotherm (K_d) model. It is recognized that some projects may need a more sophisticated model for geochemical reactions. Geochemistry of the Hanford Site vadose zone varies spatially, especially when engineering structures are present.

G. Time-Dependent Hydraulic and Geochemical Values

1. **Criterion.** The code shall be able to simulate engineered materials in the vadose zone which have hydrogeologic and geochemical properties that are time-dependent. Unless stated elsewhere, the code need not have the ability to model material property changes that are the function of the contaminants present.

2. **Requirements.** The proponent of the code shall document the ability of the code to conserve mass (fluid and contaminant) while simulating changes in hydraulic and geochemical properties that are an explicit function of time.

3. **Reason.** Because of the long time periods under consideration, material properties of engineered structures will change. The simulations must be able to account for such changes.

H. Hydraulic, Geologic, and Engineering Structure

1. **Criterion.** The code shall be capable of simulating engineered structures and various geologic features such as layering, heterogeneity, and anisotropy. The geologic features include the representation of horizontal, vertical, and tilted features.

2. **Requirements.** The proponent of the code shall document that the code can readily simulate:

   - geologic or engineered layering (including structures, tilted layers, and sloping water table levels),
   - vertical or near-vertical features (such as clastic dikes)
   - heterogeneous features,
   - transport along boreholes and through casing annuli, and
   - anisotropic conditions that would affect moisture flow or contaminant transport.

3. **Reason.** The vadose zone under the Hanford Site exhibits layering and heterogeneities. The moisture flow is known to be anisotropic because of these properties.

I. Output

1. **Criterion.** The code shall provide moisture content throughout the model domain and contaminant concentration and flux at user chosen points, internal surfaces, and/or along boundary segments; all as functions of time. The code shall also be able to calculate flow lines for user chosen source points. The code shall be able to report mass balance and mass balance errors at each time step.

   The code shall be able to report for each time step the number of iterations required for convergence if convergence is achieved. The code shall be able to report which convergence criteria is not achieved if convergence is not achieved.

2. **Requirements.** The proponent of the code shall document that the code can provide the moisture flow and contaminant transport output as stated in the criterion. The proponent shall document how the status of convergence is communicated to the user.

3. **Reason.** Past experience with preparing environmental analyses has indicated that such capabilities are necessary to adequately portray and control the model runs. Because the vadose-zone equations are non-linear, lack of convergence is a serious problem. The user of the code must have information on whether convergence was reached and in those cases where it is not reached, what was the reason.

J. Interface Between Moisture Flow and Contaminant Transport

1. **Criterion.** The code shall be able to perform three classes of simulation, 1) moisture flow only, 2) transient contaminant transport simulation based on a previously run moisture flow calculation, and 3) combined (steady state or transient) moisture flow/ transient contaminant transport simulation. In the last case, redundant input for describing the moisture flow and the contaminant transport must not be required.

2. **Requirements.** The proponent of the code shall document that the code performs the three classes of simulations. The proponent shall also document that redundant information is not needed for a combined moisture flow / contaminant transport simulation.

3. **Reason.** The three classes of simulations are needed for analyst flexibility. Often, the flow-field is established before the contaminant transport calculations are made. Multiple steady-state contaminant transport calculations can be made from one moisture flow calculation. Sometimes a single simulation of both flow and transport is more appropriate.

IV. DESIRABLE FEATURES

These items are features that the code should have, but the absence of which will not disqualify a code from initial consideration and further evaluation. However, code selection will likely depend on the applicability of those desired features identified by a project as essential for its suite of simulations. Notably poor performance on a desired feature (such as excessive cost) can be reason for code disqualification.

A. Ease of Use

1. **Feature.** The code should interface with pre- and post-processing modules that allow the user to readily set up problems and to understand results. Graphical interfaces are preferred to text interfaces. Such pre- and post-processing modules could be an integral part of the code. In particular, the capability to graphically display the numerical grid discretization along with zone identifiers, the contaminant and moisture fluxes across selected boundaries and/or regions in the modeling domain, and contours, spatial cross sections, and time histories of contaminant concentrations is highly desired. The pre- and post-processing systems can be commercial or public domain products not developed by those responsible for the vadose zone code.

   Variable grid spacing allows great efficiencies in modeling sources, discontinuities, barriers, etc, while allowing a coarse grid in less important zones. In some problems, radially symmetric, cylindrical grids will prove useful.

