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Decisional Draft

Groundwater Model Development Plan in Support of Risk Assessment

United States
Department of Energy
Richland, Washington

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1.0 INTRODUCTION

Milestone M-29-02 of the Tri-Party Agreement (TPA) between the Washington Department of Ecology (Ecology), the U.S. Environmental Protection Agency (EPA), and the U.S. Department of Energy, Richland Field Office calls for, "a plan for development of area-wide groundwater models to support risk assessment and to evaluate impacts of changing groundwater flow fields" (Ecology et al. 1990, 1991). An earlier milestone, M-29-01, identified the computer codes that will be used to evaluate migration of contaminants within soil and groundwater on the Hanford Site (DOE-RL 1991a). The reasons for conducting risk assessment and evaluating area-wide impacts of changing groundwater flow fields are briefly introduced in this section.

The National Oil and Hazardous Substances Pollution Contingency Plan states that, at an EPA National Priorities List site, "..the lead agency shall conduct a site-specific baseline risk assessment to characterize the current and potential threats to human health and the environment that may be posed by contaminants migrating to groundwater or surface water, released to air, leaching through soil, remaining in the soil, and bioaccumulating in the food chain. The results of the baseline risk assessment will help establish acceptable exposure levels.." (40 CFR 300.40(d)(4)). In support of this objective, a guideline document, "Hanford Site Baseline Risk Assessment Methodology", is currently under development and has been released in draft form (DOE-RL 1991b). This guideline identifies exposure to groundwater and surface water as one of the primary risk-driving pathways at Hanford and states that the modeling of contaminant transport may be required to provide estimates of exposure concentrations. The risk assessment methodology document acknowledges the existence of contaminated groundwater at the Hanford Site and the need to evaluate the risks posed by this contaminated groundwater. The methodology document further notes that for most of the operable units at the Hanford Site, soil currently represents the primary source of hazardous substances that potentially can be transported to other media where human contact may occur. Furthermore, although liquid disposal practices may have contributed more to migration of contaminants into groundwater in the past, infiltration due to precipitation is the probable current mechanism for transport. It is therefore apparent that groundwater contaminant transport prediction tools (i.e., models) are needed to support baseline risk assessments. These groundwater models would be used to evaluate the potential migration of contaminants within vadose zone soils to the water table and through the saturated groundwater flow system to the potentially exposed populations.

Site-specific models will be used to predict transport in the vadose zone beneath the waste site. In addition, area-wide groundwater flow and solute transport models that incorporate large segments of the Hanford Site are needed to: (1) simulate the impacts of changing subsurface effluent disposal practices on groundwater flow fields, (2) provide boundary conditions for smaller, site-specific saturated flow and transport models, (3) evaluate large-scale groundwater isolation or treatment strategies, and (4) allow simulation of the cumulative effects from multiple waste sites. These models would be large enough that their boundary conditions could be defined by well-defined physical hydrologic boundary conditions, such as river-stage (head) conditions along the Columbia and Yakima rivers and no-flow boundaries along Gable Mountain anticline and Rattlesnake Ridge.

1.1 PURPOSE

In general, this document provides a consistent framework for the development of saturated and vadose zone groundwater flow and transport models to support human health and environmental risk assessments and to evaluate the impacts of changing flow fields. Some of the specific objectives of this plan are summarized below:

- Discuss modeling needs for risk assessment and requirements for model development.
- Describe the models that will likely be used to support risk assessment and provide direction regarding how these models will be developed. This direction will help maintain consistency in approach among different groups conducting modeling for a variety of sites and applications.
- Provide guidance for remedial investigation/feasibility study (RI/FS) activities regarding the types and quantities of characterization information needed to develop models for risk assessments. This milestone was prepared to emphasize the importance of planning for the baseline risk assessment during the scoping phase of the RI/FS process, i.e., ".. a preliminary site modeling strategy should be developed during the RI/FS scoping to allow model input data requirements to be incorporated into the data collection requirements.." (EPA 1989, pg. 4-5).
- Delineate technical issues that remain to be resolved. A preliminary judgement on the relative importance and current understanding of each technical issue is provided. The priority of these issues may change as modeling objectives are better defined.

Specific action items are provided for development of both site-specific vadose-zone models and area-wide (Hanford Site) saturated groundwater models. Modeling the vadose zone is still relatively difficult , particularity for dry soils typical of Hanford, and a number of issues need to be resolved before conducting extensive vadose zone modeling.

This document focuses on the use of groundwater flow and transport models in support of risk assessments. It is recognized that other exposure pathways exist and that under specific situations and conditions these pathways can pose a significant risk, i.e., during excavation contaminants could become airborne. However, the subsurface pathway, including potential migration of contaminants through both vadose zone and saturated zone sediments, is considered the pathway of primary importance at Hanford. This is certainly the case when viewing the subject from a long-term disposal perspective. Over the years, most of the waste has either been placed in storage or "interim disposed" in these sediments. Furthermore, future plans generally assume that most wastes will ultimately be disposed in this medium.

1.2 APPROACH

In developing a modeling strategy, it should be recognized that waste sites are complex and no level of characterization and analyses will remove all uncertainty. As discussed in the following sections, the waste sites at Hanford are certainly no exception to this observation. Therefore, this plan for model development was not prepared with the intention of removing all uncertainty through characterization and analyses, but to collect and perform sufficient analyses to allow for and support an informed and defensible risk assessment. The required level of certainty and, therefore, the level of modeling and characterization, should be finalized during the RI/FS process.

2.0 MODEL DEVELOPMENT PROCESS

The model development process described is oriented toward site-specific vadose zone models to support baseline risk assessment and area-wide saturated flow and transport models. Area-wide saturated models will be used at various scales. For example, at a large scale, these models will be used to assess the impacts of changing groundwater flow fields. At smaller scales, saturated flow and transport models coud be used to predict contaminant concentrations for evaluating compliance with various regulations, i.e., predicting concentrations at the location of monitoring wells. It is expected that these models will also provide the baseline for future modeling needs, such as risk evaluation of alternative remediation approaches, assessment of future data needs, and design of groundwater extraction and/or control systems. The discussion in this section is primarily based on previous modeling experience at Hanford and a general knowledge of Hanford waste sites and the RI/FS process. It is expected that the approach for model development may evolve during implementation of the RI/FS as more is learned of the extent of contamination and processes controlling contaminant transport at Hanford waste sites.

Model development refers to preparation of input files for a computer code that will allow numerical simulation of flow and transport in vadose zone and aquifer systems. It is assumed that the computer code requires no development, modification, or refinement. The basic steps of model development include the following:

- definition of objectives
- evaluation of existing data and collection of additional data
- formulation of conceptual model
- code selection
- grid definition
- incorporation of data into model
- calibration and assessment of additional data needs.

2.1 DEFINITION OF OBJECTIVES

Model development should begin with a clear definition of the project objectives. Factors that should be considered include the intended predictions, the required accuracy of the results, and the potential future uses of the model. The project objectives will influence the choice of software, coarseness of the grid, data requirements, calibration standards, and other elements of model development. The general objectives of the models discribed in this report are to (1) support risk assessment with predictions of contaminant migration and concentrations, and (2) evaluate impacts of changing groundwater flow fields.

Specific information needed from groundwater modeling to support risk assessment is primarily predictions of contaminant concentration in groundwater and contaminant flux rates into the Columbia River. The contaminant flux rates into the river are necessary to allow prediction of concentrations in surface water. To provide this information, it will be necessary to simulate flow and transport in both the vadose and saturated zones. Presumably, simulation of vadose zone flow and transport will be necessary to predict groundwater concentrations directly beneath and very near the waste units. In addition, small-scale, fully saturated models may be necessary to predict flow and transport in the saturated zone near the source region. Area-wide saturated zone models will be necessary to simulate groundwater transport from the 200 Areas across the Hanford Site to the Columbia River and to provide boundary conditions for small-scale, site-specific models.

Evaluation of impacts from changing groundwater flow fields will likely be conducted with area-wide saturated groundwater flow and transport models. Since the primary influence on changing groundwater flow fields is effluent disposal in the 200 Areas, fulfillment of this objective will require a model that covers most of the Hanford Site from the Columbia River south and west to Rattlesnake Ridge, Cold Creek Valley, and Dry Creek Valley. A model that extends between these boundaries is necessary to allow use of well-defined boundary conditions: river stage head conditions along the Columbia River, zero-flux along Rattlesnake Ridge, and fixed-flux or fixed-head along Cold Creek and Dry Creek valleys.

It is also anticipated that application of these models will support design of groundwater monitoring and extraction systems for the purpose of assessing risk reduction associated with alternative remedial designs. These modeling needs, and others that may become apparent in the future, should be considered during the model development process to minimize future modifications.

2.2 EVALUATION OF EXISTING DATA AND COLLECTION OF ADDITIONAL DATA

A wide variety of data will be important in the quantification of groundwater flow and transport. Most of the data types needed to develop groundwater flow and transport models can be grouped into the categories shown below.

- Geologic and stratigraphic information:
  - borehole and well logs
  - geophysics
  - air photos and maps for surficial features (surface water, outcropping of bedrock).

- Saturated zone physical characteristics:
  - horizontal and vertical hydraulic conductivity information
  - storativity measurements
  - porosity measurements
  - dispersivity estimates.

- Boundary conditions:
  - natural infiltration rates
  - effluent discharge information through the years
  - upwelling from basalt
  - influx from Cold and Dry Creek valleys
  - Columbia River stage information
  - bank storage effects.

- Calibration information:
  - water table information through the years
  - plume migration through the years, including present day contaminant distribution
  - contaminant source terms.

- Vadose zone characteristics:
  - meteorological data
  - unsaturated hydraulic conductivity measurements
  - lysimeter results
  - surficial soil characteristics
  - vegetation characteristics
  - evapotranspiration
  - unsaturated sediments moisture content.

- Contaminant characteristics:
  - decay/degradation rate
  - daughter/degradation products
  - soil/water partitioning coefficients
  - solubility
  - Henry's Law constant (volatiles only).

The amount of available data at the Hanford Site regarding groundwater flow and transport varies from extensive to none. Most of the data have resulted from a wide range of programs and studies conducted under very different quality control standards and reported in multiple documents. The effort to compile and assess these data is often the most time-consuming part of developing a groundwater model. The data should be organized and catalogued to help minimize duplication of effort and maximize consistency. Note that not all the data types listed above will be necessary for all modeling applications. Data collection for a specific application should be focused on those data needs relevant to the project objectives.

2.3 FORMULATION OF CONCEPTUAL MODEL

In general, conceptual models of groundwater flow systems usually consist of hydrologic units bounded by head or flux boundary conditions, internal boundary conditions due to water injection and extraction, and hydrogeologic characteristics. The hydrogeologic characteristics are expressed using governing parameters such as permeability, storativity, dispersivity, porosity, as well as geochemical attributes. Vadose zone models also require information related to moisture content, vegetation characteristics, soil texture and layering, and moisture-permeability characteristic curves. Contaminant transport models require source and contaminant characterization, as well as groundwater velocity vectors. Important contaminant characteristics include soil/water partitioning, solubility, decay, and form (i.e., nonaqueous-phase, dissolved, particulate, leachate).

Initial formulation of a conceptual model is generally based on data ranging in scale from centimeters to kilometers. Small scale data, such as borehole logging, slug tests, and testing of borehole cores, are not necessarily representative of average bulk conditions. In many cases, governing parameters can be more accurately assessed using direct or indirect means from large-scale observations of system behavior, including water table maps, observations of plume movement and shape, long-term, multiwell aquifer tests, and geophysics. For example, in areas where water level measurements indicate steeper hydraulic head gradients, it can be surmised that the aquifer transmissivity is lower than in surrounding areas. Note that transmissivity estimates based on short-duration pump test and slug test data provide information on local aquifer conditions (on the scale of meters), and may not reflect actual aquifer conditions at the scale of the model. An additional disadvantage of small-scale, single-well pump tests and slug tests is that they do not reveal faulty well

construction that can result in inaccurate estimates of aquifer conditions. The scale of data is particularly important for dispersivity, which has been shown to range from centimeters for bench-scale permeability experiments to kilometers for regional groundwater plumes (Gelhar 1985). This wide range in measured dispersivities is due to the increase in size of geologic heterogeneities as the scale of the plumes becomes larger.

Since complete description of a hydrologic system is never possible, some interpretation and estimation is necessary. An understanding of the uncertainty in the conceptual model is important during model development. Parameters that are poorly known can be refined during calibration to better match observed hydraulic head conditions and contaminant movement.

2.4 CODE SELECTION

Completion of Milestone M-29-01 (selection of computer codes for groundwater modeling) of the TPA change package (Ecology et al. 1990) resulted in selection of four computer codes for use in development of groundwater flow and transport models. The codes are described in the M-29-01 report (DOE-RL 1991a) and are listed below:

UNSAT-H	UNSAT-H (Fayer and Jones 1990) has been developed at Hanford and is designed to simulate infiltration under typical Hanford conditions.
PORFLO-3	PORFLO-3 (Sagar and Runchal 1990) is a fully three-dimensional, integrated finite-difference, flow and solute transport computer code with a wide variety of capabilities, including coupled vadose/saturated zone analysis, retardation, radioactive decay, and conductive heat transport.
VAM3D-CG	VAM3D-CG (Huyakorn and Panday 1990) is a finite-element flow and solute transport code capable of coupled vadose/saturated zone analysis.
CFEST	CFEST (Gupta et al. 1982) is a fully three-dimensional, finite-element, saturated flow and transport code.

Selection of the proper code will depend on the intended application.

As currently planned, the UNSAT-H computer code will be used to quantify the water balance at the air/soil interface. Once the rate of infiltration is quantified, it will be used as a boundary condition for the vadose zone flow and transport models. The VAM3D-CG computer code has an evapotranspiration feature, but this feature is less sophisticated than the processes modeled in UNSAT-H and has not been calibrated to Hanford conditions. As such, VAM3D-CG will be used to provide a rough check on the results obtained using UNSAT-H.

Two computer codes (PORFLO-3 and VAM3D-CG) were selected for simulating moisture redistribution and contaminant transport in the vadose zone (DOE/RL 1991a). At the present time, both of these models are being used at Hanford in support of environmental restoration activities. The primary reasons for selecting two codes rather than one stems from the need to verify (benchmark) results and the subtle differences associated with numerical capabilities (finite element versus finite difference).

