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Professor

January 14, 1999

Mr. Douglas Hildebrand
U. S. Department of Energy
Mail Stop HO-12
P.O. Box 550
Richland, WA 99352

Dear Mr. Hildebrand:

On behalf of Charles Andrews, James Mercer and myself, I am pleased to submit our "Report of the Peer Review Panel on the Proposed Hanford Site-Wide Groundwater Model." This is our first report following the November 20, 1998 meeting at PNNL during which we were briefed on and discussed the proposed Hanford Site-Wide Groundwater Model. Each panel member has reviewed the documents and maps provided before, at and after the November meeting. The panel has maintained close contact while writing this report which is a consensus document.

If you have any questions or concerns, please do not hesitate to contact me. We look forward to our next meeting and continuation of the peer-review process.

Sincerely,

Steven Gorelick

cc: Marcel Bergeron
Michael Thompson
Richard Holten
Charles Cole
Mark Freshley

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Report of the Peer Review Panel on the Proposed Hanford Site-Wide Groundwater Model

Report prepared by:

Steven Gorelick
Charles Andrews
James Mercer

January 14, 1999

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Executive Summary

External peer review of the Proposed Hanford Site-Wide Groundwater Model was conducted in the Fall of 1998. The three-member review panel commented on three specific issues: 1) adequacy of the conceptual model and its technical capabilities to meet the anticipated uses and needs, 2) possible improvements to the modeling framework / implementation, and 3) immediate new data needs.

The Panel unanimously agreed that:

1) The concept of developing a broadly applicable site-wide groundwater model is excellent. Scientists working for the U.S. Department of Energy–Richland Operations Office have made significant progress and should be commended for their superior efforts in dealing with voluminous data and complex field conditions, and for their integrated/interdisciplinary approach to model building.

2) With regard to the issue of model adequacy, the spectrum of anticipated uses and needs is so broad, ranging from time scales of less than 1 day to thousands of years and spatial scales of meters to kilometers, that this or any general-use, site-wide model cannot be expected to be adequate for all potential uses. An initial task should be to specify a narrower, and perhaps more pragmatic, list of model uses that involve less disparate temporal and spatial scales and contaminants whose behavior can be adequately characterized by linear sorption and first-order decay.

3) With regard to improvements in the modeling framework:

    - The existing deterministic modeling effort has not acknowledged that the prescribed processes, physical features, initial and boundary conditions, system stresses, field data, and model parameter values are not known and cannot be known with certainty. Consequently, predictions of heads and concentrations in three dimensions over time will be uncertain as well.

    - A new modeling framework must be established that accepts the inherent uncertainty in model conceptual representations, inputs, and outputs. Given such a framework, the expected values of heads and concentrations, as well as the range (distribution) of predictions, would be products of the site-wide groundwater model.

    - A priority task is to construct a comprehensive list of alternate conceptual model components and to assess each of their potential impacts on predictive uncertainty.

    - Assessment can be initiated with hypothesis testing and sensitivity analysis within the general framework already established with the existing site-wide model. If uncertainties due to alternate conceptual models are significant, then a Monte Carlo analysis is required to estimate both the expected value of the prediction and its uncertainty.

4) With regard to improvements in model implementation:

The Panel has identified a series of important improvements to the current site-wide modeling effort. A few of the most significant ones are listed below.

- The calibration procedure for the current model is not defensible. Reasons include the insufficient justification for using a single snapshot of presumed steady-state conditions in 1979, over-parameterization of zonal transmissivities given an insufficient number of independent data, potential for incompatibility between pumping-test results and model representation of the aquifer, 2D model calibration for a 3D model, and use of interpolated head values.

- The existing representation of chemical reactions is limited to first-order decay and linear sorption. This representation is potentially adequate for some of the prevalent contaminants found in Hanford groundwater; however, for most of the contaminants of concern found in the vadose zone, reactive transport needs to be represented. The decision that must be made at this stage is whether or not the umbrella of the site-wide groundwater model should cover reactive transport simulation or whether chemical processes are better handled by specialized local models. If the decision is to delegate chemical processes to specialized local models, it still may be possible to use hydraulic boundary condition values from the hydraulic component of the site-wide model. If the decision is to include reactive chemistry in the site-wide model, then the simulation framework must be based on a flexible open architecture that embraces complexities such as transport of multiple species, microbial degradation, and perhaps nonlinear feedback to the flow model as aquifer or water properties change.

- The domain covered by the site-wide groundwater model must be better justified. The site-wide groundwater model simulates groundwater flow and contaminant transport only in the unconfined sedimentary aquifer in the Pasco Basin south and west of the Columbia River. The unconfined aquifer to the north and east of the river and the bedrock basalt aquifer are not represented in the site-wide groundwater model even though the major discharge area for both aquifers is the region adjacent to the Columbia River.

- Boundary conditions and boundary fluxes should be re-inspected because of some inconsistencies with existing information and because of an insufficient conceptual basis for use of these conditions for applications of the site-wide model at both large and small scales.