   The user of the code shall have control over criteria used to assess convergence of the vadose-zone equations.

2. **Proof.** The proponent of the code shall document the pre- and post-processing modules that aid user's use of the code and the user's understanding of the output of the code.

   The proponent of the code shall document the type of grid spacing available.

   The proponent of the code shall document what control the user has in specifying the criteria to assess convergence.

3. **Reason.** The ability to obtain defensible results is directly related to ease of use. If the code's input is difficult to construct or its output is difficult to understand, then the probability that the analyst will misinterpret information greatly increases.

The ability to focus the code on zones of interest allows increase efficiency in both analyst and computation resources.

Because the vadose-zone equations are non-linear, lack of convergence is a serious problem. The user of the code must have information that convergence is reached and in those cases where it is not reached, what was the reason.

B. Certification/Verification/Benchmarking

1. **Feature.** The results of the code should be tested against experimental data from Hanford Site-relevant systems. The code should be verified and benchmarked against analytic solutions and other codes.

2. **Proof.** The proponent of the code shall supply documentation of such testing. The experimental data need not be from the Hanford Site, but should reflect similar environmental conditions (dryness, geochemistry). The proponent shall also supply any information concerning verification/benchmarking simulations against other codes that are relevant for Hanford Site vadose zone-like conditions.

3. **Reason.** Although a code that predicts events thousands of years into the future is impossible to validate, it is important that the code be tested and evaluated against real conditions.

C. Reputation Among User Community

1. **Feature.** The code should be well regarded among the user and regulatory community. In particular, the code should be acceptable by the U.S. Environmental Protection Agency and the Washington State Department of Ecology for environmental analyses for the Hanford Site. The code should have been used in simulations of the Hanford Site vadose zone with the results published in externally reviewed documents.

2. **Proof.** The proponent of the code shall document examples of use of the code beyond the developing organization. The proponent shall document past application and acceptance of code results by the U.S. Environmental Protection Agency and the Washington State Department of Ecology for environmental analyses for the Hanford Site. If the code has not been accepted, then the proponent shall indicate plans for achieving such acceptance. The code proponent shall supply the names of authors, titles, and document identifiers of some of the reports which have used the code to model moisture flow and contaminant transport in the Hanford Site vadose zone. The proponent shall indicate for each report cited the type of external review that was conducted. Such external reviews shall be provided if requested.

3. **Reason.** The environmental analyses performed must gain acceptance by the regulatory agencies and by the public. A necessary condition is that the computer codes used have wide acceptance among the technical community and be accepted by the regulatory agencies. Such acceptance is more likely if the code has already been use to model the Hanford Site vadose zone with the results published in an externally reviewed paper or report.

D. Multiphase (Non-Aqueous Phase Liquid) Contaminant Transport

1. **Criterion.** For some applications, the code should be capable of simulating multiphase contaminant fluxes in one, two-, and three-dimensions. Transport processes of the NAPL include absorption into the soil moisture, diffusion, dispersion, biotransformation, geochemical degradation, and volatilization. The NAPL transport processes may be functions of the driving hydrologic processes.

2. **Requirements.** The proponent of the code shall document whether the code can simulate multiphase contaminant transport in one-, two-, and three dimensions by the listed mass transport processes both as a function of hydrologic conditions established by the moisture flow subsystem, and independent of them. The code proponent shall supply the names of authors, titles, and document numbers of some published papers or reports that document use of the code to model non aqueous phase liquid contaminant transport. In the event such documentation does not currently exist, the proponents will provide explanations of techniques capable of performing the simulations.

3. **Reason.** The ability to simulate multiphase contaminant transport, particularly carbon tetrachloride, is of great interest to the 200 Areas Remediation Program. Because of the complexity of the facilities to be simulated and the widespread distribution of carbon tetrachloride throughout the vadose zone, two- and three-dimensionality is often required for many analyses. The mass transport phenomena listed are the primary drivers for NAPL contaminant transport. A previous Hanford Site study showed that little difference in the vadose concentrations resulted when the NAPL transport was coupled with or independent of the vadose moisture advection calculations. The main difference in the coupled and independent model results was found in aquifer concentrations (Piepho 1996).