Three computer codes (VAM3D-CG, PORFLO-3, and CFEST) will be used for modeling ground-water flow and contaminant transport in the saturated sediments. At this time, it is assumed

that the finite-element computer codes (CFEST, VAM3D-CG) will be used to model conditions at all space scales of interest. The finite-element models are believed to have more flexibility when it comes to the need to simulate various geologic feature, i.e., tilting beds, discontinuous layers, etc. It is believed that VAM3D-CG has some advantages over CFEST as they relate to relocation of the water table, i.e., pressure wave propagation, operation of liquid discharge facilities, etc. The PORFLO-3 computer code is being used to simulate the flow and transport of contaminants at smaller space scales (few square miles) and its use in this capacity will continue. This is particularly true when there is a need to simulate the interaction of contaminant migration in both saturated and unsaturated conditions.

Although it is believed that the codes listed will be suitable for the majority of modeling applications, alternative codes may be used if it appears that they provide superior and necessary capabilities. Regulatory agreement should be obtained before using an alternative code.

2.5 GRID DEFINITION

In contrast to analytical models, which generally provide a single equation solution that treats the modeled region as a uniform material, numerical models discretize the modeled region into a grid of nodes and elements. The advantage of analytical models is that they provide quick solutions to problems with regular geometries and uniform materials. Unfortunately, analytical solutions cannot account for variability in material properties or irregular geometries. Numerical solutions overcome these shortcomings by discretizing the modeled region into elements and nodes with variable material properties. Then, by solving the governing equation over each element and requiring continuity between elements, a set of nodal values is obtained for the solution. Note that some of the advantages of numerical approaches are included within analytical superposition model.

Grid definition is an important aspect of models because it affects the numerical stability, accuracy, and computation time of numerical solutions. Solution techniques for simulation of contaminant transport and vadose zone flow are particularly sensitive to nodal density in areas with steep concentration or moisture gradients. In general, as the nodal spacing increases, the solution is more prone to instability (manifested by oscillations) or numerical diffusion. Past experience and factors to consider when developing a numerical grid are discussed below for both transport modeling and vadose zone flow modeling:

- Transport Modeling - The controlling factor in transport modeling is the dispersivity coefficient, since it determines the steepness of the concentration front. For transport problems, a general guideline is that nodal spacing should be < 10 times the longitudinal dispersivity. Acceptable results have been obtained for area-wide Hanford groundwater models using a nodal spacing of approximately 1,100 ft with a longitudinal dispersivity of 140 ft (GAI 1991).
- Vadose Zone Flow Modeling - Problems with instability and numerical diffusion during vadose zone flow simulations are primarily related to moisture content. This is because unsaturated hydraulic conductivity is a function of moisture content, resulting in a non-linear problem requiring iterative solution algorithms. Unfortunately, the nonlinearity becomes extremely pronounced at low soil moisture contents typical of Hanford. The nodal spacing used for a previous vadose zone modeling exercise at Hanford was as low as 0.5 m for the vertical dimension and 2.0 m for the horizontal dimensions (Smoot and Sagar 1990).

Although numerical problems associated with instability and numerical diffusion can be minimized using an extremely small nodal spacing, the amount of computational effort required to arrive at solutions can become prohibitive. This is especially true as the dimensionality of the problem increases. In a situation where the nodal spacing is reduced by half, the number of nodes increases by a maximum factor of two for a one-dimensional problem, a maximum factor of four for a two-dimensional problem, and a maximum factor of eight for a three-dimensional problem. In addition, to avoid numerical instabilities the length of the timesteps must be reduced to accommodate smaller nodal spacing, thereby further increasing the computational effort.

Solution efficiency and accuracy can be optimized given some knowledge of the project objectives and hydrologic conditions. To optimize performance of flow simulations, nodal density should be increased near regions with higher hydraulic gradients, such as near pumping wells, areas of mounding, and regions with abrupt changes in hydraulic conductivity or transmissivity. Significant stratigraphic changes (such as clay underlain by gravel) are particularly difficult to simulate in vadose zone modeling because they generally result in abrupt changes in both moisture content and hydraulic conductivity. As a result, it is advantageous to decrease nodal spacing near stratigraphic interfaces. In contaminant transport modeling, solution accuracy and stability are only affected by nodal spacing in the areas that the plume will travel through; therefore, nodal density should be increased primarily in the regions near and downgradient of the contaminant sources.

Since finite-element algorithms allow the use of nonrectangular elements, they are generally more flexible regarding nodal density than finite-difference algorithms. On the other hand, the time required to create a nonregular grid may not be worth the reduction in computational effort. For example, if only a few simulations will be performed, it may be better to use a regular grid that is easier to develop even if the simulations take longer to run. If extensive calibration is expected or sensitivity studies are planned, however, it may be advisable to commit the initial effort to create a nonregular, finite-element grid that will reduce the computation time required to perform simulations.

2.6 INCORPORATION OF DATA INTO MODEL

The conceptual model is transformed into a computer model using nodal and element parameters to describe the system. The parameters that are usually required for input into a computer model are as follow.

- Nodal:
  - spacial location
  - nodal type (continuity, fixed flux, fixed head)
  - initial condition.
- Element:
  - list of nodes that define the element
  - areal flux due to infiltration or evaporation
  - hydraulic conductivity or hydraulic conductivity function
  - storativity
  - specific yield
  - dispersivity
  - effective porosity.

For typical field applications, measured values of these parameters are usually not available for every node and element. Furthermore, although most models assume constant parameter values within each element, natural variability of these parameters likely occurs at a scale much smaller than the size of the elements. Consequently, it will be necessary to estimate or calculate average representative values using interpolation and professional judgement, or statistical techniques if an adequate data set justifies their use. Finally, model parameters can be adjusted using manual or computerized calibration techniques until simulated results match well with observed conditions.

2.7 CALIBRATION/VALIDATION AND ASSESSMENT OF ADDITIONAL DATA NEEDS

In most cases, initial simulations of a natural groundwater system will not compare well with observed conditions. The disparity between simulated and observed conditions can usually be attributed to one or more of the following reasons.

- Numerical problems - Numerical problems can usually be corrected by adjustments in the spacial grid or timestep interval, although large, multidimensional, vadose zone flow problems can be extremely difficult to solve given limited computing resources.
- Erroneous observed conditions - Inaccuracies in the observed conditions could reflect problems with data collection, analytical errors, or simply lack of information. The modeler should keep the potential for these data imperfections in mind when assessing model results.
- Deficient conceptual model - Simulated results may not match observed conditions because the conceptual model differs significantly from the actual system. Examples of processes that may be important that are usually not included in the conceptual model include: (1) upwelling from the underlying basalt aquifers, (2) significant vertical flow within an aquifer, (3) scale-dependent dispersivity, and (4) vapor transport in the vadose zone. Such problems with a conceptual model may be solvable during the calibration process, but in some cases may be due to fundamental limitations of the model or lack of information.
- Incorrect model parameter values - Adjusting model parameters to obtain better comparison between simulated results and observed conditions is the primary goal of the calibration process. Given the inaccuracy and/or lack of measured parameters, such as hydraulic conductivity, storativity, and porosity, calibration entails refinement of the assumed model values until the match between simulated results and observed conditions is acceptable.

Because observed hydraulic head conditions are reliable and usually available (given enough wells and water level measurements), calibration of saturated flow models is relatively staightforward. One potential problem with calibration of saturated flow models is that a unique solution for the hydraulic head distribution is not available if all the boundary conditions are either no-flow or fixed head. In other words, if the model does not contain a flux condition of significant magnitude (relative to total flux through the model), increasing or decreasing all the hydraulic conductivities in equal proportion will result in the exact same hydraulic head distribution. The only difference is that the amount of flux through the model will be increased or decreased in proportion to the change in hydraulic conductivities. To obtain a unique solution, it is necessary to apply a significant hydrologic stress (i.e., nonzero flux) at one or more locations in the model. This nonzero flux can take the form

of pumping or injection at wells, cribs, and trenches, distributed infiltration due to precipitation, or groundwater influx from upgradient valleys. Distributed infiltration and groundwater influx from Cold Creek and Dry Creek valleys are poorly characterized at Hanford and are not suitable for calibrating hydraulic conductivity. Fortunately, effluent discharge to the subsurface has had a significant effect on groundwater flow at Hanford in both the 200 East and 200 West areas and the amount of discharge has been recorded. If a model accurately predicts both the mounding resulting from effluent discharge in the 200 Areas and general site-wide hydraulic head conditions, it is likely that the hydraulic conductivities are of the correct order of magnitude.

Several models of saturated flow conditions at the Hanford Site have been calibrated in the past. The approaches used for two of these models are described below.

- GGWP - A saturated groundwater flow model using the Golder Groundwater Package (GGWP) computer code was initially developed in 1989 and further refined in recent years (GAI 1991). This model was calibrated manually to hydraulic head conditions measured both in 1944 (before effluent discharge commenced at the Hanford Site) and in December 1979 (after 35 yr of effluent discharge). Hydraulic head conditions were significantly different for these two different times, with approximately 80 ft of groundwater rise near the 200 West Area and 30 ft near the 200 East Area. Hydraulic conductivities were adjusted until a reasonably good match was obtained for both points in time. The advantage of calibrating to these very different hydraulic conditions is that the model should be more capable of correctly simulating future conditions given changes in effluent disposal practices. The calibration was further verified by a general correlation between observed tritium plumes and simulated groundwater travel times, although the simulated travel times did require estimation of a second parameter, effective porosity. Effective porosities were assumed to be related to hydraulic conductivity, and ranged from 0.15 to 0.25.

- CFEST - Calibration of a saturated groundwater model of the Hanford Site using the CFEST code was recently reported (Jacobson and Freshley 1990). This model was calibrated to hydraulic head conditions observed in December 1979, using an automated inverse technique initially developed by Neuman (1980). Jacobson and Freshley (1990) also simulated transient behavior of the groundwater flow system between 1980 and 1985, during a period of changing effluent disposal practices. The automated inverse technique can greatly reduce the effort required to calibrate the model, thereby providing more opportunity to conduct sensitivity analyses.

In addition, contaminant distributions can provide useful calibration information regarding the direction and magnitude of groundwater velocity vectors. The governing processes important in contaminant transport modeling include advection, dispersion, retardation, transformation, and source behavior. Unfortunately, these factors can influence observed plume behavior in ways that appear similar, and it is generally not possible to obtain a unique solution for most contaminants. These difficulties are minimized for mobile contaminants with known decay behavior, such as tritium. In the case of tritium, the unknown variables are reduced to advection, dispersion, and source term. If the source term is relatively constant, then the effects of advection and dispersion are generally quantifiable. The advection factor is characterized by element groundwater velocity vectors obtained from a groundwater flow model. As such, advection is generally not calibrated with a transport model, although comparison of simulated and observed transport behavior can provide information

regarding the accuracy of a groundwater flow model. The dispersivity parameters affect the spread of the plume, both with regards to diffusion and shape. A discussion of dispersivity at Hanford is provided by Golder Associates, Inc. (GAI) (1991).

Calibration/validation of vadose zone flow and transport models is considered to be more difficult than saturated flow and transport models. This difficulty results from the problems associated with collecting and characterizing the various system variables. For example, the collection and use of representative soil samples to establish moisture-retention characteristics under partially saturated conditions is subject to debate. Similarly, transport properties vary as a function of moisture content and this further complicates the collection and interpretation of data collected in the field.

3.0 USE OF MODELS AT HANFORD

This section provides a description of how subsurface groundwater flow and contaminant transport models will be used at the Hanford Site in support of risk assessments and evaluation of changing groundwater flow patterns.

3.1 GENERAL MODELING FRAMEWORK

It is assumed that some level of modeling will be performed in support of each operable unit. A preliminary decision on an appropriate level of modeling should be made during the initial phases of the RI and should be consistant with the risk assessment methodology currently under development (DOE-RL 1991b). The decision should be based on what is needed to prepare the baseline risk assessment and provide sufficient justification for recommending various remedial actions. Planning for the human health and environmental risk assessments prior to preparing the work plan is an essential step in the process. As discussed in Section 2.1, a statement on the objectives of the risk assessment will be the first step in development of groundwater models.

Once the objectives have been defined, the data that are required to support this analysis can be defined and a plan to secure this information can also be defined. The site and waste characterization component of the RI/FS process is intended to determine the characterization of the site as well as the nature and extent of contamination. Quantitative risk assessments, like site and waste characterization, require that data be collected to support the anticipated needs. These needs will vary depending on the level and extent of the modeling activity. Furthermore, the objectives and general approach to modeling decided on during the scoping phase should be reviewed and revised as the RI data are collected and evaluated. Table 3-1 provides a summary on the use of groundwater flow and transport computer codes and models during the RI/FS process.

Table 3-1. Role of Modeling in the RI/FS Process.

RI/FS activity	Data flow	Computer codes/models
Scoping		
Evaluate existing data and develop conceptual model	--------->	Select mathematical models
Identify risk assessment objectives	<---------	Conduct sensitivity/worst-case analysis
Identify initial data quality objectives and prepare RI/FS work plan	<---------	Identify critical model parameters
Phase I - RI		
Field investigation	<---------	Groundwater modeling to assist well placement
Define nature and extent of contamination	--------->	Calibrate and refine model simulations
Develop preliminary baseline risk assessment and evaluate "no action" alternative	<---------	Contaminant identification - Exposure assessment - Toxicity assessment - Risk characterization
Phase I and II - FS		
Identify/screen treatment technologies	--------->	Select models to evaluate risk assessment alternatives and estimate uncertainties
Phase II - RI		
Refine data quality objectives	<---------	Data input for models
Conduct field investigations	--------->	Boundary conditions for models
Treatability investigations	--------->	Calibrate models, reduce uncertainties
Finalize baseline risk assessment	<---------	Perform final risk assessment
Phase III - FS		
Further define, evaluate, and compare alternatives	<---------	Modeling of risk assessment alternatives

During the scoping phase of the RI/FS process, a conceptual model of the waste site is prepared to visualize the relationship between the contaminant sources, release mechanism, transport routes, and potential receptors. The conceptual model is based on existing knowledge. Based on this conceptual model, a decision on the role and use of models in support of the baseline risk assessment will be defined. The results of this assessment should be discussed and agreed on by the team preparing the characterization work plan. Once the team reaches agreement on the nature and extent to which models will be used, the requirements to support modeling can be defined. These requirements can then be used to define appropriate data needs that will be used to help structure the work plan. If models are available, they may be used to perform sensitivity analyses to establish the relative importance of the various model parameter and to help quantify data quality objectives (DQO).

During the Phase I RI, groundwater flow and transport models can be used for various purposes not related to risk assessment. During the early period of the Phase I RI, they may have value in helping to define the location of sampling wells. As field data become available, groundwater flow and transport models can be used to help interpret data. As more data become available, these data will be used to revise the conceptual model and eventually used to calibrate the model. In this mode, revising the conceptual model and calibrating the model are visualized as two activities that proceed in parallel. Once the groundwater flow and transport models have been calibrated, these models will be used to support the baseline risk assessment.

