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A Nontechnical Guide to Groundwater Modeling: With Specific Reference to the U.S. Department of Energy's Hanford Site

Natural Resources Defense Council (NRDC)

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About the Author

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1.0 Introduction

1.1 PROJECT BACKGROUND

As part of a 1998 court settlement between the U.S. Department of Energy (DOE) and 39 plaintiffs consisting of nonprofit public interest groups, DOE established a $6.25 million Citizens' Monitoring and Technical Assessment Fund to provide money to nonprofit, nongovernmental organizations and federally recognized tribal governments raising issues related to the nuclear weapons complex. The Fund was established to help those groups procure technical and scientific assistance to perform technical and scientific reviews and analyses of environmental management activities at DOE sites. (See http://www.nrdc.org/nuclear/9812doe.asp).

The administering organization for the Fund is RESOLVE, Inc., a neutral nonprofit dispute resolution organization with special expertise in the environmental arena and offices in Washington, D.C., and Portland, Oregon. The mission of RESOLVE, founded in 1977, is to mediate controversial environmental issues and promote the effective use of conflict resolution in public decision making.

Funds for this project were awarded to the Natural Resources Defense Council under MTA Fund grant 01-014. The Natural Resources Defense Council has in turn engaged Dr. Peter Willing to complete the project.

1.2 PURPOSE OF THIS DOCUMENT

This document is intended to be a practical report addressing groundwater modeling in the U.S. Department of Energy's nuclear weapons complex that will permit community organizations to more effectively oversee and understand DOE environmental cleanup actions. The nuclear weapons program is distributed among 13 major facilities in 10 states and dozens of smaller facilities. The concept here is to focus on the groundwater modeling activities in some of the cleanup decisions and to suggest how members of the public can ask questions to help them understand the end results. The original intent was to paint a more diverse picture by examining three different facilities, but logistical and resource constraints have limited the inquiry to the Hanford site in the state of Washington. The author hopes that insights gained at Hanford will be applicable elsewhere. The purpose is to produce a guide that will help an informed and motivated member of the public understand a report on a technical modeling exercise and understand the information upon which the originating agency is relying.

This report focuses specifically on understanding the limitations of models that deal with groundwater and transport and fate of underground contaminants, in both saturated and unsaturated conditions. It does not attempt to deal directly with predicted health effects from the contaminants. Results from groundwater or vadose zone modeling cannot be divorced from evaluation of the observational data that are used to feed the models.

The reader will note the use of chemical symbol shorthand in the document. Reference to a periodic table of the elements may be useful to the lay reader; a convenient example can be found at http://en.wikipedia.org/wiki/Periodic_table_%28wide%29. The modern convention for denoting isotopes of radionuclides is used, in which the superscripted isotope number precedes the element symbol. The paper also uses scientific numerical notation accompanied by standard decimal notation.

Sources of information include the written materials cited in the reference section, many of which are available in electronic form. Other sources include numerous individuals who are now working for, or have in the past worked for, the Department of Energy or its contractors or regulators. Information sources also include knowledgeable individuals who have been active observers of the Department of Energy's environmental programs for many years. Unfortunately, the author's attempt to meet directly with key practitioners and users of groundwater models were rejected (Spane, 2006). A compensating circumstance was the opportunity for the author to attend the public sessions of a Review Panel Workshop on Remediation Decision Tools for Central Plateau Operable Units, held in Richland, Washington, on August 9–11, 2006.

2.0 A Groundwater Primer

This section of the report introduces the reader to basic quantitative concepts in groundwater modeling. We do not expect the reader to apply Darcy's Law, solve differential equations, or select appropriate ratios for contaminant mobility. However, the reader and interested citizen will obtain great value by having a basic understanding of the technical underpinnings of this important and evolving science. Two aspects of groundwater behavior greet the beginning student. The first, logically as well as historically, is the movement of water under the earth's surface. The second concerns the transport and fate of groundwater contaminants of various descriptions. A section on each follows.

2.1 GROUNDWATER FLOW

This section covers only the most elemental concepts of groundwater behavior, in lay terms. The curious reader is encouraged to consult various texts such as Freeze and Cherry (1979), Fetter (2001), or Domenico and Schwartz (1990) for more thorough treatment of groundwater flow and contaminant transport.