- Spatial variability of recharge should be treated geostatistically to determine expected values, spatial correlation, and estimated uncertainties.

5) With regard to collection of new data:

- The Panel believes that it is premature to initiate a campaign to collect new data. The highest priority is to adopt a broader modeling framework that accepts conceptual model uncertainty. Within this new framework the site-wide model would serve as an important tool to help guide new data collection efforts. First, the degree of likely impacts of the various sources of uncertainty can be assessed through analysis of all uncertainties including those introduced by alternate conceptual models. Second, the worth of new data for reducing costs and risks can be evaluated. Only then can the issue of additional data collection be logically addressed.

- The integration of the site-wide model with a geographic information system (GIS) is an excellent means to preserve the site data for applications at a variety of spatial scales. The Panel recommends that both *data-bases* (original field measurements) and *information-bases* (interpretations or interpolations) be maintained. For example, details in well logs found in the data-base could be used to develop a geostatistical model for scales smaller than that found in the interpreted hydrogeologic facies information-base.
- The Panel recommends that the site-wide groundwater model be thought of as a flexible and evolving platform for analyzing groundwater flow and contaminant transport. The model itself must not be stagnant because, as more data are collected, it is likely that the conceptual model of the groundwater system will change. In addition, new predictive capabilities undoubtedly will be desired. The adopted model framework must be one in which new concepts can be tested and enhancements readily included. It must have the capability of being modified to test alternative conceptual models, reflect the most recent consensus conceptual model, and address differing concerns regarding water resources and water quality.

Introduction

This report is the product of a peer review of the Proposed Hanford Site-Wide Groundwater Model by a panel of three external reviewers who have been contracted by Pacific Northwest National Laboratory (PNNL) on behalf of the US DOE Richland Operations Office (DOE/RL). The external panel members are Dr. Steven Gorelick, Stanford University (Panel Chair), Dr. Charles Andrews, S.S. Papadopulos and Associates, Inc., and Dr. James Mercer, HSI GeoTrans, Inc. The charge of the Panel was to review the Proposed Hanford Site-Wide Groundwater Model and specifically address three questions:

1. Is the conceptual model and technical capabilities embodied in the numerical implementation of the proposed site-wide groundwater model adequate to meet the anticipated needs, requirements and uses for the Hanford Site?
2. If not, what model refinements/modifications or alternative conceptual models should be investigated to further improve the conceptual model and its numerical implementation to meet the anticipated Hanford Site needs, requirements, and uses?
3. Are there major conceptual model, parameter, and data uncertainties that can and should be resolved by collection of additional data and information in order for the proposed model to be adequate for Hanford Site needs, requirements, and uses?

The Panel reviewed the documents listed in Appendix A and met on November 20, 1998 with representatives of DOE, PNNL, Washington Department of Ecology, and the Yakima Indian Nation. Presentations were made on the Site-Wide Groundwater Model and briefly discussed (see Appendix B for the meeting agenda). The scope of the Panel's work includes a follow-up meeting within the next year, after PNNL's response to this report.

Definitions and Understanding of Panel

The following concepts are defined and used by the Panel in this report:

- **Site-wide groundwater model** (SGM) is the application of the CFEST-96 code to the conditions at the Hanford Site for prediction of steady-state and transient saturated flow in 3D and dissolved-phase transport of contaminants of concern.

- **Anticipated uses, needs, and requirements** for the SGM are defined in two parts as:

  Anticipated Uses -- The SGM would be applied to a range of problems including: current and near-term impacts of operations facilities and proposed waste-disposal facilities; planning, design, and evaluation of remediation strategies including monitoring, natural attenuation, hydraulic control/containment, and contaminant removal/cleanup; long-term performance assessment involving risk assessment and management; and assessment of site-wide cumulative environmental impacts.

Anticipated Needs and Requirements -- To meet these anticipated uses, the SGM needs to have the capability to interface with vadose-zone models of flow and transport; risk assessment models; specialized, high-resolution, local-scale simulation potentially involving reactive chemical processes, and perhaps more sophisticated models of surface-water – groundwater interactions (both hydrologically and chemically). Thus, the SGM must be applicable to different problems involving a wide-range of processes and complexity. Furthermore, the SGM must handle disparate spatial scales extending from local facility areas to regional site-wide, and temporal scales ranging from less than 1 day to 10,000s of years.

- **Alternative conceptual models** are different constructs of the geometry of the model domain, number and configuration of hydrogeologic units, hydrologic and chemical stresses, initial conditions, boundary condition types and values, as well as processes that control the behavior and response of groundwater flow and contaminant transport. Each alternative construct is a conceptual model.

- **Numerical implementation** is the translation of a conceptual model into the input data for a numerical code, CFEST-96.