It is anticipated that groundwater modeling will be conducted by Westinghouse Hanford Company or its subcontractors as directed by the unit manager responsible for an RI/FS. Modeling needs will become apparent during scoping of the RI, planning and execution of the risk assessments, and perhaps during the design of remediation systems. Some of the information needs related to risk assessment are indicated in Figure 3-1. In general, these information needs are concerned with the potential for contaminants to reach humans or other biota, and predictions of contaminant concentrations at the point of exposure.

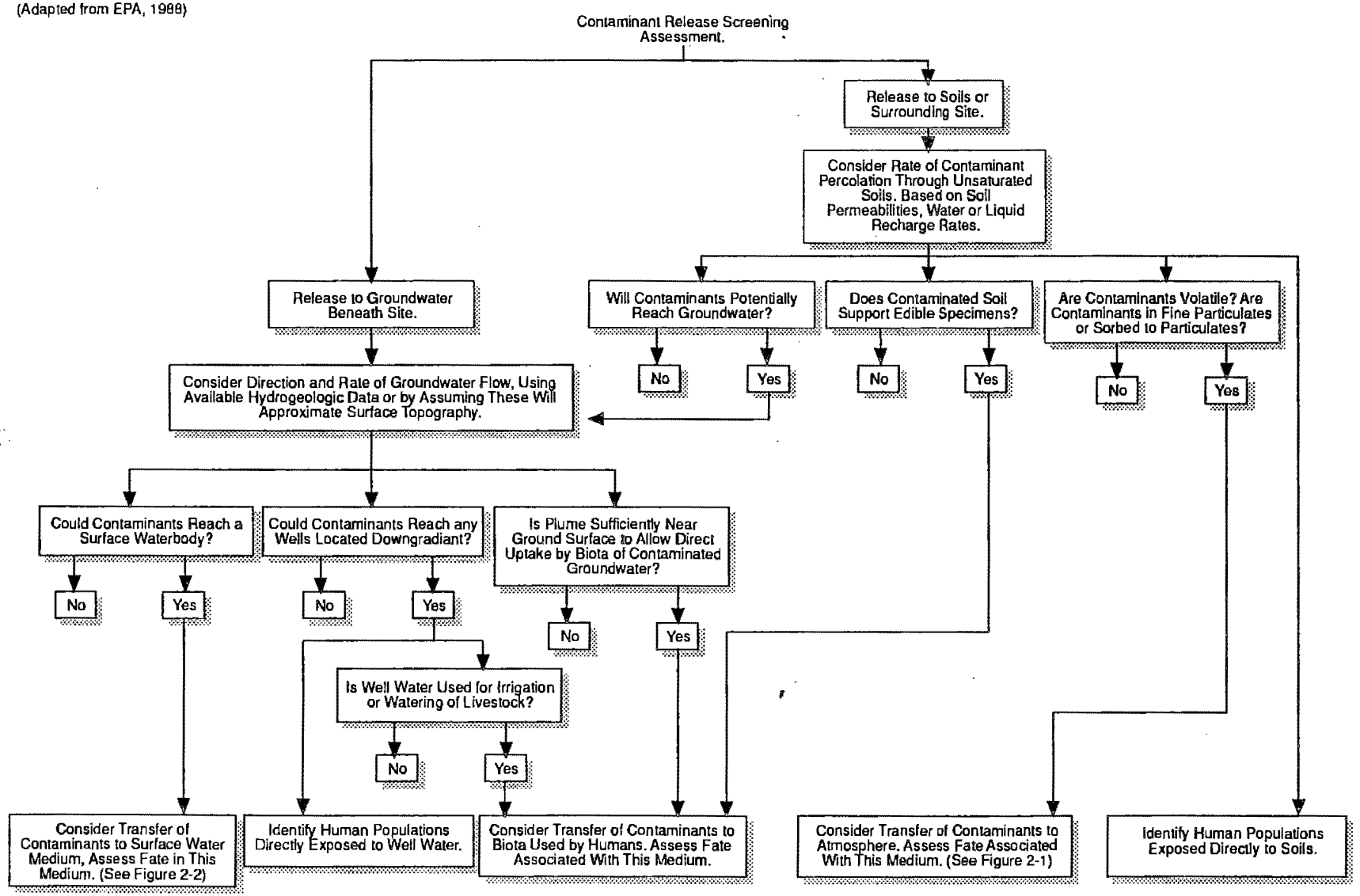
Groundwater modeling performed in support of RI/FS activities should also account for: (1) use of appropriate model complexity; (2) space scale and use of telescoping models; and (3) site-wide coordination of modeling efforts.

3.1.1 Model Complexity

The complexity of the model should be consistent with the objectives of the exposure assessment. Simple calculations or analytical models may be sufficient for screening purposes, while more complex numerical models may be required to support situations where the geometry is complex and/or more detailed analyses may be required to support final record of decision (ROD). It is expected that detailed numerical modeling in support of risk assessment will only be performed for those situations where the amount of risk is similar in magnitude to allowable standards. In cases where contaminant inventory is small, the waste form is extremely stable, and/or the constituents are relatively benign, the amount of risk may be many orders of magnitude less than allowable standards. Alternatively, in situations where large quantities of relatively toxic constituents are free to migrate, the risk may be clearly unacceptable. Simple analytical models will be relied on to identify these situations, thereby significantly reducing the time and resources that would be expended if extensive numerical modeling were performed for all situations. This multitiered approach to modeling is recommended by the EPA (1988, p. 100).

Figure 3-1. Environmental Fate Screening Assessment Decision Network: Soils and Groundwater.

(Adapted from EPA, 1988)



If it is anticipated that detailed numerical modeling will eventually be required, it may be most economical to begin development of a more powerful numerical model during the early screening stages of exposure assessment. The decision between initial use of simple analytical codes or more powerful numerical codes should be carefully weighed on a unit-by-unit basis. Input from the regulators should be encouraged during screening assessments to help identify the appropriate level of modeling.

3.1.2 Space Scale and Use of Telescoping Models

It is anticipated that models will be developed for different space scales, ranging from < 100 ft of vadose zone directly beneath a waste site, to a Hanford area-wide saturated zone model covering several hundred square miles. The scale of the model will be consistent with the modeling objectives. For example, if the objective is to predict groundwater concentrations directly beneath a waste site, the model could be constrained to simulate flow and transport in the vadose and saturated zones directly beneath the waste site. If estimates of groundwater concentrations downgradient of the site are needed, it will be necessary to develop saturated zone flow and transport models. The scale of these models will depend on where prediction of contaminant concentrations are required, i.e., small-scale, local models will be sufficient near the site and large-scale, area-wide models will be necessary far from the site.

One limitation of local-scale saturated flow models is that well-defined boundary conditions are usually not available near the site. Area-wide models are usually extended to geologic features that define defensible boundary conditions (such as the no-flow boundary defined by Rattlesnake Ridge). One method for estimating boundary conditions for local-scale models is to use a telescoping grid approach that uses the results of area-wide models to define boundary conditions around the perimeter of a local-scale model within the area-wide model. An example of the telescoping grid approach is provided by Ward et al. (1987).

3.1.3 Site-Wide Coordination

Modeling efforts for different operable units at Hanford will be coordinated to ensure consistency and minimize effort. It is likely that different RI/FS units will use overlapping or similar models. The characteristics of these models, including general conceptual elements, flow and transport parameters, boundary conditions, and level of complexity, should be consistent. Methods for maintaining consistency include: (1) having the same personnel either conducting or reviewing all modeling efforts; (2) maintain-ing up-to-date data packages for use by all groups performing groundwater modeling; and (3) requiring documentation of all modeling activities at the site, including complete disclosure of information sources, assumptions, input and output data files, and interpretation of results.

Development of area-wide groundwater models will likely be required for multiple RI/FS groundwater operable unit investigations. Instead of having an area-wide model developed for each groundwater operable unit, it would be more efficient to have a single group maintain area-wide models. To accommodate the individual needs of different operable units, it is conceivable that multiple versions of these area-wide models with slight variations may be developed. It is important that fundamental elements of the different versions are consistent, including aquifer geometry, flow and transport parameters, and boundary conditions.

3.2 VADOSE ZONE MODELING

To perform a risk assessment, it is necessary to predict the maximum contaminant concentrations in groundwater directly beneath and downgradient from a waste site. Vadose zone modeling of some form will be necessary to determine these concentrations. Relative to saturated groundwater modeling, however, vadose zone groundwater modeling is characterized by significant numerical difficulties and greater uncertainty regarding conceptualization and parameter estimation. In many vadose zone modeling situations, it may be advisable to use simple models and conservative assumptions to estimate exposure concentrations. Simplified analytical methodologies for estimating groundwater concentrations from vadose zone soil concentration are introduced. The appropriate level of modeling and data collection for risk assessment at individual sites should be determined during the RI/FS.

3.2.1 Screening Methodologies

It is proposed that a screening methodology be used to scope and define the need for vadose zone flow and transport models. Based on this approach, simplified analytical techniques will be used. Start with a simple analytical model and systematically add detail. The analyst can evaluate first hand the relative importance of the various processes and parameters using a limited amount of data. Once the important processes and parameters have been identified, this information can be factored into the preparation of the work plan. As such, the benefits are twofold. First, the investigator is allowed to assess qualitatively the relative importance of each process and parameter as it relates to the situation at hand. Secondly, the analyst is in a better position to define and propose the level of modeling that should be considered in structuring the work plan.

Although it has been assumed that detailed vadose zone flow and transport modeling will be required to support a level of decisions regarding Hanford Site remediation, it must be remembered that modeling should not become an end in itself. During the planning, the analyst must strive to select the most simplified model and/or method of analyses that will satisfy the needs of the risk assessment. Additional information on the use of a screening methodology in support of scoping vadose zone flow and transport models is provided in Appendix A.

3.2.2 Technical Issues

The extent to which vadose zone flow and transport model will be used for predicting future risk is not fully known at this time. It is assumed that at waste sites in which significant vadose zone contamination is found, the transport of these contaminants to groundwater will need to be modeled to predict risk, justify remedial actions, and support an ROD. The overlying concern in using vadose zone models is the uncertainty of how well modeling results represent actual contaminant transport. The simulation models rely on various assumptions and approximations of the physical system and before the modeling results can be accepted, the more important of these assumptions should be test and the accuracy of contaminant transport predictions should be demonstrated. Some of these assumptions and relating modeling issues have been identified and are addressed in this section. Each

of these issues has been assigned a relative level of importance, and a near-term plan for resolving the most important of these have been identified.

(1) Calibration/Validation of Vadose Zone Flow and Transport Models. The need for some level of calibration/validation of models is considered a major issue. It is generally assumed that a technically defensible performance/risk assessment can be accomplished only with validated and/or calibrated models.

Calibration and validation are activities designed to test the realism of the vadose zone flow and transport model. From a philosophical perspective, calibration and validation are very different. When addressing the subject of calibration, it is generally assumed that both the conceptual and numerical models are correct or adequate. Therefore, to calibrate a model, model parameters are simply adjusted within an acceptable range based on site-specific measurements to arrive at a best fit. Validation on the other hand, examines in more detail the realism of both the conceptual and numerical model. In reality, state-of-the-art limitations preclude our ability to truly validate a groundwater flow and transport model. These limitations relate primarily to the difficulty in obtaining field measured data to compare with simulated vadose zone conditions. Furthermore, validation is site specific and consequently it's utility if achieved at one location is limited when considering application of the model at another location.

In light of these limitations, an interim goal is to provide a general level of testing at various or representative locations across the Hanford Site has been adopted. The objective of these analyses is to provide a reasonable assurance that the vadose zone flow and transport models provide a reasonable representation of reality. The results from this testing will be evaluated against risk assessment needs to determine if additional calibration/validation work is required. Additional discussion on possible future calibration/validation activities is provided in Appendix B.

(2) Evaluating Applicability of Models for Estimating Unsaturated Hydraulic Conductivity for Hanford soils. Resolution of the models used to represent unsaturated hydraulic conductivity is considered a major issue. The current approach uses a single measurement of saturated hydraulic conductivity combined with a closed-form expression (e.g., the van Genuchten-Mualem theory) to predict over the entire range of moisture content, the unsaturated hydraulic conductivity values that routinely vary over six to eight orders of magnitude for Hanford soils. A study is underway to establish the appropriateness (or inappropriateness) of the current approach of estimating unsaturated hydraulic conductivity values that have been proposed for waste-site characterization and modeling activities in various RI/FS work plans.

(3) Groundwater Recharge Estimates. Quantification of recharge is considered a major issue. Data from lysimeter studies conducted by Gee (1987) indicate that infiltration rates at Hanford range from 0 to 10 cm/yr. The higher rates appear to be associated with unvegetated, gravelly surfaces. Since most of the Hanford Site is covered with some type of vegetation, the average infiltration rate is likely to be far less, perhaps close to zero. Estimating groundwater recharge (i.e., net water infiltration through surface soils with subsequent transmission to the underlying unconfined aquifer) is particularly difficult for an arid site such as Hanford. This is because of the fact that the recharge estimation errors for an arid site can often be on the same order of magnitude as precipitation or evapotranspiration.

(4) Applicability of Arya-Paris Model. The importance of this issue will be addressed once the current ongoing study has been completed. The Arya-Paris model is a convenient procedure for translating the particle-size distribution data into a soil-moisture characteristic data. Bulk density as well as the particle-size distribution are the only data needed for application of the Arya-Paris model. A preliminary study is ongoing to demonstrate the success or failure of using the Arya-Paris technique of using the particle size distribution data for estimating the soil-moisture characteristic curves for Hanford soils. Presence of a significant correlation between the particle size distribution and soil-moisture characteristic curves can lead to a large cost reduction in site characterization activities aimed at obtaining moisture retention curves at Hanford. Future plans are contingent on the results of the ongoing work. As currently planned, the preliminary study is scheduled to be completed this fiscal year (9/30/92).

(5) Moisture-Dependent Anisotropy. At the present time, this issue is considered of minor importance. Variable, moisture-dependent anisotropy in unsaturated soils is an effective, large-scale (macroscopic) flow property which results from media textural heterogeneities at a smaller scale. For saturated media, an averaging of the heterogeneities in geologic media at the smaller scale leads to an effective hydraulic conductivity value, at the larger (macroscopic) scale, with the lateral hydraulic conductivity value becoming much larger than the vertical hydraulic conductivity. For unsaturated media, recent stochastic analyses suggest that the lateral to vertical hydraulic conductivity ratio increases with a decrease in moisture content of the soils; i.e., the anisotropy increases with a decrease in saturation. A preliminary study will be performed to evaluate, through a combined numerical simulation and field study, the effects of smaller-scale heterogeneities that are present in the Hanford soils on macroscopic moisture-dependent anisotropy. If it is demonstrated that the moisture-dependent anisotropy is a significant process for Hanford soils, appropriate credit can be assigned to account for such a phenomenon in computing groundwater travel times and radionuclide flux rates. Work on this issue has not been initiated.