Most people have a clearer picture of the behavior of surface waters than they do of groundwater. One of the most obvious differences between them is visibility. Streams and rivers are typically more accessible for measurement, monitoring, and sampling. Groundwater is largely hidden except for access in wells and springs. Groundwater and surface water travel at dramatically different speeds. Table 1 illustrates this point.

The two forces of gravity and friction control flowing water systems, whether they be surface or groundwater. The far greater friction in soil and rocks accounts for the large disparity between surface and groundwater flow velocities. In practical terms the effects of gravity on flow velocity is expressed in terms of hydraulic head, or vertical distance over which gravity is operating in a given situation. As is evident from Table 1, water in the ground moves orders of magnitude more slowly than it does in surface streams.

2.1.1 The Saturated Zone

Groundwater behavior is governed by characteristics of the water itself and of the medium through which it flows. These characteristics interact and affect each other strongly. One characteristic of water is fluid density: Salt water, for example, is denser than fresh, and freshwater from a river mouth will float above seawater. Water is more viscous at lower temperature than at higher; this can be appreciated by watching how readily cold water

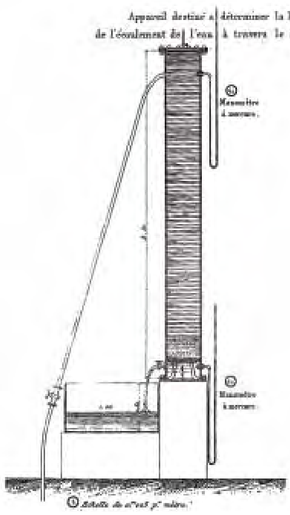
Table 1. Comparison of Flow Velocities in Natural Waters

Condition of Flow	Typical Flow Velocity, Feet per Second
Fast, turbulent river	10–15
Slow, meandering stream	2–4
Intake screen—slow enough to avoid juvenile fish impingement	0.5
Groundwater under steep gradient in coarse gravel	3×10^{-3} , or 0.003
Groundwater under moderate gradient in fine sand	3×10^{-5}, or 0.00003
Groundwater under moderate gradient in silty clay	3×10^{-8}, or 0.00000003

runs out of a frying pan, then heating it up and noting how much “thinner” the water appears. The amount of void space and the grain shape of soil particles affect how quickly water molecules move among them.

Henry Darcy set about defining the relationships among these characteristics in France in the mid-nineteenth century through a series of ingenious experiments and careful observations that became the foundation for understanding fluid flow in porous media.

Figure 1. Henry Darcy’s Experiment



Darcy’s Law can be plainly stated as follows: Flow in a porous medium is equal to the hydraulic conductivity of the medium multiplied by the cross-sectional area of the medium, multiplied by the change in height over the flow path divided by the length of the flow path. In mathematical notation, this becomes

$$Q = -KA\left(\frac{h_a - h_b}{L}\right)$$

where Q = flow volume (units L^3/T, $Length^3/Time$)
K = hydraulic conductivity (units L/T)
A = cross-sectional area of flow cell (units L^2)
ha = initial head (units L)
hb = head at downhill end of flow cell (units L)
L = length of flow cell (units L)

This equation produces a negative value for gradient, which indicates that the flow is from a position of higher head to one of lower head.

As an example, flow through Darcy’s permeameter column in Figure 1 of length 2.5 m and diameter of 0.35 m, loaded with clean sand with an assumed K value of 86.4 m/day and a head difference ha - hb = 0.7 m, would be 2,330 liters per day.

We include this detailed explanation not in the expectation that many readers will attempt to apply Darcy’s Law, but in the hope of encouraging a basic conceptual understanding of the forces that govern fluid movement through earth surface materials.

The range of applicability of Darcy’s Law extends to both saturated and unsaturated conditions; to both steady state and transient conditions; to homogeneous (similar matrix characteristics in all directions) and isotropic (similar void space geometry in all directions) conditions. It applies to laminar flow but not turbulent flow; to Newtonian fluids like water but not fluids such as paints, clay suspensions, debris flows, or cornstarch in water, which sometimes behave as solids.