- A **sub-model** of the SGM is an application of the CFEST-96 computer code in which the spatial discretization is reduced in a sub-region of the area modeled in the SGM to allow for the more precise definition of hydraulic and contaminant sources and sinks, and/or to allow for the more accurate solution of the governing equations. The hydraulic boundary conditions for the sub-model are calculated either explicitly or implicitly from the SGM. A **specialized local model** is the numerical implementation of a conceptual model other than that used in the SGM to simulate groundwater flow and contaminant transport in a sub-region of the area modeled in the SGM. The hydraulic boundary conditions for a specialized local model are calculated explicitly from the SGM. An example of a specialized local model would be a reactive-chemical transport model developed to simulate chromium behavior in the vicinity of a reactive wall.

Review Comments on Questions Posed by PNNL to Panel

Question 1:

Is the conceptual model and technical capabilities embodied in the numerical implementation of the proposed site-wide groundwater model adequate to meet the anticipated needs, requirements and uses for the Hanford Site?

Given the broad anticipated needs, requirements, and uses as defined above, the Panel concludes that the SGM is inadequate at this stage. No single model may be adequate for all of the anticipated needs and uses.

Question 2:

If not, what model refinements/modifications or alternative conceptual models should be investigated to further improve the conceptual model and its numerical implementation to meet the anticipated Hanford Site needs, requirements, and uses?

Conceptual Model

The modeling framework for the SGM does not acknowledge that the physical and chemicals processes, internal 3D structure, flow and solute stress locations and magnitudes, 3D initial conditions, 3D boundary conditions, field data, and model parameter values are not known and cannot be known with certainty. Therefore, predictions of heads and concentrations in 3D over time will be uncertain as well.

The Panel recommends that:

1. The concept of uncertainty be acknowledged and embraced from the outset. A new modeling framework should be established that is stochastic rather than purely deterministic. Both the expected values of heads and concentrations as well as the range (distribution) of predictions should be products of the model.
2. Each type of application of the SGM will have different requirements depending on the consequence of uncertainty in predictions.
   - To assess the relative importance of uncertainties due to alternative constructs of processes, features, stresses, and parameter values, hypothesis testing and sensitivity analysis can be used to evaluate the likely range of predictions.
   - For cases in which the only significant source of uncertainty is the estimated model parameter values, then Monte Carlo analysis or first-order analysis of uncertainty on the parameter values alone can be used to determine the expected value of the prediction and its uncertainty.

- If uncertainties due to alternate constructs are significant, then a full Monte Carlo analysis is required to estimate the uncertainty of predictions.

3. Alternative conceptual models should be developed and investigated. Some examples are:

   - The effects of larger-scale regional flow on the Hanford Site-Wide Groundwater Model domain, including flow through the basalt, flow through faults and fractures, and vertical flow through the lower boundary
   - Chemical processes in both the aqueous phase and between solids and water
   - The existence of immobile-domains and solute movement via diffusive mass-transfer (kinetics)
   - Evapotranspiration (for example, at West Lake and other areas where the water table is near the land surface or along the river)
   - The existence of non-aqueous phase liquids
   - Focused recharge
   - Boundary conditions and values (e.g., inflows and their consistency with stream flow measurements, or impermeability of the lower boundary).

   The importance of these and other conceptual model features must be evaluated before assuming that uncertainty in hydraulic conductivity is the only source of uncertainty in predictions.

Because these are just a few examples, the Panel believes that a priority item is to construct a comprehensive list of alternative conceptual model components and assess each of their potential impacts on predictive uncertainty. One method of assessment is hypothesis testing within the framework of the existing SGM. Tools that will aid in this hypothesis testing include water-balance calculations, particle tracking, and sensitivity analysis. If these tools are inappropriate to evaluate the impact of any particular source of uncertainty on predictions, then Monte Carlo analysis is recommended.

Numerical Implementation

The recommended modifications and refinements of the numerical implementation include:

Model calibration
Representation of contaminant chemistry
Boundary conditions
Boundary fluxes
Recharge
Dispersivity (and mixing versus spreading)
Effective porosity versus specific yield
Storage coefficient values
Subscale spatial variability
Representing diffusive mass-transfer

Measured (versus observed) heads and concentrations
Initial conditions in 3D
Interfaces and output needs
Flexible model framework.

Following is a brief discussion of each recommendation.

Model calibration:

The calibration process and consequent estimates of hydraulic conductivity are not defensible. Reasons for this are the following:

1) Parameter estimation was based on the selection of a single snapshot of hydraulic heads in 1979 that was assumed to represent steady-state conditions. Given the transient nature of areal recharge and source fluxes from disposal of wastewater, this approach is questionable. Further work should aim to justify this assumption and/or to perform a transient calibration.

2) The zonal parameterization of transmissivities resulted in 262 parameter values that were estimated. The data used in the inverse procedure considered 217 hydraulic heads and 52 local estimates of transmissivity. This is a clear example of over-parameterization. Resulting transmissivity estimates lead to simulated heads that match observed heads, but the predictive value of the model is low.