(6) Effects of Hysteresis in Modeling Vadose Zone Flow. This issue is also considered of minor importance. Literature data on vadose zone hydrology indicate that the field soils behave as a highly anisotropic media under unsaturated conditions. Yet laboratory and in-situ permeameter experiments indicate that these soils are very nearly isotropic in their saturated state. The anisotropy in hydraulic conductivity appears to be dependent on the hydraulic state of the medium, textural heterogeneities, and hysteresis-enhanced moisture-dependent variation in unsaturated hydraulic conductivity. Work on this issue has not been initiated.

(7) Use of Lumped Recharge Estimate Versus Event-Based Simulations. This issue is assumed to be of minor importance at Hanford. All vadose zone flow and transport simulations performed to date at Hanford use a lumped, average input for recharge estimates (e.g., centimeters per year). The importance of using an event-based input, with the associated surface water balance, on the groundwater travel time and radionuclide flux rates to the water table is relatively unknown. It is proposed that a study be performed to evaluate, through a combined use of field lysimeter data and numerical simulations, the relative effects of using a precipitation event-based simulation versus a lumped, average estimate for infiltration recharge. By accounting for infiltration, evapotranspiration, and runoff processes for each precipitation event separately, the effects of using the two approaches on the moisture plume through the vadose zone in the 200, 300, and 100 areas will be quantified. Work on this issue has not been initiated.

Other technical issues relating to vadose zone transport include vapor transport and multiphase flow. Vapor transport will be important for volatile constituents, particularity under dry conditions with little recharge. Multiphase flow could be important in both the vadose and saturated zones for constituents present as liquid product. It is anticipated, however, that multiphase flow and vapor transport will only be important in a few situations. The carbon tetrachloride release in the 200 West Area is considered the most significant situation where multiphase flow and vapor transport have important roles. Since carbon tetrachloride has already reached the water table in the 200 West Area, it may be possible to conduct risk assessments without performing significant modeling.

3.2.3 Vadose Zone Data Needs

A listing of the data needed to support vadose zone flow and transport modeling is provided in Appendix C. Specifying the specific data needs for an operable unit risk analysis will be part of the RI/FS work plan, and will depend on the nature of anticipated modeling activities.

3.3 SATURATED FLOW MODELING

Risk assessments will require prediction of contaminant concentrations downgradient from a waste site, including both groundwater and surface water. Saturated zone modeling of some form will be necessary to determine these concentrations. In general, saturated zone modeling capability is better developed than vadose zone modeling capability. The primary limitations in saturated groundwater models relate to incomplete characterization of the hydrogeologic system. These limitations can result in significant errors in contaminant plume travel times and spacial distribution. Since risk assessments are generally based on the maximum concentration in groundwater and surface water, regardless of location and time, errors in plume shape and velocity are tolerable. The specific needs of the risk assessment must be kept in mind when determining data needs and developing saturated groundwater models.

Prediction of future groundwater flow patterns resulting from changes in effluent disposal practices will require use of a area-wide saturated groundwater flow model. Future development should be based on knowledge gained from development and use of previous area-wide groundwater flow models.

3.3.1 Screening Methodologies

Saturated zone modeling will be necessary to predict groundwater concentrations downgradient of the source region and to predict fluxes into the Columbia River. Although complex numerical models can be used to simulate saturated zone flow and transport, significant information can be obtained using screening methodologies and analytical models. Potentially applicable approaches are outlined below.

As discussed in the risk assessment methodology (DOE-RL 1991b), risk assessments will be based on the maximum concentrations in groundwater and surface water without concern for where and when these concentrations occur. For mobile constituents from liquid effluent disposal facilities, the highest concentrations currently measured in groundwater should be a good representation of future maximum concentrations in groundwater. For nonmobile constituents that have not yet reached

groundwater, the maximum groundwater concentration should occur directly beneath the waste site, and can be estimated using screening approaches for vadose zone transport outlined in Appendix A.

Approximating the maximum concentration in surface water can be performed using approaches analogous to those described in Appendix A for the vadose zone. The most conservative approach would assume that the maximum concentration in groundwater will eventually show up in surface water. Factoring in the effects of dispersion, sorption, and decay can be accomplished using analytical transport models or hand calculations. In contrast with the vadose zone, groundwater flux rates in the saturated zone are easier to observe and predict given sufficient water level measurements and hydraulic conductivity measurements. The dilution effects of mixing in the Columbia River can be estimated using a mixing approach similar to that in Appendix A for a vadose zone plume entering the saturated zone, except that the mixing depth extends some distance into the river, and the flux rate in the river is dependent on the stream depth and velocity. The effects of retardation and decay can be dealt with in the same manner as for the vadose zone.

3.3.2 Technical Issues

Technical issues considered most important for groundwater modeling at the Hanford Site are summarized below. The importance of these technical issues with regards to decision making was not qualitatively assessed (with sensitivity studies, for example) in this report. The importance of technical uncertainty will vary for different operable units. For example, groundwater influx from Cold Creek and Dry Creek will likely be important for transport modeling in the 200 Areas, but will not significantly affect modeling of contaminant transport in the 100 Areas. Since project objectives should be the motivating force behind modeling efforts, investigation of a technical issue should not be conducted until the significance of the issue has been carefully assessed.

(1) Need for three-dimensional models: Most of the saturated groundwater flow models used at the Hanford Site to date have been two-dimensional. Assumptions included in two-dimensional models include no vertical flow (thus, vertically homogeneous hydraulic conductivity), groundwater flux conditions (including infiltration, leakage, and groundwater pumping) applied equally over the entire thickness of the aquifer, and vertical mixing of a contaminant plume over the entire thickness of the aquifer. These assumptions may be significant oversimplification for actual groundwater systems that commonly include one or more of the following: layered stratigraphy, significant variation of hydraulic conductivity with depth, infiltration at the top of the model, and partially penetrating wells. In addition, since most contamination enters groundwater at the water table and vertical dispersivities are close to zero, the typical groundwater plume remains close to the water table and experiences little vertical spreading. Because concentrations in groundwater samples collected from typical monitoring wells are an average of the concentration over the screened interval, the vertical mixing assumption is generally valid for aquifers with saturated thicknesses similar to well screen intervals, which are typically 10 to 20 ft at Hanford. As the saturated thickness of an aquifer increases, however, the degree of dilution at the source is increasingly overestimated. In previous transport modeling at Hanford, this overestimation of dilution at the source was compensated for by increasing the contaminant mass influx rate (GAI 1991). For example, if the aquifer was 100 ft thick beneath the source, the mass influx rate at the source was increased by a factor of 5 (the aquifer thickness divided by the typical screened interval). This correction resulted in more realistic concentration predictions for wells screened near the water table but also increased the total contaminant mass in the aquifer.

The advantage of three-dimensional models is that they facilitate simulation of vertical flow, layered systems, vertical dispersivity, partial well penetration, and other three-dimensional factors typical of actual hydrogeologic systems. The primary disadvantages of three-dimensional models are the computational demands of solving three-dimensional grids (see Section 2.5), and the lack of three-dimensional data. Furthermore, the problems with modeling transport using two-dimensional models are not easily solved using three-dimensional models. For example, in horizontally layered systems, contaminant plumes do not usually experience much vertical spreading, resulting in extremely high vertical concentration gradients (e.g., LeBlanc 1984). Simulating these high gradients without very small nodal spacing in the vertical direction (on the order of several meters or less) will result in extreme numerical dispersion that can invalidate the solution. Other than for small, site-specific models, increasing the number of vertical layers, such that numerical dispersion is sufficiently reduced, usually results in unacceptable computational demands. This situation means that area-wide transport modeling is practically impossible in three-dimensions.

One means to obtain the advantage of three-dimensional flow modeling without the transport difficulties, is to model flow in three-dimensions and transport in two-dimensions using the velocity vector results for the upper regions of the aquifer. This approach would be most useful for situations with no significant natural or artificial infiltration and negligible vertical gradients.

(2) Natural infiltration rate: The amount of recharge due to natural infiltration is uncertain, although it appears to vary from <0.1 cm/yr (0.04 in/yr) up to 10 cm/yr (3.9 in/yr) depending on soil and vegetation conditions (Gee 1987). The importance of natural infiltration on the site-wide hydrologic system can be assessed by comparison with other sources of groundwater flux across the site. In the 200 Areas, average effluent discharge to the subsurface between 1943 and 1980 has been estimated to approximate 32,500 L/min (8,600 gal/min) (Zimmerman et al. 1986). Influx from Cold Creek and Dry Creek valleys has been estimated to range from 7,600 L/min (2,000 gal/min) (Jacobson and Freshley 1990) to 114,000 L/min (30,000 gal/min) (GAI 1991). In comparison, a natural infiltration rate of 2.0 m (0.8 in) over the approximately 520 km^2 (200 mi^2) of Hanford Site that lie south of the Columbia River would contribute approximately 2,800 L/min (740 gal/min). Given these flux estimates, it is apparent that natural infiltration will be more significant with regards to flow patterns in the saturated zone when effluent discharge to the subsurface is discontinued.

(3) Upwelling from basalt: The amount of influx upwelling from the underlying basalt aquifers into the water table aquifer has not been quantified. A study performed by Graham et al. (1984) indicated that an upward hydraulic gradient generally existed between the basalt aquifers and the unconsolidated deposits. Due to the low hydraulic conductivity of the basalts, the rate of upwelling from the basalt is likely quite low. However, in regions where the basalt aquitards have been eroded away, such as near Gable Mountain Gap, the basalt aquifers are directly connected to the water table aquifer and the rate of upwelling may be quite high. The importance of upwelling near Gable Mountain Gap may require additional investigation.

(4) Groundwater influx from Cold Creek and Dry Creek Valleys: Similar to groundwater influx from infiltration, the importance of influx from Cold Creek and Dry Creek valleys is relative to the other sources of recharge to the site. As mentioned above, estimates of influx from Cold Creek and Dry Creek range from 7,600 L/min (2,000 gal/min) to 114,000 L/min

(30,000 gal/min). The sources of recharge in these valleys include areal infiltration, runoff, and irrigation. In addition, upwelling from the underlying basalts may significantly impact the flow rate out of these valleys. Estimates of influx from these valleys could be refined with better characterization of the stratigraphy and hydraulic conductivity where Cold Creek and Dry Creek valleys enter the Hanford Site.

(5) Dispersivity: Dilution and spreading of contaminant plumes is largely determined by dispersivity. Model dispersivities used in the past were based on analysis of observed tritium plumes at the Hanford Site (GAI 1991). As discussed in Section 2.3, scale dependence should be considered when determining what dispersivity is appropriate. For many modeling applications, dispersivity may not be very important. For example, for predictions of maximum groundwater concentrations near a contaminant source, it is probably best to assume no dispersion. To predict concentrations in the Columbia River, it is most important to know the total contaminant mass flux rate into the river. Therefore, dispersivity will only be important for predicting the distribution of groundwater concentrations downstream of the source before the plume reaches the Columbia River.

(6) Measured parameters: Values of model parameters, such as hydraulic conductivity, storativity, and effective porosity, are the primary variables that affect groundwater flow and transport simulations. Although these parameters can be estimated during calibration exercises, it is desirable that the parameters used in the model resemble field measurements. Hydraulic conductivity is the only parameter necessary to perform steady-state flow simulations (assuming the base of the aquifer is well defined). Estimates of hydraulic conductivity can be calculated using results from both slug tests and pump tests, although pump tests measure a larger portion of the aquifer than slug tests and generally allow more reliable interpretation. Storativity is only required for transient flow simulations. Because storativity estimates require pumping tests of long enough duration to observe drawdown in at least one observation well (rarely performed at Hanford), very few estimates of storativity are available. Effective porosity is only required for simulation of transport problems. Although laboratory tracer tests on sample cores may be useful, effective porosity estimates should be based on field tracer tests.

3.4 ROLE AND USE OF UNCERTAINTY AND SENSITIVITY ANALYSIS

An evaluation of the uncertainty associated with calculating the concentration of contaminants is an important part of the baseline risk assessment. A reasonable approach to assessing this uncertainty involves the use of sensitivity analyses. Sensitivity analysis is usually defined as the adjustment of parameters within a reasonable range of site-specific values to examine or quantify its effect on the result (contaminant concentration). This type of sensitivity analysis is subjective and its use for an application will need to be examined on a case by case basis.

In addition to parameter sensitivity analyses, it is recommended that the sensitivity of major assumptions be evaluated. For example, simplified models generally use averaged parameters and assume a homogeneous medium for representing flow under saturated conditions. Although it is generally believed that such simplifications are valid if conservative or bounding parameters are used, this assumption will need to be examined. For example, if the soil is nonhomogeneous, a preferential pathway may exist and this could result in a short circuit of the flow pathway. These types of conditions and assumptions need to also be evaluated on a case-by-case basis.

Application of uncertainty analyses techniques using stochastic techniques (e.g., Monte Carlo simulations) are not recommended at this time, primarily due to their limited application and absence of generally accepted procedures. Application of such techniques may become more accepted and useful in the future, particularity in light of the large uncertainties associated with vadose zone modeling.

4.0 PLAN FOR DEVELOPMENT OF HANFORD GROUNDWATER MODELS

4.1 VADOSE ZONE PLAN

Discussion of the technical issues that surround the use of vadose zone models was provided in Section 3.2.2 and discussion of the data (model parameters) required to support the application of vadose zone flow and transport models was provided in Section 3.2.3. This section discusses a near-term plan that will lead toward the resolution of these issues and data needs and provide recommendations and guidance on the use of vadose zone flow and transport modeling.

4.1.1 Calibration/Validation of Vadose Zone Flow and Transport Models

Calibration/validation is generally viewed as the major issue surrounding the use of vadose zone flow and transport models at Hanford. The plan outlined in this section is designed to establish or test the overall veracity of vadose zone flow and transport modeling through a series of selected Hanford Site case studies. These case studies are the result of several liquid releases that have occurred on the Hanford Site and that have been characterized to some extent. Completion of these studies does not remove or alleviate the need to calibrate/validate models to site-specific conditions when then models are used in support of risk assessments. The successful completion of these activities simply provides the necessary reassurance that these codes/models can be applied with reasonable confidence across the Hanford Site.