E. Additional Contaminant Transport Capabilities

1. **Feature.** For some applications, the code should be able to modify the chemical distribution coefficient (K_d value) of the linear sorption isotherm model based on moisture content or other environmental conditions. The code should also be able to modify the diffusion parameter based on moisture content. The code should be able to model sorption-enhanced dispersivity. The ability of the code to simulate more complex geochemical modeling may be important for some projects (for example, by using the Langmuir sorption isotherm model, the Freundlich sorption isotherm model, or a full reactive geochemistry model).

2. **Proof.** The proponent of the code shall document whether the code has the ability to modify the K_d value and/or the diffusion parameter based on moisture content or other environmental conditions and whether the code can model sorption-enhanced dispersivity. The code proponent may submit additional capabilities that may be advantageous to Hanford Site projects.

3. **Reason.** A general feature of the K_d experiments is the dependence of the K_d value on pH. Research has also shown that the chemical distribution coefficient (K_d value) of uranium depends on moisture content. It is also expected that diffusion is also moisture dependent and that sorption-enhanced dispersion can be significant. For some projects, a more sophisticated geochemical model than the K_d model may be required.

F. Additional Moisture Flow Capabilities

1. **Feature.** For some applications, the code should have the ability to use different representations (including table lookup) for hydraulic conductivity and moisture retention as a function of moisture content. The code should be able to model saturation-dependent anisotropy for dry moisture regimes. The code should have the ability to distinguish between wetting and drying conditions and include these effects in the flow calculation. For some projects, the ability to model multiphase flow will be important. For other projects, the ability to model thermal effects, evapotranspiration, and varying density fluids may be important.

2. **Proof.** The proponent of the code shall document the functional representations available in the code to represent hydraulic conductivity and moisture retention as well as the ability to treat saturation-dependent anisotropy. The proponent shall document how the code treats moisture hysteresis. The code proponent may submit additional capabilities that may be advantageous to Hanford Site projects.

3. **Reason.** Because many of the analyses will involve dry conditions, various functional representations of a single experimental data set may provide different calculational results. The ability to determine the sensitivity of calculational results to functional representation is important. Saturation-dependent anisotropy and moisture hysteresis effects may affect calculational results. Because of the various types of wastes and hydraulic conditions considered by the various projects, different projects will have different flow simulation requirements.

G. Decay Products

1. **Feature.** For some applications, the code should be able to treat the effects of complex decay chains (for example, the decay of uranium).

2. **Proof.** The proponent of the code shall document those features of the code which allow different contaminant transport properties to be assigned automatically to progeny by the code based on position in the radioactive decay chain.

3. **Reason.** The transport of the actinide radionuclides and their daughters are important to Hanford Site environmental analyses. However, the contaminant transport of various radioelements may differ, principally because of the differences in geochemical interaction.

H. User Support

1. **Feature.** The better the user support by the code developer, the better the code for Hanford Site analyses.

2. **Proof.** The proponent of the code shall document available user support (including applicable costs). The code proponent shall also document relevant instances of user support.

3. **Reason.** Much of the cost of using a code is the time that it takes an analyst to understand and apply the code. The better the user support, the better the answer will be and the more efficient the code will be to use. However, the benefit of technical support must be weighed against its cost.

I. Speed of Execution

1. **Feature.** The faster the code simulation for a given degree of accuracy, the better is the code for Hanford Site applications. Such speed could come from the superiority of algorithms, the better implementation of methods, and/or the greater use of hardware features.

2. **Proof.** The proponent of the code shall provide evidence of the relative speed of the code.

3. **Reason.** Many of the problems run for Hanford Site analysts might take days to complete. Thus, speed of execution is an important consideration.

J. Non-Proprietary Codes

1. **Feature.** Proprietary codes should be used only if they provide a distinct advantage over public domain codes and only if the author(s)/custodian(s) allow inspection and verification of the source code. If a proprietary code is used, access to the source code must be made available by lease or purchase to Richland Operations Office and to the Office of River Protection (both of the Department of Energy) and its contractors (and their agents for verification) and to any oversight agencies.

2. **Proof.** The proponent of the code shall document whether the code is proprietary. If the code is proprietary, then the code proponent must document that the source code can be inspected and the access to the source code is available by purchase or lease. The proponent shall also supply the licensing cost (and any other mandatory fees for the use of the code).

3. **Reason.** The Department of Energy has a responsibility to ensure that the code behaves as claimed. It is desirable that others can confirm the investigation made by the Hanford Site. The cost of the code should not be a major fraction of the cost of analyst. If it is, the code may not be acceptable.