3) Hydraulic conductivities for each of the model layers were calculated based on transmissivities estimated from a 2D model of the entire unconfined aquifer. The panel believes that, in general, hydraulic conductivities in a 3D model should be estimated using a 3D inverse model. Short of 3D estimation, an assessment must be undertaken regarding the use of detailed stratigraphy and "text-book value" hydraulic conductivities as the basis for disaggregating transmissivities for a 2D unconfined aquifer into hydraulic conductivities in 3D.

4) The head data used in the inverse model were, in fact, not head data. Rather, they were interpolated values at model node locations. These interpolated values carry a bias. The parameter estimation procedure provides two pieces of information: the parameter estimates and the covariance of these estimates. When the "data" used in the inversion process are values interpolated at all nodal locations, the covariance of the parameter values is artificially reduced and the estimates are unreliable. That is, the creation of data through interpolation leads to biased estimates of model parameter values and artificial estimates of model parameter uncertainty.

5) The Panel is also concerned about the effect of using transmissivities from wells that are partially screened in the aquifer to serve as observed transmissivities for the entire thickness of the alluvial aquifer. An additional concern is the selection of weights used in the matching procedure for heads and transmissivities.

6) Within the framework suggested earlier, parameter uncertainty estimates are an essential part of the model and its ability to provide an expected range of predicted values. Proper parameter estimates and parameter uncertainty estimates (covariances) should be developed and used to assess the uncertainty in predicted heads and concentrations.

Representation of contaminant chemistry:

The site-wide model is capable of representing transport of individual non-interacting solutes undergoing first-order decay and linear sorption. First-order decay is appropriate to represent radioactive decay, and may be appropriate for representing simple degradation processes. These processes are a small subset of all possible chemical processes, and may not be adequate for some compounds of major concern at the Hanford Site. As it stands, the responsibility for the use of the limited chemistry in the SGM to simulate a particular contaminant rests on the model user.

The use of K_ds is an engineering approach to represent the retardation of contaminants due to sorption. Such an approach restricts the use of the model for prediction of the behavior of the majority of contaminants of concern at the Hanford Site. For applications involving the migration of tritium through the aquifer, the chemical processes in the SGM (decay and no sorption) are adequate. For other contaminants, such as carbon tetrachloride, the model may provide reasonable predictions if no volatilization occurs, water quality is nearly constant, and the chemistry can be represented by first-order decay and linear sorption. In any application of the SGM, justification of the engineering approach to retardation is needed.

Boundary conditions:

The locations and types of boundary conditions specified in 3D over time must be re-inspected. In general for large-scale applications to the Hanford site, the specified head boundary corresponding to rivers is adequate. However, the use of a specified head along the Columbia River may be inadequate for small-scale sites near the river or for short-term analyses potentially affected by the river. For example, the observed and predicted water levels for 1996 near the 100-B, C Area indicate flow directions that are at right angles to each other. In such cases, time-dependent heads and/or head-dependent fluxes should be considered. The specified head boundary along the Yakima River may be better represented by a head-dependent flux for some cases.

Boundary fluxes:

Assuming that the locations of lateral boundary fluxes are reasonable, there is an inadequate conceptual model of the existing boundary fluxes. Based on the map of recharge values used during calibration and the locations of Gable Butte and Gable Mountain, significant internal boundary fluxes apparently exist and are not considered in the active model domain. Similarly, fluxes along the western boundary are non-zero only along a small portion. Given the large drainage area in the Rattlesnake Hills and associated mountain area, some rationale must be supplied for assuming no-flow conditions, and/or those boundary fluxes must be reconsidered. Stream flow in upstream reaches of Dry Creek and Cold Creek are a likely lower boundary on underflow from these areas. A comparison of upstream stream-flow values and boundary fluxes is needed; for example, the 1997 USGS estimates of recharge from the creeks to the alluvial system are lower than values used in the calibrated model. A uniform 3D distribution of values along each flux-boundary was assumed. Some rationale for this distribution is needed, or these values must be redistributed in a less arbitrary manner. Along the western boundary it appears that boundary fluxes may in fact be leakage from Cold and Dry Creeks within the Hanford Site, in which case most of the flux should be apportioned to the upper part of the aquifer.

The no-flow boundary between the basalts and the alluvial material at the base of the model may not be appropriate for areas of increased vertical permeability such as in the area northeast of the 200-East Area and in known or suspected fault areas. Further documentation of the justification for the treatment of the lower boundary throughout the domain needs to be provided. Such documentation should begin with the conceptual model and should include a water balance that accounts for flow in the basalts.

Recharge:

Areal recharge is potentially the dominant source of water to the aquifer. The spatial distribution of recharge appears to have varied greatly in the past. As such, it is unclear how simulation of future events should represent this distributed water flux. The recharge map constructed by Fayer et al. (1996) is a good starting point to determine an average recharge map and a companion map of recharge uncertainty. Once available, this information can be used in identifying the range of model predictions (mentioned previously). In addition, the Panel recommends that experts at PNNL develop a strategy to represent the spatial distribution of recharge for a range of climatic conditions, consequent vegetation, and antecedent soil moisture conditions.