Recently, two activities have been performed that support the validation/calibration of Hanford Site partially saturated flow and transport models. These include: (1) a validation of the PORFLO-3 computer code and conceptual model using the Las Cruces field data(Rockhold and Wurster 1991; and, (2) a calibration of the PORFLO-3 computer code using field data collected on the T-106 single-shell tank leak (Smoot and Sagar 1990).

Three activities are planned for FY 1992 that will address the need to validate/calibrate vadose zone flow and transport models. A status and plan for each of these activities is presented in the following paragraphs.

4.1.1.1 <u>Injection Test Site</u>. An effort is ongoing to use data from the injection test site in the 200 East Area to validate a vadose zone flow and transport model that uses VAM3D-CG. During FY 1991, the test data were reduced to a format useable in the VAM3D-CG. During FY 1992, numerical simulation will be performed and the results compared against the experimental data. Moisture-retention curves for soil samples collected in situ will be used to support these analyses. This study is scheduled to be completed during FY 1992.

4.1.1.2 200-BP-1 Plume Modeling. PORFLO-3 is being used to evaluate and interpret field data collected at waste sites in the 200-BP-1 operable unit. The nature and extent of contamination at several waste sites and characterization of this contamination in terms of model parameters required by PORFLO-3 is being collected in the field. This work was initiated in FY 1991. Results from preliminary analyses have been reported during Unit Manager meetings. As additional site characterization data become available, the information is incorporated into the model. Additional discussion on validation/calibration activities in support of 200-BP-1 operable unit is provided in Appendix B. It is recommended that ongoing activities be revised, if necessary, to reflect these guidelines. Existing budget and work scope constraints are recognized and must be factored into any adjustment.

4.1.1.3 300 Area Promethium Release. A data set from an unplanned release of promethium-147 is provided in Section 3.1.2.2.5 of the 300-FF-1 operable unit work plan. Based on a cursory review, it appears that this release has been characterized well enough to justify a preliminary vadose zone flow and transport analyses. A plan for using this data set, augmented with addition information from future characterization, is being assessed. This work is being performed in support of 300-FF-1 and the results from the preliminary analyses should be available by the end of this fiscal year. The PORFLO-3 variable saturated flow and transport computer code is being used to perform these analyses.

In addition to the activities described above, a rationale for continuing the validation/ calibration of variably saturated flow and transport models at the Hanford Site is provided in Appendix B. It is recommended that future vadose zone flow and transport models validation activities follow these guidelines to the extent possible. A study will be performed to identify a set of waste sites that, once characterized, will provide a database suitable for the purpose of validating vadose zone flow and transport models. The objective will be to define a set of sites that cover the spectrum of anticipated application (need for vadose zone flow and transport models) across the Hanford Site. The results from this study will be presented at the workshop discussed in the proposed workshop. During the conduct of this study, meetings will be held bi-monthly to status progress. The first meeting is scheduled to be held in January 1991.

4.1.2 Plan for Resolving Other Issues

4.1.2.1 Validating the van Genuchten-Mualem Theory. A study is ongoing to assess the validity of the van Genuchten-Mualem theory. A "library" of core samples from various boreholes and for various soils exists at the Hanford Site. These samples and the ongoing collection of moisture characteristics data will serve as the data to verify the van Genuchten-Mualem relationships for the unsaturated hydraulic conductivity for Hanford soils. Based on the core sample data and soil samples collected at various operable units, laboratory-measured data will be obtained on the saturated hydraulic conductivity and the moisture-characteristic curves (i.e., the moisture content versus pressure head). Based on core data, independent, laboratory-measured estimates will also be obtained for the unsaturated hydraulic-conductivity curves (i.e., the unsaturated hydraulic conductivity versus moisture content) for the major soil types at Hanford. These independent measurements will serve as a basis for verification of applicability (or nonapplicability) of the various estimating techniques (van Genuchten-Mualem, Brooks-Corey, Campbell relationships, etc.) for the Hanford soils, especially at the relatively low moisture contents. This study will provide some important data on the moisture characteristics for the Hanford soils. Results from this study will provide useful data to correlate the measured hydraulic conductivity values to bulk density and particle-size distribution

for the Hanford soils. The presence of a significant correlation would allow extensive use of the Hanford Site particle-size database for estimation of the unsaturated hydraulic conductivity.

The results from this preliminary assessment are scheduled to be available by the end of this fiscal year. A need for follow-on work will be defined at that time based on the results of these findings.

4.1.2.2 Groundwater Recharge. At the present time, the subject of groundwater recharge is included as a task in the Protective Barrier Development Program (Adams and Wing 1986). Although no specific study has been identified to quantify recharge across the Hanford Site, it is proposed that a study be performed to provide a defensible estimate of infiltration and groundwater recharge of meteoric water under current climatic conditions for the full range of soil and plant cover associations found in the 200 East, 200 West, 300, and 100 areas, and that this study by interated into the ongoing study that supports the Protective Barrier Development Program. Existing data on multiyear lysimeter studies, combined with drainage analyses (using Richards' equation), will be used to: (1) produce preliminary estimates of recharge; (2) document uncertainties contained in the estimates for various aggregate areas (i.e., 200 East, 200 West, 300, and 100 areas); and (3) provide a detailed study plan to improve recharge estimates at the Hanford Site. The preliminary estimates based on lysimeter data will later be compared to estimates obtained by use of environmental tracers (e.g., ^{36}Cl or tritium). In lieu of this proposal, it is proposed that estimates of recharge become a subject of the aggregate area studies and the various other work plan formulations currently underway. In either case, it is recommended that the UNSAT-H model discussed in Section 2.4 be used for the purpose of quantifying recharge.

4.1.2.3 Applicability of Arya-Paris Model. As discussed in Section 3.1.1, a study is ongoing to assess the utility of applying the Arya-Paris model to describe the moisture characteristics for Hanford soils. A recommendation on the viability of using this formulation will result from this preliminary evaluation. Work on this task is coupled to the ongoing work on the van Genuchten-Mualem theory described previously.

4.1.3 Other Activities

4.1.3.1 Guideline for Single-Shell Tank Field Characterization Activities. A study is underway to define soil characterization needs to support vadose zone flow and transport modeling in support of assessing the potential for contaminant migration in the vicinity of single-shell tanks. The objective of this study is to define DQO and to discuss the rationale to support these specification. The expectation is that detailed vadose zone flow and transport models will be required to assess the risk to human health and the environment resulting from past tank leaks.

4.1.3.2 Use of Area-Wide Data Sets Versus Site-Specific Data. As stated in Section 4.1.3.1, a question that has recently surfaced involves the development and use of area-wide data versus site-specific data sets. This basically is a restatement of the question "How much data are required to characterize a site?" This question can only be answered in terms of the end objective. Based on the specific need, acceptance criteria and/or DQO need to be defined before this question can be answered. It is recommended that this approach (definition of objectives or development of DQO) be used during the stucturing of all future work plans.

4.1.3.3 Soil/Water Partitioning Coefficients. The quantification of distribution coefficients for various radionuclides has been an ongoing activity at Hanford for many years. The database is updated periodically. The recent updating of this database that is most germane to baseline risk assessments performed in support of Hanford Site remediation activities has been provide by Serne and Wood (1990) as well as Ames and Serne (1990). It is recommended that a technical baseline be established for assigning soil/water partitioning coefficients in support of risk assessment activities. It is proposed that this baseline be established and that this baseline emphasize the work performed at Hanford over the years. In addition, a guideline on the use of geochemical models in support of risk assessments should be prepared. Finally, it has been speculated that, under very dry soil conditions, that partitioning could become the most important transport consideration. It is proposed that a study be performed to address this aspect of transport.

4.1.3.4 Guidance Document on Screening Methodologies and Defining the Need for Vadose Zone Modeling. It is recommended that a document be prepared to guide the formulation (i.e., screening methodologies, defining need, specification of data, etc.), for applying vadose modeling under both wet and dry conditions. Completion of the guideline for defining vadose zone modeling needs in support of single-shell tank field characterization will provide a basis for developing the guideline for wet conditions. A guideline for using vadose zone flow and transport models under dry conditions will be prepared. This activity will support the choice of location for the 216-W-5 Burial Ground. A discussion on the use of vadose zone flow and transport models in support of this facility will be part of the performance assessment required by the Department of Energy requirement (DOE-RL 1989). As stated previously in Section 3.3, it is recommended that the quantification of release rate from the various waste forms be addressed in facility-specific work plans. Once the contaminants find their way into the soil column, it is assumed that one of the other guideline documents (wet or dry) can be applied.

4.1.3.5 FY 1992 Workshop. It is proposed that a workshop be held during September 1992 to present the results of work completed during this fiscal year. The workshop will provide a basis for defining future activities. Proposed topics to be discussed at the workshop include the following.

- The preliminary results and observations on validation of the van Genuchten-Mualem formulation for Hanford soils.
- A status report on groundwater recharge studies being performed at Hanford (see Section 4.1.2.2).
- Discussion of the rationale to support development of the DQO in support of single-shell tank vadose zone soil characterization.
- Progress report on the development of the guideline to support vadose zone flow and transport under dry conditions.
- Summary of vadose zone model calibration/validation activities. In addition, the candidate waste sites that have been identified to support future vadose zone validation work will be discussed.

4.2 PLAN FOR DEVELOPMENT OF AREA-WIDE SATURATED ZONE MODELS

This section presents a plan for the development of a numerical model to simulate the movement of water and contaminates in the uppermost unconfined aquifer underlying the Hanford Site. Westinghouse Hanford Company proposes to develop a model of the flow and transport system using the VAM3D-CG numerical computer codes (Huyakorn and Panday 1990) which will be implemented in a two-dimensional mode. The flow model would be constructed first, followed by the contaminant transport model. As work progresses, a decision will be made as to the utility and feasibility of developing a partial or fully three-dimensional flow model. The need to develop three-dimensional flow models is not certain at this time. Contaminant transport is expected to remain a two-dimensional simulation. An existing computer code, VAM3D-CG, was selected to allow the simulation effort to concentrate on the development and incorporation of the considerable geologic, hydrologic, and groundwater quality database currently available. Additional hydrogeologic characterization data of the Hanford Site collected under the RI/FS and other remedial programs will be incorporated into the models as they become available.

The resulting model will simulate the variable-thickness upper unconfined aquifer system with expansion capabilities to handle the uppermost confined system. No decision is believed possible at this time on the need for this latter capability. On a theoretical basis, the VAM3D-CG implements momentum and continuity relationships to simulate flow. Contaminant transport is represented by an advection dispersion formulation. Reversible contaminant partitioning relationships and radioactive decay are also included. The numerical equations are solved using very efficient numerical algorithms based on finite-element formulations.

The implementation will use a large (on the order of 1/4 square mile) grid discretization. The grid size is variable. This large grid size is proposed to make the model useful for site-wide forecasting of the impacts of large-scale remedial measures.

Recognizing that a considerable effort is currently ongoing in the areas of data collection and interpretation, Westinghouse Hanford Company proposes to start immediately on the model input preparation. This approach will allow the model to be operational in the shortest time frame possible. New characterization data and changes in flow conceptualization will be incorporated as they become available. This approach recognizes and plans for the need to continually update the hydrogeologic conceptualization of the Hanford Site that is incorporated in the model.

Toward the completion of the two-dimensional effort, meetings will be held with Ecology and EPA to evaluate the need and utility of expanding the two-dimensional effort into three dimensions. This decision will be based on an examination of the remaining needs for risk assessment, the availability of three-dimensional data, and computational requirements.

4.2.1 Purpose

The purpose of this modeling effort is to develop a numerical model supported by a credible data base that can be used to:

- Predict changes in the groundwater contaminant concentrations over time to assist in estimating the level of exposure to a receptor for purposes of risk assessment.

- Establish starting conditions (initial and boundary) for smaller scale localized models of the saturated flow system needed to evaluate the potential impacts of certain remedial measures.
- Estimate impacts to the groundwater flow system to changes in discharges to cribs, ditches and ponds. (Major changes are currently proposed under both the M-17-00 Milestone.)
- Estimate the flux of liquids and contaminants to the Columbia River.
- Establish the need and feasibility of other models for risk assessment and remediation.

The process of selecting a model and developing the input information will naturally provide consistency for other modeling efforts to follow. This initial effort will also be useful in developing guidance for the quantity and location of additional data needs to fill in areas of limited understanding.

4.2.2 Preliminary Model Selection

A preliminary decision was made to proceed with the VAM 3D-CG model based on the following:

- VAM 3D-CG is numerically and technically sophisticated.
- Limited additional model development is expected.
- Active numerical support from the developer is available, if needed.
- VAM models are also being used by Westinghouse Hanford Company to model vadose zone and multiphase flow.
- Simulation of two- and three-dimensional flow regimes are possible with the same code.

As data collection proceeds and implementation begins, the model selection will be confirmed by numerical testing of the code.

4.2.3 Assumption and Limitations

Presented below are a number of assumptions and a brief discussion on their implications to the numerical effort. No level of importance is intended by their respective order in the list.

- A two-dimensional formulation of the flow system is sufficient for the purposes of risk assessment. The corollary assumption is that flow in the upper unconfined system is believed to be essentially horizontal. The added complexities of a site-wide three-dimensional flow simulation are believed to outweigh the expected improvement in the evaluation of risk. Complexities include: limited site-wide hydraulic head data with depth, limited stratigraphic data north of Umtanum Ridge, and significantly increased computational demands. A fully three-dimensional approach would orient the effort toward resolving simulation problems at the expense of hydrogeologic issues.

- A two-dimensional formulation of the contaminant transport system is sufficient to meet the purposes of risk assessment. This is based on the assumption that most contaminants enter the saturated system from above and little vertical dispersion occurs. An additional dimension would yield significant increase in numerical difficulties and is not supported by the existing data base.
- Sufficient data exist to allow model input development to begin while Westinghouse Hanford Company simultaneously collects and interprets new information. This assumption recognizes that a number of models have already been developed and that the hydrogeologic conceptualization will change as additional characterization is conducted.
- The model will simulate dilute contaminants which are miscible in water. Floaters and sinkers, i.e., immiscible fluids, are beyond the scope of an area-wide model and need to be handled on a separate basis.
- The model will discretize the site into variable-sized, large planar areas having variable thickness to account for large scale changes in hydrologic transport characteristics. Other scales and models will be needed to handle unique chemical or localized hydrologic conditions.

4.2.4 Approach

Table 4-1 presents the list of task elements for the model implementation. The first two columns of Table 4-1 present task elements common to the implementation of the VAM models. The third column presents a list of data packages used to update the hydrogeologic conceptualization and provide other technical information for use in model implementation.