K. Version

1. **Feature.** The version of the code should be a recent version, preferably the latest one that has been fully tested, of a family of codes. For codes that are well established, the use of a well-tested version may outweigh the use of the newest, but less tested version.

2. **Proof.** The proponent of the code shall document the history of code versions and shall indicate where the particular version submitted falls in this history.

3. **Reason.** Computer codes have errors. Also, developers of codes learn how to better implement features of their codes. Thus, the latest version of a code usually is preferable to an earlier version.

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Appendix A. Comparison with other Documents

Table A-1. DOE Guidance (Case 1988)	
Description	This Document
Model important transport and exposure processes	III.A, III.B
Address problem scenarios of concern	III.A, III.B
Function properly for the particular climate and geographical region	II.D
State of the art in a given modeling area	IV.J, general
Spatial and temporal simulation capabilities	III.A, III.B
Ability to accept site-specific characterization data	II.D
Flexibility to eliminate irrelevant processes	handled by individual projects
Existence of adequate documentation	II.A

Table A-2. NRC Guidance (Kozak 1989a)

Description	This Document
Implement models of NUREG/CR-5453, Vol. 3 (Kozak 1989b)	II.A, III.B
Have sufficient and adequate documentation	II.B
Been extensively used or accepted by user community	IV.C
A public code is preferred to a proprietary code unless the proprietary code has some outstanding or unique feature	IV.I
Most recent version of a family of codes is preferred	IV.J
Complexity of the code should be commensurate with the amount of information available about the physical setting	III.A, III.B
Codes that can be run on existing NRC machines or personal computers are preferred.	II.B
Groundwater codes that can simulate both saturated and unsaturated zones are preferred.	Groundwater flow not in scope
Codes that simulate both flow and transport are preferred.	III.J, made mandatory
Handle time-dependent source injection rate	III.C
Capability to account for radioactive decay chains are preferred	IV.F

Table A-3. TWRS Undisturbed Vadose Zone Code Selection (Mann 1998)		
Ident	Description	This Document
II.A	The code shall be documented	II.A
II.B	The code shall be available for use on common computers	II.B
II.C	The code shall be maintained under a software quality management program	II.C
II.D	The code shall allow the use of site- and facility-specific data/standards/guidelines	II.D
II.E	The code shall have diagnostic monitoring capability during run-time	II.E
III.	The code shall be based on appropriate scientific principles and well established engineering equations	III.
III.A	The code shall be capable of simulating two- and three--dimensional flow of water of a constant density in an isothermal setting under both steady state and transient conditions	III.A
III.B	The code shall be capable of simulating contaminant fluxes in two- and three-dimensions as a function of driving hydrologic processes and mass transport phenomena, including advection, hydrodynamic dispersion, molecular diffusion, and adsorption	III.B
III.C	The code shall be capable of incorporating time-dependent upper boundary conditions (i.e., a variable infiltration rate). The code shall be capable of simulating homogeneous and non-homogeneous Dirichlet and Neumann boundary conditions.	III.C;
III.D	The code shall be able to accept a specified time-dependent release rate from one or more volume sources and from disconnected surface sources and then simulate the release until the inventory is depleted.	III.D
III.E	The code shall be able to use van Genutchen - Mualem and Brooks-Corey relationships to represent moisture retention and unsaturated conductivity functions	III.E
III.F	The code shall be able to represent geochemical retardation using the linear sorption isotherm or K_d model where the value for K_d depends only on the contaminant and on spatial position.	III.F
III.G	The code shall be able to simulate engineered materials in the vadose zone which have hydrogeologic	III.G

Table A-3. TWRS Undisturbed Vadose Zone Code Selection (Mann 1998)