Dispersivity (and mixing versus spreading):

The selection of dispersivity values based solely on model element sizes and the Peclet number criterion is problematic for the following reasons: 1) Any physical interpretation of dispersivity values is lost. 2) An empirical or theoretical relationship between dispersivity and travel distance scale is not used. 3) The resolution of the mesh dictates the dispersion of the plume. That is, a very fine mesh will result in a simulated plume dominated by advection; this simulated plume will display little lowering of the plume peak as the plume travels and a small degree of spreading. Alternatively, a course mesh will show that as the plume travels, its peak will be greatly reduced and the plume will become elongated.

The transverse dispersivities are unlikely to be 1/5 of the longitudinal dispersivity for all scales of interest. Furthermore, vertical transverse dispersivity values are most likely smaller than the horizontal transverse dispersivity values. Our understanding is that CFEST-96 does not have the capability for specifying different vertical and horizontal transverse dispersivities; we recommend that the code be modified to incorporate this feature.

The Panel recommends that an independent method be used to estimate dispersivity values and that mesh spacing be selected such that the Peclet criterion is met.

It also must be recognized that the concentrations produced by the SGM do not represent local values when using large field-scale dispersivities. If the SGM is integrated with a multi-species interactive chemical module that relies on accurate prediction of local concentrations, then the issue of predicted concentrations due to local mixing (versus those predicted using a macrodispersion-approach) must be addressed.

Effective porosity vs. versus specific yield:

Although the values used for effective porosity and specific yield may sometimes be similar for a given aquifer material, there is no physical justification to base effective porosity values on measured specific yield values. There is considerable ambiguity in the literature regarding the term *effective porosity*. For purposes of the SGM, effective porosity is the quantity by which the seepage velocity must be multiplied to obtain the Darcy velocity. The seepage velocity is the average speed that water travels between two points due to advection. Specific yield is the drainable porosity, i.e., the volume of water that can be drained by gravity from a unit volume of initially saturated porous medium. In general, specific yield represents a much smaller fraction of total porosity than does effective porosity. Effective porosity values must be estimated, and the impact of their uncertainties must be assessed.

Storage coefficient values:

The error introduced by using wrong storage coefficient values may be responsible for some predictive errors. For example, hydrographs for Areas 5, 6, 7, 8, and 9 show an observed pulse of water. This pulse propagates through the subsurface faster and with a higher amplitude than does the simulated pulse of water. This comparison suggests that the storage parameter used in the simulation may be too high, or the hydraulic conductivity may be too small as the rate of propagation of the pulse is related to the ratio of hydraulic conductivity to the storage coefficient.

Subscale spatial variability:

Spatial variability of hydraulic parameters exists at scales smaller than that of the hydrogeologic facies. This small-scale variability may be important to model applications involving specific sites. The geologic data, such as well logs, should be maintained apart from the interpreted hydrogeologic-facies information. Such segregation would enable modelers of particular applications to go back to the data and potentially extract smaller-scale information about fine structures and parameter values. Work is needed to estimate the geostatistical parameters at the sub-hydrogeologic facies scale.

Representing diffusive mass-transfer:

It is noted that in almost all applications of groundwater transport models the simulated plume of a contaminant exhibits much less tailing (late arrival of mass) than is observed in the field. There are a number of processes that can explain the observed tailing, but in many instances the dominant process is diffusive mass-transfer from an immobile domain to a mobile domain. In alluvial sedimentary groundwater systems, the immobile domain may well correspond to zones of lower hydraulic conductivity, such as silt or clay lenses, within an aquifer unit. Experience suggests that, in any situation in which the effective porosity is significantly smaller than the total porosity, transfer to and from an immobile domain likely is important. In these cases, the immobile domain can be thought of as a functionally stagnant volume of water corresponding to the difference between the total porosity and the effective porosity.

The Panel believes that tailing of contaminant plumes is likely to be significant in the unconfined aquifer at the Hanford site. Therefore, the SGM will overestimate the rate at which contaminant plumes migrate and dissipate after a source has been removed because diffusive mass-transfer to and from immobile domains is not considered. The Panel recommends that diffusive mass-transfer be addressed by modifying CFEST-96 to permit the option of including a mobile-immobile domain formulation.

Measured versus observed heads and concentrations:

In much of the previous groundwater modeling work, the predictive value of the groundwater flow and transport models has been evaluated by comparing contour maps of observed data to contour maps of simulated data. The Panel notes that contour maps of observed data are interpretations of data and not the actual data. The Panel strongly recommends that when assessing the predictive value of models, the observed data be compared to simulated data on a point-by-point (well-by-well) basis, and that this comparison is done in an accepted statistical framework (see for example, ASTM D5447-93 Standard Guide for Application of a Ground-Water Flow Model to a Site-Specific Problem).