Implementation of the area-wide flow model would begin with a review of past numerical efforts and build on the existing database. This approach would provide a useable model in the shortest timeframe possible. The flow model would be calibrated to historic flow conditions and applied to future flow scenarios. Currently, Milestone M-17-00A and M-17-00B (Ecology et al. 1990) presents a status of effluent discharge plans and would form the basis for future flow scenarios. Negotiations and agreements with EPA and Ecology on new facility sitings and expected groundwater discharge permits would provide another source of information for developing future scenarios.

Column two of Table 4-1 presents the major task elements in the implementation of a contaminant transport model. The initial task is to evaluate the groundwater data and sort/select those constituents important to risk assessment and for which a significant database exists to develop a credible model. It is expected that a two-dimensional model of the contaminant transfer will be sufficient for risk assessment and other needs. Flow simulation results will be used to drive the contaminant transport portion of VAM3D-CG. This implements the assumption that little vertical dispersion occurs in the Hanford saturated groundwater system and keeps the simulation balanced in relation to the availability of data. VAM3D-CG is proposed for use to complete this milestone. This model will be evaluated in detail as work begins to fully establish its capabilities and ease of use. Should a problem develop or a better alternative present itself, Westinghouse Hanford Company will notify Ecology and EPA of any proposed changes and implement a change after receiving EPA and Ecology approval.

Table 4-1. Task Elements, Saturated Two-Dimensional Flow and Transport Model Implementation.

	EPA and Ecology Approval	
Two-Dimensional Flow Implementation	Two-Dimensional Transport Implementation	Data Packages
Review past modeling efforts	Select groundwater constituents of interest	Update Ringold and Hanford formation lithology/ stratigraphyy
Review existing data		Update and correlate aquifer property data to lithology
Test VAM3D-CG	Test VAM3D-CG	Update and complete artificial recharge estimates
Develop conceptualization: Stratigraphy Hydrostratigraphy Boundary conditions Initial conditions Calibration data	Develop Estimates: (specific yield, dispersivity, partition coef.) Initial conditions Boundary conditions Calibration data	Select calibration data sets
Development of site discretization		Develop future flow scenarios
Calibrate model to historic flow conditions	Calibrate model to selected plumes	
Run future flow scenarios	Run future contaminant transport scenarios	
Report	Report	
	Final summary report	

Key to the implementation of a hydrology and transport model is the development and interpretation of the voluminous quantities of data currently available. RI/FS groundwater remediation activities have provided the opportunity to update the current knowledge of the stratigraphy and lithology in large areas of the Hanford Site. Completion of the first two tasks listed in column 3 of Table 4-1 are dependent on the completion of various groundwater operable units and groundwater aggregate area management studies (AAMS) in the 200 Areas. The remaining three tasks are outside the basic needs of existing RI/FS program and will be completed for the modeling effort alone.

The magnitude of the data collection, analysis, and interpretation effort makes commitment to when new information will be available for modeling difficult, if not impossible. Each operable unit will face changes in schedule and scope as remediation proceeds. However, geologic and hydrologic information is being collected and analyzed for each groundwater operable unit and AAMS. As key portions of the information become available, they will be incorporated into the model, as needed. With a few exceptions, the implementation of the site-wide model will use existing and currently "planned-for-collection" information.

4.2.5 Long Term Recommendations

As planning for the development of a Hanford-wide model was undertaken, it became evident that a number of hydrology related tasks of long duration were needed for an implementation of remediation measures, credible risk assessments, and general support to ROD. Each is briefly described below:

- Four to five deep characterization boreholes are needed in the 100 Areas north of the Umtanum Ridge anticline. These holes are needed to fill gaps in the stratigraphy, the vertical component of flow, and aquifer properties.

- Runoff measurements in Cold and Dry creeks should be continued. These measurements are the only source of reliable information on what may be the dominant source of naturally occurring groundwater recharge on the Hanford Site.

- Aquifer pump tests with nearby observation wells are needed, particularly in aquifers of intermediate transmissivities. Much of the conductivity data on the reservation need to be supported with a limited number of well-designed and implemented aquifer tests.

- A program to quantify the rate and variation of natural infiltration is recommended. Such a program will be needed to support a nonaction alternative to ultimately decide if buried wastes are to be removed or left in place. The existing program to quantify natural infiltration was discussed in Section 4.1.2.2.

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APPENDIX A

VADOSE ZONE SCREENING METHODOLOGY

A.1 INTRODUCTION

To predict the maximum concentration in groundwater directly beneath a waste site it is conservative to base the calculation upon the vadose zone contaminant concentration, the water flux rate through the vadose zone, the amount of dilution in the saturated zone, and the rate of removal due to radioactive decay, or chemical and biological degradation. The approach outlined below begins with the simplest and most conservative conceptual model: that groundwater concentrations will eventually equal vadose zone concentrations. Additional components of the conceptual model can be incorporated as deemed necessary and applicable.

A.2 BASE METHOD

If the effects of decay and saturated zone dilution are excluded, concentrations in the saturated zone will eventually equal contaminant concentrations presently existing in vadose zone pore water. As a result, it is no longer necessary to estimate the water flux rate through the vadose zone and the only information needed is the existing concentration in vadose zone pore water. Unfortunately, vadose zone source characterization usually provides information on soil concentrations, not vadose zone pore water concentrations. For most contaminants, determining the concentration in pore water associated with soil concentrations is difficult given the potential for sorption and precipitation reactions. A conservative method to determine the water concentration in the vadose zone would be to assume that the bulk (or total) concentration was entirely associated with the pore water. This assumption is equivalent to a soil/water partitioning coefficient of zero and complete dissolution of the contaminant. Given these assumptions, the equivalent water concentration (C_{w1}) can be calculated from bulk soil concentration (C_b), the volumetric moisture content (Th), and the soil dry density (d), using the following equation:

$$C_{w1} = C_b * d / Th \qquad (1)$$

For example, given a bulk soil concentration of 10 mg/kg (dry soil), a volumetric moisture content of 20%, and a soil dry density of 1.6 kg/L, the maximum possible water concentration would be 80 mg/L.

In summary, the above method for determining groundwater concentrations that would result from vadose zone contamination uses the following conservative assumptions:

- no sorption
- no solubility limitations
- no mixing in groundwater.

Calculating the groundwater concentration using these assumptions would be the most conservative estimate possible. Because such a conservative approach will likely overestimate groundwater concentrations, it may be desirable to utilize more reasonable characterizations of contaminant behavior. General methods for incorporating the effects of sorption, solubility, and

groundwater mixing are outlined below. Note that the screening methodologies described in this section do not provide information regarding the time history of contaminant transport. As presently outlined in the risk assessment methodology (DOE-RL 1991b), the predicted future maximum is the governing exposure concentration and time history is not important.

A.3 SORPTION EFFECTS

Most contaminants have some chemical interaction, or sorption, with the soil matrix. Generally, the amount of sorption is expressed using the soil/water partitioning coefficient, or K_d parameter, and it is assumed that the sorption is linear with concentration, completely reversible, and not limited by kinetic factors. Because K_d's can be affected by water chemistry, soil mineralogy, and organic content of the soil, they are typically quite difficult to quantify. Furthermore, it is likely that non-linear behavior, irreversible sorption, and kinetic limitations can be important factors in contaminant sorption. Note that experimental results often indicate that contaminant K_d's can range over several orders of magnitude for different soil samples. Conservatively low estimates of contaminant K_d's, based upon existing data in the literature, laboratory experiments, or observations of field behavior, should be used. Typical units for K_d are l/kg. The relationship between soil concentration (C_s) and water concentration (C_{w2}) is expressed as:

$$C_s = K_d * C_{w2}$$

Given that bulk soil concentration C_b can be expressed as:

$$C_b = C_s + C_{w2} * Th/d$$

The equivalent water concentration can be calculated from the bulk concentration by substituting for C_s and solving for C_w to obtain the following equation:

$$C_{w2} = C_b / (K_d + Th/d) \qquad (2)$$

For example, given a bulk concentration of 10 mg/kg (dry soil), a partitioning coefficient of 2.0 L/kg, a moisture content of 20%, and a dry soil density of 1.6 kg/L, the water concentration would be 4.7 mg/L. This concentration is 1/17th of the previous concentration estimate that did not address the effects of sorption.

A.4 SOLUBILITY LIMITATIONS

Solubility of a contaminant limits the maximum possible water concentration. If the water concentration calculated using Equations 1 or 2 exceeds the solubility of the contaminant, it suggests that the soil sample may contain nondissolved liquid or solid phases of the constituent. Typically, organic solvents may be present as pure liquid phase, while metals and other inorganic constituents may be present as solid precipitate or bound in particulate matter.

Solubility estimates may be based on existing data in the literature, leachability experiments, and observations of field behavior. Because solubility can be affected by a multitude of factors, including temperature, pH, ionic composition, redox conditions, and the presence of other constituents, solubility estimates should be used with some knowledge of their variability.

Furthermore, maximum concentrations under field conditions may be limited by chemical kinetics or diffusion. This means that although the concentration in water that contacts a pocket of pure phase liquid or precipitate may be at saturation, the water concentration several millimeters away may be considerably less than saturation. As a result, even at highly contaminated sites, measured water concentrations in the field are rarely within one order of magnitude of the solubility limit. In the interests of being conservative, the solubility limit should be used as the concentration of a contaminant in soil water if calculations using Equations 1 or 2 exceed the limit of solubiity.

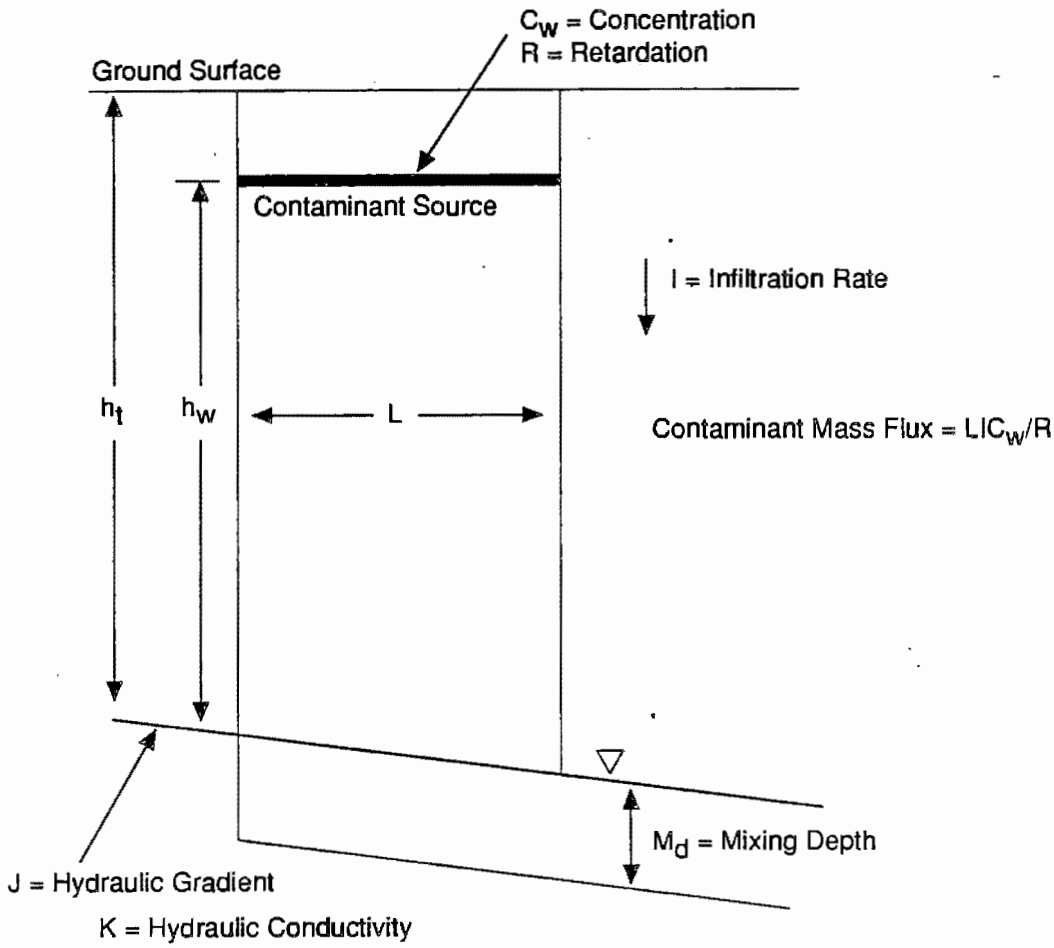
A.5 GROUNDWATER MIXING EFFECTS

Dilution of vadose zone concentrations due to mixing with saturated zone groundwater is only important in situations where the flux of contaminated water downward through the vadose zone is much less than the saturated groundwater flux beneath the waste site. Clearly, groundwater mixing would not be important for modeling contaminant transport beneath an active liquid effluent disposal facility receiving significant volumes of discharge. On the other hand, groundwater mixing could be very important beneath a solid waste facility underlain by a gravel aquifer, where the groundwater flow rate would be on the order of hundreds of meters per year and the groundwater flux rate may be tens of meters per day. The methodology described below allow quantification of the effects of groundwater mixing on contaminant concentrations beneath a waste site.

It is important to note that by excluding the effects of groundwater mixing the previous methodologies only required a single value for concentration (presumably a likely maximum concentration), and did not rely upon the distribution of contamination. As described below, however, to assess the effects of mixing in the saturated zone, it is necessary to account for contaminant distribution.

The methodology described below for estimating mixing in the saturated zone essentially mixes the downward contaminant flux (through the vadose zone) into the horizontal groundwater flux beneath the waste site. Figure A-1 illustrates the general approach. The total groundwater flux in the saturated zone is a function of the Darcy flux in the saturated zone and the mixing depth. As will be discussed below, these factors can generally be constrained by a factor of two or three with minimal effort. The total mass flux of contaminant through the vadose zone is a function of concentration (including distribution parallel to the groundwater flow direction), retardation, and the water flux through the vadose zone. Concentration in the vadose zone can be approximated using field sampling results and the techniques described above. Methodologies for estimating the remaining factors (saturated zone Darcy flux, mixing depth, retardation, and vadose zone flux) for low infiltration rates are described below.

Figure A-1. Screening Methods for Estimating Effects of Mixing in the Saturated Zone.



$$\text{Water Flux} = JKM_d + LI$$

$$\text{Saturated Zone Concentration} = \frac{LIC_w/R}{JKM_d + LI}$$

A.5.1 Saturated Zone Darcy Flux

The flux of water in the saturated zone (q_{sat}) can be estimated from the hydraulic gradient (J) and hydraulic conductivity (K) using Darcy's law:

$$q_{sat} = J * K$$

Generally, the hydraulic gradient can be estimated from water level measurements or groundwater modeling results to within a factor of two. The hydraulic conductivity can be estimated from properly performed pump test or slug test results to within a factor of two or three. Pump test results are generally more reliable than slug test results. Since lower flux results in less mixing, lower values of hydraulic gradient and hydraulic conductivity are considered conservative when considering contaminant concentration.