Ident	Description	This Document
	and geochemical properties which are time-dependent	
III.H	The code shall be capable of simulating engineered structures and various geologic features such as layering, heterogeneity, and anisotropy. The layering shall not be restricted to a horizontal representation.	III.H
III.I	The code shall provide moisture content throughout model domain and contaminant concentration and flux at user chosen points, internal surfaces, and/or along boundary segments; all as functions of time. The code shall also be able to calculate flow lines for user chosen source points. The code shall be able to report mass balance and mass balance errors at each time step.	III.I
III.J	The code shall be able to perform a moisture flow simulation only, a steady-state contaminant transport simulation based on a previously run moisture flow calculation, and a combined moisture flow / contaminant transport simulation.	III.J
IV.A	The code should interface with pre- and post-processing modules that allow the user to readily set up problems and to understand results. Graphical interfaces are preferred to text interfaces. Such pre- and post-processing modules could be an integral part of the code.	IV.A
IV.B	The results of the code should be tested against experimental data from Hanford-relevant systems. The code should be verified and benchmarked against analytic solutions and other codes.	IV.B
IV.C	The code should be generally known and accepted by user and regulatory community	IV.C
IV.D	The code should have capabilities beyond the linear sorption isotherm model	IV.D; added examples
IV.E	The code should have capabilities beyond the use of van Genutchen/Mualem equations	IV.E; added examples
IV.F	The code should be able to treat the effects of complex decay chains	IV.F
IV.G	The code should have good user support	IV.G

Table A-3. TWRS Undisturbed Vadose Zone Code Selection (Mann 1998)		
Ident	Description	This Document
IV.H	The code should execute efficiently	IV.H
IV.I	Proprietary codes should be used only if they provide a distinct advantage and only if the code is available for inspection	IV.I
IV.J	Recent versions of a code family are preferred	IV.J

Table A-4. Savannah River Performance Assessments (WSRC 1992)		
Ident	Description	This Document
1R	Code shall be based on appropriate scientific principles and well established engineering equations	III
2R	Code shall be verified	II.A
3R	Code shall be documented	II.A
4R	Code shall be maintained under a software QA and management program	II.C
1S	Code should allow site- and facility-specific application	II.D; Make mandatory
2S	Transport code should be capable of tracking waste inventory over time and computing fluxes at designated locations	III.B, IV.D; Some items made mandatory
3S	Code should be validated	IV.B
4S	Degree of complexity should be consistent with the quantity and quality of data and the objectives of the computation	Covered by scope of activity
5S	Hardware requirements should not be exotic	II.B; Made mandatory
6S	Proprietary codes should be used only if they provide a distinct advantage and only if the code is available for inspection	IV.I
7S	Ease of interfacing code output with other codes is desired	IV.A
8S	Familiarity with the code is desirable	Code familiarity not addressed because we do not know code users. Implication captured in IV.A

Table A-5. Codes to be Used in Hanford Risk Assessments (DOE/RL-91-44)		
Ident	Description	This Document
2.1(1)	The complexity of the model should be consistent with the objectives of the risk assessment	Final selection will rest with the individual projects. However, this concept was used through the creation of this document.
2.1(2)	Use of the models will be factored into the RI/FS process during the planning stages and considered throughout the RI/FS	Requirement on individual projects
2.1(3)	Modeling efforts associated with remediation of various wastes at the Hanford Site will be coordinated to ensure consistency and transferability of data and results, thereby minimizing effort.	The Hanford Groundwater / Vadose Zone Integration Project has been established to meet this requirement. This effort is an outgrowth of the coordination requirement.
2.1(4)	Improvements in modeling capabilities will be encouraged	This effort is seen as an attempt to meet this requirement.
2.1(5)	Use of software for risk assessment not included in this document will be allowed given sufficient justification	The process outlined in this document is designed to provide sufficient justification
2.1(6)	Uncertainty and parameter sensitivity will be qualified with nonprobabilistic approached	Approach taken in this document
3.1.1	Availability	II.B
3.1.2	User Support	IV.G
3.1.3	Useability	IV.A
3.1.4	Portability	II.B
3.1.5	Modifiable	II.C
3.1.6	Reliability	IV.B, IV.C
3.2.1	Air transport	not applicable
3.2.2	Surface water flow and transport	not applicable
3.2.3.1	Infiltration	not applicable

Table A-5. Codes to be Used in Hanford Risk Assessments (DOE/RL-91-44)		
Ident	Description	This Document
3.2.3.2	Vadose zone flow and transport:	
	moisture-dependent hydraulic conductivity relationships for different soils types	III.A; IV.E
	hystersis	IV.E
	flexible in specifying vadose zone thickness	II.D
	layered soils	III.H
	discontinuous stratigraphic layers that are tilting in places	III.H
	first order, linear sorption/desorption processes, using an effective distribution coefficient	III.F, IV.D
	radioactive decay	IV.F
3.3.3.3	Saturated flow and transport	not applicable

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