Initial conditions in 3D:

The vertical extent of the contaminant plumes at the Hanford site is poorly defined, and as a result, the initial concentration conditions for contaminant transport simulations have a large uncertainty associated with them. This uncertainty must be considered in making predictive simulations. In the most recent modeling analysis, the thickness of the contaminant plume was the calibration parameter, and a value of 25 meters was assigned in the calibration process. There are clearly many other uncertain parameters in the SGM, and the calibration of thickness may be meaningless. The Panel notes that one of the reports indicates that the tritium plume in some areas is over 60 meters thick. As noted below, the Panel does not advocate installation of new monitoring wells at this time to better define the vertical extent of groundwater contamination. Even with a large number of wells to monitor the vertical distribution of contaminants, uncertainty associated with the vertical definition of contaminants will exist due to the large size of the Hanford site and the complexity of the stratigraphy. Therefore, the SGM framework must have a method for dealing with this uncertainty.

Interfaces and output needs:

Selected Computer Code

An important factor in the selection of CFEST-96 was the availability of the source code. The Panel agrees that this is an important criterion. The implementation of the SGM by groups other than PNNL requires the use of CFEST-96 as well as supporting codes, such as GEOFEST. It is important that the suite of codes (i.e., simulation model, inversion model, GIS, and data translators) be available, their interaction be documented and to a certain degree be user friendly.

The Panel concludes that CFEST-96 is an appropriate computer code to use for the site-wide groundwater model for a subset of the anticipated uses. The Panel notes though, that there are several other computer codes that would also be appropriate for the SGM. There is currently a large knowledge base at DOE/RL on the application of CFEST-96, and an automated system has been developed to create input files from the hydrogeologic databases and to process the output files from CFEST-96. Given that a large investment has already been made in the application of CFEST-96 and that the code has many of the required capabilities, it is sensible to use this code. The Panel has noted some changes that would be useful in the CFEST-96 code (such as the ability to use both horizontal and vertical transverse dispersivities and the ability to simulate mobile-immobile domain mass-transfer). The Panel has assumed that making these changes in CFEST-96 would be relatively straightforward.

The Panel is concerned that a high degree of specialized knowledge will be required to use the SGM (and CFEST-96). As a result, regulators, tribal nations, and other stakeholders may not have the expertise to use the SGM. The Panel recommends that DOE/RL provide training workshops on the use of the SGM, including the use of pre- and post-processors. The Panel has assumed that model source and executable codes, and all model-input files will be made available to concerned parties.

A vision for the SGM is the use of the simulated groundwater contaminant concentrations and contaminant fluxes as input data for other computer analysis programs (for example, risk assessment programs). The Panel believes that the output format is sufficiently well documented and flexible that simple computer programs can be developed to provide the linkage with other analysis programs. Development of the SGM at this stage should provide for easy access to output of simulated head and contaminant values and fluxes over space and time.

Sub-Models of the SGM and Specialized Local Models

The SGM is an appropriate tool for analyzing groundwater flow and contaminant transport on a large scale. For addressing many issues that involve groundwater flow and contaminant transport on a smaller scale, it may be appropriate to use a sub-model of the SGM or a specialized local model. In either case, the SGM can be used to define hydraulic boundary conditions for a model of the smaller-scale problem. The Panel recommends that pre- and post- processors be developed, if they do not already exist, so that it is relatively easy to create sub-models of the SGM and to create the hydraulic boundary conditions for specialized local-scale models. It is difficult to anticipate requirements of the specialized local models, but it is important that thought be given to how they might interface with the SGM.

For the development of specialized local models it is essential that an up-to-date, easy to use geologic database be maintained. In models of small regions, it is very likely that the appropriate number of hydrogeologic units will differ from that defined in the SGM. The geologic database will be needed to define these hydrogeologic units on a refined scale.

The Panel anticipates the specialized local-scale models will be developed primarily to analyze the migration of contamination whose behavior in the subsurface cannot be simulated accurately with first-order decay and linear sorption. In some cases, where there is a significant inventory of the contaminant in the vadose zone, coupled unsaturated-saturated models of small regions may be required to answer the questions posed. Specialized local models may also be developed for areas where short-term transient effects, such as variations in river stage, are important.

Flexible Model Framework:

The Panel recommends that the modeling framework for the SGM permit evolving sophistication of groundwater flow and contaminant transport. The SGM must not be stagnant because as more data are collected, it is very probable that the conceptual model of the groundwater system will change. The framework must be setup so that modifications are possible to test alternative conceptual models and to properly reflect the current consensus conceptual model.

Question 3

Are there major conceptual model, parameter, and data uncertainties that can and should be resolved by collection of additional data and information in order for the proposed model to be adequate for Hanford Site needs, requirements, and uses?