A.5.2 Mixing Depth

Actual mixing depths beneath a waste site are generally not well known. However, it can generally be assumed that the mixing depth at an extraction well would be no less than the well screen interval. A typically small screen interval on the order of 3 m should be sufficiently conservative. If the aquifer thickness is less than a typical short well screen interval, it may be assumed that the mixing depth would correspond to the aquifer thickness.

Across much of the Hanford Site, the water table is found near the bottom of the Hanford formation. Where this occurs, the saturated portion of the Hanford formation may form a potential flow path and in mixing may be confined to this zone of higher permeability. Under these conditions, the mixing depth may be limitd to the local saturated thickness. This layer may be <3 m.

A.5.3 Retardation

The movement of contaminants in the vadose zone can be slower due to sorption than the movement of water. This slowing is commonly expressed using the retardation coefficient, which is defined as the rate of water movement divided by the rate of solute movement. The retardation coefficient can be calculated using the following equation:

$$R = 1 + d * K_d/Th$$

For example, if soil density equals 1.6, K_d equals 2, and moisture content equals 0.2, the retardation factor would equal 17. Because K_d values are quite variable, conservative values should be assigned.

A.5.4 Vadose Zone Flux

In general, the factors that determine the rate of water influx into in the vadose zone beneath a Hanford waste site includes: (1) relatively rapid drainage resulting from elevated moisture conditions associated with effluent discharge, and (2) relatively slow drainage due to infiltration of precipitation. The first driving force is dominant at liquid effluent facilities during effluent disposal to the subsurface. After effluent disposal is discontinued, soil moisture gradually returns to natural conditions and infiltration of precipitation becomes the dominate driving force. Infiltration of precipitation is the only driving force beneath solid waste sites (assuming minimal amounts of free liquids).

The rate of water flux in the vadose zone due to natural infiltration is dependent upon precipitation, the type of surface soil, and vegetation. Measured infiltration rates range from 0 to approximately 10 cm/yr. A conservative value should be used for the analysis.

Since many waste units requiring risk assessment were previously liquid effluent disposal facilities, the current and future rate of water flux through the vadose zone will be somewhere between the rate that existed during active use and the rate due to natural infiltration. One possible method to limit the range of possible flux rates is to estimate the average rate of drainage from the soil column since discharge was discontinued. Since flux rates should decline with time, the average flux rate in the past should be a conservatively high estimate for future flux rates. This method for estimating the average flux rate in the past relies upon the following parameters: the average moisture content in the soil column when effluent discharge was discontinued (Th_i), the current average moisture content of the soil column (Th_c), the total height of the soil column above the water table (h_t), the distance between the water table and the contaminant source (h_w), and the time since effluent discharge ended (T_e). The average flux rate (q_{ave}) at the contaminant source location since effluent discharge ended can be calculated using the following equation:

$$q_{ave} = (h_t - h_w) * (Th_i - Th_c)/T_e \qquad (3)$$

Figure A-1 illustrates the meaning of h_t and h_w. If information on moisture contents are not available then conservative estimates may be utilized. If moisture contents vary with some pattern (e.g., increasing with depth) it may be useful to partition the soil column into discrete segments.

If the flux rate calculated using Equation 3 were to continue unchanged into the future, it is clear that eventually all excess moisture in the vadose zone would be drained. At this point, the flux rate would return to the normal rate associated with precipitation. The amount of time (T_d) required to drain excess moisture from the soil column above the source region can be calculated using the following equation:

$$T_d = (h_t - h_w) * (Th_c - Th_n)/q_{ave} \qquad (4)$$

where th_n equals the specific retention of the vadose zone soils. The distance (X) that the contaminant would have traveled during the time T_d can be calculated using the following equation:

$$X = T_d * q_{ave}/(Th*R) \qquad (5)$$

Substituting Equation 4 for T_d in Equation 5 and simplifying reduces the equation to the following:

$$X = (h_t - h_w) * (Th_c - Th_n)/(Th_n * R) \quad (6)$$

It is evident from this equation that the distance a contaminant will travel before the water content and flux rate return to natural conditions is independent of the average flux rate assumed in the equation. The distance above the water table (h_s) at which the rate of contaminant flux into the water table will occur at normal infiltration rates is the point where h_w equals X. This height can be determined by substituting in h_s for both X and h_w in Equation 6 and rearranging:

$$h_s = A * h_t/(1+A)$$

where,

$$A = (Th_c - Th_n)/(Th_n * R)$$

For example, given the following parameters: h_t = 100 m, R = 17, th_c = 20%, and th_n = 10%; it follows that h_s equals 5.6 m. Any contamination within 5.6 m of the water table will enter the saturated zone at the elevated infiltration rate, while contamination more than 5.6 m above the water table will enter the saturated zone at the natural infiltration rate.

A.6 EXAMPLE APPLICATION

To illustrate the methodologies outlined above, a hypothetical example of dilution in the saturated zone is provided below. To estimate the saturated zone concentration it is necessary to divide the contaminant mass flux by the total water flux. The water flux can be calculated by adding the total water flux in the vadose zone and the total flux in the saturated zone:

$$\text{Total Water Flux} = J * K * M_d + L * I$$

where J = water table hydraulic gradient, K = saturated hydraulic conductivity, M_d = the thickness of the mixing zone, L = width of vadose zone plume parallel to the direction of flow in the saturated zone, and I = infiltration rate. These parameters are illustrated on Figure A-1. The contaminant flux can be calculated with the following equation:

$$\text{Contaminant Flux} = L * I * C_w$$

where C_w equals the water concentration in the vadose zone and can be calculated using either Equation 1 or 2. Dividing the contaminant flux by the water flux results in the following equation:

$$\text{Saturated Zone Concentration} = L * I * C_w/(J*K*M_d + L*I)$$

Using this equation, and given the following parameters:

C_w = 4.7 mg/L = 4,700 mg/m^3
I = 0.1 m/yr = 0.00027 m/d
L = 20 m
J = 0.001
K = 100 m/d
M_d = 3 m

the saturated zone concentration would equal 0.083 mg/L, equivalent to a mixing factor of 1/57.

A.7 RADIOACTIVE, CHEMICAL, AND BIOLOGICAL DECAY

The importance of decay is dependant upon the rate of decay and the travel time through the vadose zone. Radioactive decay rates are generally known with a fair degree of certainty. Chemical and biological decay rates are usually poorly known. A methods for determining the travel time is provided below.

The travel time (T_t) can be estimated given the estimated water flux rates (q), the distance from the source elevation to the water table (h_w), the moisture content (th), and the retardation coefficient (R) using the following equation:

$$T_t = h_w * th * R/q \qquad (7)$$

If the methodology described above for vadose zone flux rate indicates that the flux rate changes during transport of the contamination, then h_w should be divided into two segments (X_1 and X_2) corresponding to the distance traveled at each flux rate. For example, consider the previous example with h_s (the distance traveled by the contaminant during drainage of water content above normal conditions) equal to 5.6 m. Assuming effluent discharge was discontinued 5 years previously, contamination is located 80 m above the water table, the initial moisture content was 0.3, and the parameters using in the previous examples, the average flux rate during those 5 yr due to moisture above natural conditions can be calculated using Equation 3:

$$q = (100\text{-}80 \text{ m}) * (0.3\text{-}0.2)/5 \text{ yr} = 0.4 \text{ m/yr}$$

This flux rate would be in addition to the flow associated with natural infiltration (0.1 m/yr). The amount of time required to drain the remaining excess moisture can be calculated using Equation 4:

$$T_d = (100\text{-}80) * (0.2\text{-}0.1)/0.5 = 4 \text{ yr}$$

During those 4 yr, the distance traveled (X_1) could be determined using Equation 7 and solving for X_1:

$$X_1 = 4 \text{ yr} * 0.5 \text{ m/yr} / (0.1*17) = 1.2 \text{ m}$$

The remaining 78.8 m (X_2) would be traveled at the normal infiltration rate of 0.1 m/yr, and the total travel time can be calculated using Equation 7:

$$T_t = 4 \text{ yr} + 78.8 \text{ m} * 0.1 * 17 / 0.1 \text{ m/yr} = 1{,}344 \text{ yr}$$

Given a first-order decay constant (k), the rate of decay can be determined using the following equation:

$$C = C_i * e^{(-k * Tt)}$$

The half-life of the constituent is equal to 0.693/k. Continuing the example described above, and assuming a half-life of 100 yr, the concentration would be reduced by a factor of 9×10^{-5} before it reached the water table.

APPENDIX B

RATIONALE FOR VALIDATION OF VADOSE ZONE FLOW AND TRANSPORT MODELS

B.1 INTRODUCTION

The issue of subsurface model validation is complex and although subsurface flow and transport models are being used at Hanford in support of risk assessments, the value and potential utility of such modeling is not fully understood at this time. In this appendix, the issue of validation for subsurface models is further reviewed and a strategy for assessing the adequacy of vadose zone flow and transport models is provided. This strategy acknowledges major constraints in the development of valid models. For example, sites are being studied for remediation and perhaps valid models may be needed to support decisions regarding remediation in the near future. As such, the need for and continuing challenge associated with valid subsurface flow and transport models is generally acknowledged. Most importantly, as the subject of validation is pursued, it is further acknowledged that a coherent strategy is not a substitute for consensus (Walsh 1990). As will be discussed, a continuous review and consensus is assumed during the validation process.

B.2 DEFINITIONS

The International Atomic Energy Agency (1982) provided a definition of validation that has stood the test of time in the very dynamic arena of high-level radioactive waste studies. Validation is defined as:

> "A conceptual model and the computer code derived from it are validated when it is confirmed that the conceptual model and the computer code provide a good representation of the actual processes occurring in the real system."

Definitions have been presented by others; however, all require that three issues be addressed; identification of model performance measures and field observables of interest, determination of the necessary accuracy for useful predictions, and selection of the range of conditions anticipated for model application.

Validation is always imperfect, and, in a very real sense, it can not be achieved in absolute terms. This is because our knowledge of governing processes and the geologic setting is always increasing as our understanding through laboratory and field studies continues to expand. It is also widely acknowledged that validation is site-specific. The imperfect and site-specific aspects of validation make the assertion that a model is valid both subjective and relative to existing knowledge. That is, validation can only be perfect relative to what is known. Furthermore, the appropriateness of applying a validated site-specific model to an adjacent site will always be judged relative to the proximity of the two sites, their similar structure and process conceptualization, and the character of waste disposal practices applied at each site.

Validation requires a distinction between conceptualization of a site and modeling of that site. Conceptualization relies upon our understanding of geologic structure, dominant processes, and boundary and initial conditions. Through the validation process, a review of the geologic structure and processes will yield insight into additional measurements that will be needed to improve our confidence in a valid model. Modeling relies upon an accurate conceptualization and uses governing equations, numerical methods, computer algorithms, and input data to produce numerical simulations of events. These models will be used for purposes of predicting possible future events and provide a basis for remediation.

B.3 VALIDATION PROCESS

Each of the steps in the model development process should be validated to ensure that a "good representation of actual processes occurring in the real system" is achieved Currently, most validation efforts are preceded by the selection of the code and involve the selection of an experiment, the specification of boundary and initial conditions, the completion of model simulations, and the comparison of predictions to field data. Few validation efforts begin with an impartial assessment of the purpose and objective that has lead to the decision to simulate the environment. Rarely are model performance measures and criteria for successful simulations explicitly adopted prior to conducting simulations.

In addition to the predictive-comparison validation, the validation process needs to include a statement of purpose, scope, and objective, the review and evaluation of all available data, and the conceptualization of the site leading to code selection and ultimately to the evaluation of modeling results. The overall validation process could make use of a variety of techniques for evaluating subjective decisions made by analysts throughout the modeling process. Experts could review the data available and the steps taken to arrive at the conceptual model of the site. The code flow chart, input, output, and coding logic can be reviewed in detail to ensure the correctness and accuracy of specific elements or calculations made in any model. The code to be used to model a site should be tested to ensure an appropriate degree of variability exists in model results in response to variation of process model parameters. This would serve as a reality check prior to the conduct of site-specific sensitivity or uncertainty analyses.

B.4 A RATIONALE FOR MULTIPLE VALIDATION GROUPS

Because of the complexity and subjective nature during the creation of a site-specific model, it has been shown to be of value to have more than one group performing the validation. They cross verify one another, explore and resolve differing interpretations, and reach a consensus regarding the validity of the site model. Generally speaking, economics determine the extent to which multiple groups can be employed. If multiple groups cannot be maintained throughout the validation process, it is still desirable to have multiple groups duplicate the early phases of validation, and have a single group perform the final simulations, and appropriate sensitivity and uncertainty assessments.

B.5 A STRATEGY FOR CREATING VALID MODELS OF HANFORD SITE VADOSE ZONE SITES

While it is widely accepted that model validation is site-specific, it is proposed that (1) the physical proximity of waste sites at Hanford within specific operational areas (200 East and West, 300 and 100 areas), (2) the similarities of disposal practices (cribs and trenches or dry disposal), and (3) the similarities of alternate remediations will lead to the validation of models for application at one or more classes of sites. Each class would be distinguished from others by unique aspects of its geologic structure, dominant processes, or key issues and performance measures.

For example, geologic profiles within the vadose zone differ between 200 East and 200 West areas because of the different erosion and deposition episodes that have occurred at the two locations; this despite the fact the two Areas are less than 2 mi apart. However, within the 200 West Area a generic geologic cross section may be discovered and be used in model validation. Note, the applicability of a validated model to a new site will still require a review to ensure structure and dominant processes are the same at both sites. In another example, a north-south geologic profile from the U.S. Ecology site through the 200 East Area may reveal significant differences in the soils and sediments underlying the U.S. Ecology site and the submarine reactor burial trench at the north-east corner of 200 East Area. Therefore, use of the same model at these different site might not be justified. Thus, although validation of vadose zone models may proceed to explore validation as a generic issue, the greatest potential for success lies in first identifying zones within 200 East and 200 West Areas having significant similarities in the underlying geologic profile.

Disposal practices vary. Disposal practices can influence the vertical location and mobility of wastes disposed to the vadose zone. Wastes have been disposed in the subsurface at Hanford in solid (dry) and liquid form. Some liquid disposals have been long-term and completely saturated the entire soil column, others have been of short duration. Liquid discharges have had a variety of chemical characteristics, e.g., pH was quite low in some cases and must be accounted for in our conceptualization of contaminant mobility. Once discontinued, both long- and short term liquid releases require that the analyst conceptualize and be able to simulate the redistribution of liquid in the vadose zone and its continued drainage to a new equilibrium state, if one is ever achieved.