It is expected that reports such as this will conclude with the statement, "more data are needed." The Panel has elected to avoid such a recommendation at this time for two reasons. The first is the inability to judge the relative importance and impacts of alternate model constructs on predictions and predictive uncertainty. The second is, given its limited scope and mission, the Panel is unable to appraise the degree to which existing historical data (such as hydraulic heads and concentrations in 3D, information on boundary fluxes, and hydraulic test results) have been assembled and interpreted. The highest priority is to address the conceptual model uncertainty and model implementation issues described previously in this report. Then, within the model uncertainty framework the SGM would serve as an important tool to help guide new data collection efforts. Once the degree of likely impacts from the various sources of uncertainty is assessed, the worth of new data to reduce costs and risks can be evaluated, and the issue of additional data collection can be logically addressed.

The use of a GIS is a valuable approach to consolidate data and information used for model input and should be continued. The Panel encourages the project to distinguish between *data-bases* and *information-bases* in the GIS. For example, a contour map of head measurements is an example of an information-base while the data themselves are part of a data-base. Well logs would be components of a data-base, while hydrostratigraphic interpretations are part of an information-base. This distinction is important because certain analyses must rely on the data and not the information, and vice versa.

Conclusions

This Review Panel has addressed three specific issues: a) adequacy of the conceptual model and its technical capabilities to meet the anticipated uses and needs, b) possible improvements to the modeling framework / implementation, and c) immediate new data needs.

The Panel has unanimously agreed that:

1. The concept of developing a broadly applicable site-wide groundwater model is excellent. Scientists working for the U.S. Department of Energy – Richland Operations Office have made significant progress and should be commended for their efforts in dealing with voluminous data, complex field conditions, and integrated/interdisciplinary approach to model building.

2. With regard to the issue of model adequacy, the spectrum of anticipated uses and needs is so broad -- ranging from time scales of less than 1 day to thousands of years and spatial scales of meters to kilometers -- that this or any general-use site-wide model cannot be expected to be adequate for all potential uses. An initial task should be to specify a narrower, and perhaps more pragmatic, list of model uses that involve less disparate temporal and spatial scales and contaminants whose behavior can be adequately characterized by linear sorption and first-order decay.

3. With regard to improvements in the modeling framework:

   - The existing deterministic modeling effort has not acknowledged that the prescribed processes, physical features, initial and boundary conditions, system stresses, field data, and model parameter values are not known and cannot be known with certainty. Consequently, predictions of heads and concentrations in 3D over time will be uncertain as well.

   - A new modeling framework must be established that accepts the inherent uncertainty in model conceptual representations, inputs, and outputs. Given such a framework the expected values of heads and concentrations, as well as the range (distribution) of predictions, would be products of the SGM.

   - The geometry of the site-wide model must be better justified. The site-wide groundwater model only simulates groundwater flow and contaminant transport in the unconfined sedimentary aquifer in the Pasco Basin south and west of the Columbia River. The unconfined aquifer to the north and east of the river and the bedrock basalt aquifer are not represented in the site-wide groundwater model even though the major discharge area for both aquifers is the region adjacent to the Columbia River.

- A priority item is to construct a list of alternate conceptual model components and assess each of their potential impacts on predictive uncertainty.
- Assessment can be initiated with hypothesis testing and sensitivity analysis within the general framework already established with the existing site-wide model. If uncertainties due to alternate conceptual models are significant, then a Monte Carlo analysis is required to estimate both the expected value of the prediction and its uncertainty.

4. With regard to improvements in model implementation:

   The Panel targeted a series of important improvements to the current site-wide modeling effort. A few of the most important ones are listed below.

   - The current model calibration procedure is not defensible. Reasons include the insufficient justification for using a single snapshot of presumed steady-state conditions in 1979, over-parameterization of zonal transmissivities given an insufficient number of independent data, potential for incompatibility between pump-test results and model representation of the aquifer, 2D model calibration for a 3D model, and use of interpolated head values.
   - The existing representation of chemical reactions is limited to first-order decay and linear sorption. Although potentially adequate for some of the prevalent contaminants found in Hanford groundwater, for most of the contaminants of concern found in the vadose zone, reactive transport needs to be represented.
   - Boundary conditions and boundary fluxes should be re-inspected given some inconsistencies with existing information and because there is an insufficient conceptual basis for use of these conditions for applications of the site-wide model at both large and small scales.
   - The spatial representation of recharge should be represented as a parameter having an expected value and estimated uncertainty.

5. With regard to new data collection efforts:

   The Panel believes that it is premature to initiate a campaign to collect new data. The highest priority is to adopt the broader modeling framework that accepts conceptual model uncertainty. Within this new framework, the site-wide model would serve as an important tool to help guide new data collection efforts. First, the degree of likely impacts of the various sources of uncertainty can be assessed through analysis of all uncertainties including those introduced by alternate conceptual models. Second, the worth of new data for reducing costs and risks can be evaluated. Only then can the issue of additional data collection be logically addressed.