Similarly, alternate remediations may differ markedly in the physical, hydraulic, geochemical, or microbiological processes they impose upon the subsurface system. These processes may create a nonisothermal regime. They may even modify the geologic structure or the physical-hydraulic properties of the site.

The strategy for validation of vadose zone flow and transport models is to identify classes of similar sites, disposals, and perhaps remediations such that validation efforts can proceed efficiently. The transferability of valid models will also be investigated. Selection of sites will be based on geologic structure, disposal practices, remediation options, and perhaps other issues considered relevant to site restoration decisions. The model validation process may be applied to one or more of the selected sites.

B.6 SELECTION OF APPROPRIATE SITES

Limited resources, (i.e., time, money, and personnel), require that ongoing site characterization activities be used as much use as possible to validate the flow and transport models. Use of controlled experiments remains a possibility. However, their application towards the validation of flow and transport models would need to be justified based upon these limited resources. Thus, rather than select sites for the purpose of establishing valid models of flow and transport, a strategy that relies on the use of ongoing site remedial investigations that have the greatest potential for providing complete data sets of sufficient quality to conduct a thorough validation study has been adopted. Accordingly, the concurrent development of our knowledge of a site and of a valid modeling capability for that site is an acknowledged constraint.

Selecting sites where the releases (quantity, timing, and quality) are well documented and accurate is of most value and perhaps represents a requirement. It is assumed that highly probable boundary and initial conditions associated with a past disposal operation can be established through the study of undisturbed soils surrounding the waste disposal site.

It is assumed that one or more sites within each operational area (i.e., 200 East and West, 300, and 100 areas) will be of potential interest because of unique geologic structure, disposal practice, and/or remediation alternatives. To this end, three sites within the 200-BP-1 operable unit are now being characterized; 216-B-57, 216-B-43, and 216-B-49. Each of these present an opportunity to examine a number of contaminants with various attenuation characteristics. The 200-BP-1 operable unit lies within the 200 East Area in the immediate vicinity of B Plant. As discussed in Section 4.1, it is assumed that the characterization of waste sites within the 200-BP-1 operable unit will be used for purposes of validation.

Another potential near term candidate is assumed to be the 200-UP-2 operable unit. This operable unit is located in the 200 West Area and could provide an opportunity to validate models and examine the transferability issue for models on the 200 Area plateau.

Process trenches within the 300 Area, i.e., the 300-FF-1 operable unit, currently present an opportunity to validate flow and transport models for a shallow vadose zone deposit. A possible site is the promethium-147 release site discussed in Section 4.1. Other candidate sites within the 100 Areas or near the Columbia River have not been identified at this time. Although considerable analyses has been performed in support of the 100-N Area waste sites and these sites may qualify.

B.7 IMPLEMENTATION OF THE VALIDATION PROCESS

The need for the overall validation process outlined below satisfies a longer-term objective that goes beyond the calibration/validation process described in the body of this report. Overall validation is directed at the creation of valid computational and forecast capabilities for studies that go beyond the baseline risk assessment. While it is acknowledged that the validation efforts outlined here occur concurrently with the RI process, validation is not simply applying models within the RI context. This results from the fact that the remedial investigation of a waste site may strongly focus the calculation of risk. For example, if all contaminants released at a waste site are immobile, the remedial investigation activities in support of the baseline risk assessment may concentrate on the quantification of chemical partitioning between the water and solid phase. As such, simplified flow and transport models may be used to support the baseline risk assessment under this situation. Within

this context, it is recognized that flow and transport modeling is only one component of the risk calculation.aspect of the may be are only one component of the risk calculation. As discussed in Section 2.0, those responsible for the quantification of the baseline risk assessment may employ a relatively unsophisticated modeling approach for baseline and perhaps very conservative simulations. On the other hand, for other situation, detailed flow and transport analyses may be required. Under these conditions, resolution of the flow and transport model validation issue will require examination of waste site with models of some complexity or sophistication with regard to both geologic structure and dominant processes.

B.7.1 Purpose, Scope, and Objective

A clear statement of the purpose, scope, and objective of the operable unit or waste site simulation is needed; particularly as it relates to validating the flow and transport model. Consideration should be given to the relationship between what is simulated for the site-specific study as opposed to what will be needed to validate flow and transport models. For example, the site-specific study may focus on exposure, health effects, and risk; however, flow and transport models will only forecast point concentration or mass flux. Essentially, legal and regulatory requirements must be translated to flow and transport quantities and related to field observable quantities.

B.7.2 Data Review and Evaluation

It is essential that all existing data be reviewed, reanalyzed, and evaluated. This is done to determine the spatial and temporal correlation of data, and to discover possible correlations in model parameters that are derived from the data. It is essential the validation study perform such a review and reevaluation of existing data because it provides them with the best possible overall understanding of the site structure and active processes. Certainly, as data are gathered during the RI process, they would be merged with the existing data and analyzed. During this step in the validation process, additional data needed for process models or to discriminate among alternate equally likely conceptualizations may be identified and gathered. Once identified, such data would be essential to enhance the confidence in our conceptualization and modeling of the site and its alternate remediations. It is anticipated that needed data can be developed from clean soil or core samples taken from the region surrounding but not impacted by past operations at the waste site. One of the most important aspects of the data review will be the evaluation of the quality of influent data which serves to quantify the timing, amount, and chemical character of the waste. Confidence in our characterization of the waste introduced to the environment relates directly to our ability to establish confidence in short- or long-term forecasts of waste migration and fate in the vadose zone. Because validation is truly a confidence and consensus building activity, one must begin with a strong foundation of confidence in the waste or source characterization, (i.e., timing, amount, and characteristics).

B.7.3 Conceptual Model and Scenarios of Interest

Conceptual models that take into account the geologic structure and hydrologic setting, the disposal practice, and the alternate remediation options are at the heart of the simulation objective and validation process. The geologic or geometric structure of the original site and of any engineered features of the disposal or remediation need to be considered in the conceptual model. Transport pathways communicating contamination to receptor locations must be identified and their flow and

transport characteristics determined. Active processes need to be identified and evaluated for the natural system, the disposal period, and each of the alternate remediations. The sophistication of the conceptual model(s) must be consistent with the purpose of the simulation and the complexity of the site structure and processes.

B.7.4 Performance Criteria and Acceptance Standard(s)

In this phase of the validation process, the parameters of interest are reviewed. This review, draws upon our earlier statements of purpose, scope, and objective. Key parameters for the risk assessment will have been traced back to key parameters for the flow and transport simulations. Going a step further, model performance measures are related to field observable quantities in this step of the validation. For example, point values of contaminant concentration may be the required output from the flow and transport simulations. However, prediction of point values of contaminant concentration may not be possible to achieve with any confidence in the highly variable geologic deposits underlying the Hanford Site. For the purpose of validating flow and transport models we may need to examine integrated quantities that extract us from the; point-in-space/moment-in-time issue, and enable us to compare models to larger scale measurements or estimates of contamination. Examples are the mass of contaminant within a larger spatial interval or stratigraphic unit of the geologic profile, and the mass of contaminant passing through a plane of interest over a period of time. These larger scale observables may enable us to address flow and transport model validation within a heterogeneous environment.

In addition to performance criteria, the range of model performance will need to be addressed. The range of performance will establish the range of sensitivity and uncertainty simulations necessary to demonstrate confidence in our simulations. Finally, it is essential that the needed accuracy of simulations be specified a priori so that they are useful in the decision making and risk taking process.

B.7.5 Code Selection and Assignment of Model Parameters

Consistent with the purpose, available data, and conceptualization(s), the site model should have the capability to address all probable conceptualizations and scenarios. The flow and transport code(s) selected as the primary tool in creating the site model should be able to address the most complex geometry and processes envisioned. All existing data will then be used to determine lumped model parameters. For example, if soil layers are included in the conceptual model, the existing data will be used to define physical location and process model parameters for each layer. If a homogeneous profile is envisioned, then analyses of the data would be undertaken to define a single equivalent porous medium. If a random porous medium were envisioned, then a probability density function of soil properties representing the overall soil profile would be generated from the data and used to create one or more realization of the soil profile. Similarly, initial and boundary conditions would be developed from site information for the needed simulations.

On selection, the code can be tested for generic sensitivity by using the range of conditions foreseen in the performance criteria section. Such a generic study could be undertaken on a relatively simple cross section for a variety of process model situations. This would facilitate analysis of model sensitivity by ensuring model response is realistic for the range of conditions envisioned in a simple setting before addressing all the complexity an actual site.

The overall correctness of soil physical-hydraulic property models and data needs to also be addressed in the context of the model application. The sensitivity of the selected code to the anticipated range of soil properties should be tested for generic response prior to site-specific simulations. This should be done for two reasons; to ensure a correct physical-hydraulic response and to ensure stable performance of the computational package.

The potential impacts of alternate geometric structure should also be explored. Alternative conceptualizations could be tested. This could reveal the acceptability of a variety of possible simplifications, (e.g., soil layers or a completely homogeneous profile; random and uncorrelated distributions, or spatial correlated distributions. The value of two-dimensional as opposed to three-dimensional conceptualizations could be examined in a generic setting prior to investing in a very detailed three-dimensional field study.

B.7.6 Model Calculations, Sensitivity, and Uncertainty

While the simulations of greatest interest during an RI may be future scenarios, (i.e., the baseline case and alternate remediations), the validation process will be most interested in the forecast of events from the beginning of the disposal operation up to the present day. This is precisely why the quality of the waste source data is of paramount importance. Today's understanding of the distribution of the contaminants; their position and concentrations in the environment provide us with the needed reality check on our forecast. Various data set manipulation techniques may be used to simulate the events and check the accuracy of the simulation. A partial data set may be employed to setup and run the simulation with the remainder of the data used to evaluate model performance.

Validation is about establishing confidence in the models and the modeling results. Sensitivity and uncertainty analyses should be conducted to define our level of confidence in model results based on the known range of model parameters and our level of uncertainty regarding dominant structures and processes.

B.7.7 Evaluation of Results for Acceptability

Performance criteria and acceptance standards were established early in the validation process. They were based on our intended use of the model results, the level of confidence or risk found acceptable. This aspect of validation would appear straight forward but it probably isn't. Certainly, if the model results and our confidence in them is satisfactory, we would have a valid model. If results or our level of confidence is unsatisfactory at least two alternatives can be pursued; 1) by further review of the data, or collecting additional data, and reconceptualizing the site and its alternate remediations, we could achieve satisfactory flow and transport simulations based on a validated model, or 2) no reasonable level of effort to collect more data, reconceptualize the problem, or develop new models can provide the quality of modeling results needed in the time frame at hand. In the first case, additional resources (time, money, people) can contribute to the solution through valid models. In the latter case, the decision making process would proceed without the benefit of modeling results of sufficient confidence. It is almost certain that less risky decisions will be taken in these cases and that significantly greater resources may be invested in more conservative remediations.

B.8 REFERENCES

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Walsh, W. J., 1990, "Making Science, Policy, and Public Perception Compatible: A Legal/Policy Summary, or Do We Want to Clean Up Hazardous Sites or Just Scream and Yell at Each Other?" in Ground Water and Soil Contamination Remediation: Toward Compatible Science, Policy, and Public Perception, National Academy Press, Washington, D.C.

APPENDIX C

DATA REQUIREMENTS FOR MODELING FLOW AND TRANSPORT

C.1 CLIMATIC DATA

1.1 Precipitation Data (From Meteorological Measurements)
- 1.1.1 Rainfall
- 1.1.2 Snowmelt
- 1.1.3 Runoff From Precipitation Events (Field-Measured)

1.2 Potential Evapotranspiration Data (From Meteorological Measurements)
- 1.2.1 Air Temperature
- 1.2.2 Relative Humidity (Wet and Dry Bulk)
- 1.2.3 Wind Speed
- 1.2.4 Solar Radiation

C.2 PLANT AND VEGETATION DATA

2.1 Transpiration Function (Field-Measured)
- 2.1.1 Plant Type and Depth of Root System
- 2.1.2 Plant Density

2.2 Plant Cover
- 2.2.1 Leaf Area Index (Field-Measured)

C.3 FLOW DOMAIN CHARACTERISTICS

3.1 Size of Flow Domain (Based on Field Data)
- 3.1.1 Spatial Discretization (Numerical Input)
- 3.1.2 Temporal Discretization (Numerical Input)

3.2 Boundary Conditions
- 3.2.1 Flow (Field-Measured Moisture Contents or Fluxes)
- 3.2.2 Contaminant Transport (Field-Measured Concentration or Mass Fluxes for Various Species)

3.3 Initial Conditions
- 3.3.1 Flow (Field-Measured Moisture Contents or Pressure Potentials)
- 3.3.2 Contaminant Transport (Field-Measured Concentrations for Various Contaminant Species)

3.4 Depth to Water Table (Field-Measured)

3.5 Thickness and Hydraulic Properties of the Unconfined Aquifer (Field-Measured)

3.6 Location and Rates of Pumping/Injection Wells (Field Data)

C.4 SOIL CHARACTERISTICS (These are considered to be the critical hydrologic parameters)

- 4.1 Heterogeneity and Anisotropy (Field-Measured)
  - 4.1.1 Layering (Thicknesses and Continuity of Various Layers)
  - 4.1.2 Anisotropic Characteristics of Various Layers
- 4.2 Moisture Characteristic Curves for Each Layer
  - 4.2.1 Moisture Content Versus Pressure Potential Curves (Field- or Laboratory-Measured)
  - 4.2.2 Hydraulic Conductivity Versus Moisture Content Curves (Field- or Laboratory-Measured or Derived From Moisture Content Versus Pressure Potential Curves)
  - 4.2.3 Hysteresis Data for Wetting and Drying Cycles (Field- or Laboratory-Measured)
- 4.3 Soil Bulk Density and Porosity for Each Layer (Field- or Laboratory-Measured)

C.5 CONTAMINANT TRANSPORT PARAMETERS

- 5.1 Diffusion Coefficients (Laboratory-Measured or Obtained From Literature)
- 5.2 Hydrodynamic Dispersion Coefficients (Laboratory-Measured or Obtained From Literature)
- 5.3 Retardation Coefficients (Laboratory-Measured or Obtained From Literature)
- 5.4 Radioactive Decay Constants (Laboratory-Measured or Obtained From Literature)

C.6 CONTAMINANT SOURCE CHARACTERISTICS

- 6.1 Major Radionuclides and Their Concentrations
- 6.2 Mass Source Loading Rate for Radionuclides