   The integration of the site-wide model with a GIS is an excellent means to preserve the site data for applications at a variety of spatial scales. The Panel recommends that data-bases (original field measurements) and information-bases (interpretations or interpolations) both be maintained. For example, this would enable details in well logs found in the data-base to be used to develop a geostatistical model for scales smaller than that found in the interpreted hydrogeologic facies information-base.

The Panel recommends that the site-wide groundwater model be thought of as a flexible and evolving platform for analyzing groundwater flow and contaminant transport. The model itself must not be stagnant because, as more data are collected, it is likely that the conceptual model of the groundwater system will change. In addition, new predictive capabilities undoubtedly will be desired. The model framework adopted today must be one in which new concepts can be tested and enhancements readily included. It must have the capability of being modified to test alternative conceptual models, reflect the most recent consensus conceptual model, and address concerns regarding water resources and water quality.

APPENDIX A
DOCUMENTS REVIEWED BY THE PANEL

Chiaramonte, G.R., Denslow, C.W., Knepp, A.J., and others, 1996: **Hanford Sitewide Groundwater Remediation Strategy - Groundwater Contaminant Predictions;** Report prepared for the U.S. Department of Energy, BHI-00469, Rev. 1, September 1996.

Cole, C.R., Wurstner, S.K., Bergeron, M.P., and others, 1997: **Three-Dimensional Analysis of Future Groundwater Flow Conditions and Contaminant Plume Transport in the Hanford Site Unconfined Aquifer System: FY 1996 and 1997 Status Report;** Report prepared for the U.S. Department of Energy under Contract DE-AC06-76RLO 1830, December 1997.

Fayer, M.J., Gee, G.W., Rockhold, M.L., and others, 1996: **Estimating Recharge Rates for a Groundwater Model Using a GIS;** Journal of Environmental Quality, Volume 25, no. 3, , pages 510-518, May-June 1996.

Ford, B.H., 1995: **200-UP-1 Vertical Profiling Activity Summary Report;** Report prepared for the U.S. Department of Energy, BHI-00149, January 1995.

Thorne, P.D., and Chamness, M.A., 1992: **Status Report on the Development of a Three-Dimensional Conceptual Model for the Hanford Site Unconfined Aquifer System;** Prepared for the U.S. Department of Energy under Contract DE-AC06-76RLO 1830, November 1992.

Thorne, P.D., and Newcomer, D.R., 1992: **Summary and Evaluation of Available Hydraulic Property Data for the Hanford Site Unconfined Aquifer System;** Prepared for the U.S. Department of Energy under Contract DE-AC06-76RLO 1830, November 1992.

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Thorne, P.D., Chamness, M.A., Vermeul, V.R., and others, 1994: **Three-Dimensional Conceptual Model for the Hanford Site Unconfined Aquifer System, FY 1994 Status Report;** Prepared for the U.S. Department of Energy under Contract DE-AC06-76RLO 1830, November 1994.

U.S. Department of Energy, 1998: **Preliminary Draft: Recommendations for Selection of a Site-Wide Groundwater Model at the Hanford Site - Volume I - Section 1-8, References;** DOE/RL-98-xxx, October 1998.

U.S. Department of Energy, 1998: **Preliminary Draft: Recommendations for Selection of a Site-Wide Groundwater Model at the Hanford Site - Volume II - Appendices;** DOE/RL-98-xxx, October 1998.

Wurstner, S.K., Thorne, P.D., Chamness, M.A., and others, 1995: **Development of a Three-Dimensional Ground-Water Model of the Hanford Site Unconfined Aquifer System: FY 1995 Status Report;** Prepared for the U.S. Department of Energy under Contract DE-AC06-76RLO 1830, December 1995.

APPENDIX B - MEETING AGENDA

Friday, November 20, 1998

8:00 – 8:05	Opening Remarks	Steven Gorelick, Chair
8:05 – 8:15	Introduction	Doug Hildebrand, DOE RL
8:15 – 8:45	Review of Needs and Requirements	Marcel Bergeron, PNNL
8:45 – 10:00	Review of Proposed Conceptual Model	Paul Thorne, PNNL
10:00 – 10:15	Break	
10:15 – 12:00	Proposed Conceptual Model (continued)	Paul Thorne, PNNL
12:00 – 1:00	Lunch	
1:00 – 1:15	Regulator/Stakeholder Issues	Dib Goswami, Washington State Department of Ecology
1:15 – 3:00	Review of Numerical Implementation of Conceptual Model	Charles Cole, PNNL
3:00 – 3:15	Break	
3:15 – 5:15	Numerical Implementation (continued)	Charles Cole, PNNL
5:15 – 6:00	Open Discussion	

Peer Review Team:

Dr. Steven M. Gorelick, Stanford University, Panel Chair
Dr. Charles Andrews, S.S. Papadopulos and Associates, Inc.
Dr. James W. Mercer, HSI-Geotrans, Inc.