Table 2. Important Fluid and Medium Characteristics Controlling Groundwater Behavior

Fluid Characteristics	Characteristics of the Medium
Viscosity (resistance to flow)	Porosity (% of void space)
Density	Grain size, shape, packing
Compressibility	Compressibility
Temperature	Permeability (ability to transmit a fluid)
Surface tension	

The unique properties of water account for its role as a solvent or vehicle for transport of groundwater contaminants: It has a polar molecular structure (2 hydrogen molecules, 1 oxygen). The molecule is asymmetrical, which allows hydrogen bonding and makes it a good solvent for polar and ionic compounds (e.g., salts). It exists in solid, liquid, and gaseous phases at earth surface temperatures and pressures. Water's function as a solvent is what makes it significant in terms of transport of solutes, or contaminants.

Groundwater contaminants come in many varieties with different behaviors: There are dissolved (salt) and suspended (mud); there are light and dense nonaqueous phase liquids (LNAPL and DNAPL). Some persist a long time, and others undergo rapid natural attenuation. Contaminants include organic chemicals, inorganics, radionuclides, and biological agents (viruses and bacteria). All are amenable to mathematical modeling.

2.1.2 The Vadose Zone

A key component in understanding groundwater behavior is the vadose zone, or unsaturated zone above the water table. Recharge or replenishment of deep aquifers depends on precipitated moisture (rain or snow) passing through the vadose zone to the water table. In areas where the water table is close to the surface, the vadose zone is less extensive and plays a lesser role in an overall assessment of groundwater flow and contaminant transport. However, in dry areas typical of the intermontane western United States, such as the Idaho National Engineering Laboratory, the Nevada Test Site, and Hanford, Washington, the vadose zone can be hundreds of feet thick and can play a major role. Typically the domain of soil scientists, the vadose zone has been relatively neglected (Fetter, 1994), even though it is a whole field of interest in itself, with its own set of analytical approaches and modeling solutions. For further information, visit the U.S. Geological Survey Toxic Substances Hydrology Program, at http://toxics.usgs.gov/definitions/unsaturated_zone.html; or the Vadose Zone Journal (http://vzj.scijournals.org/), published by the Soil Science Society of America.

2.2 TRANSPORT AND FATE OF GROUNDWATER CONSTITUENTS

Partial differential equations are the basis of many analytical models (see Fetter, 2001, for numerous examples). While they may be somewhat intimidating to the uninitiated, they are a simple and elegant notation for conveying an explicit quantitative relationship among the contaminant, the fluid properties of the water, and the properties of earth in which the water and contaminants move.

In dealing with the movement of contaminants in groundwater, the classical advection-dispersion equation is the starting point. Advection refers to the movement of a solute with the groundwater, at its average velocity. Hydrodynamic dispersion refers to the sum of molecular diffusion, usually negligible, and mechanical dispersion caused by the circuitous routes that individual molecules of solute follow through the grains of a porous medium. The advection-dispersion equation looks like this:

$$\frac{\partial C}{\partial t} = \left[D_x \frac{\partial C}{\partial x} + D_y \frac{\partial C}{\partial y} + D_z \frac{\partial C}{\partial z} \right] - \left[v_x \frac{\partial C}{\partial x} + v_y \frac{\partial C}{\partial y} + v_z \frac{\partial C}{\partial z} \right]$$

To explain this idea of fate and transport in nonmathematical terms, it helps to visualize a representative cube of soil with a volume of 1 cubic centimeter, like the building block of a numerical flow model (see Figure 3). The cell can be much smaller, infinitesimally small in space, and its changing conditions can be analyzed at an infinitesimally small time step. The equation describes two of the processes that are going on in the cell. Note that there are two sets of square brackets, and three terms in each set. The first set of brackets describes the changes due to dispersion, and the second set describes the changes due to advection. The negative second term indicates that the advective flux is from higher to lower concentration. The three terms in each set represent the three dimensions in space, two horizontal dimensions x and y, and one vertical dimension z.

The concentration gradient C/x is the driving force for hydrodynamic dispersion Dx; so that dispersion is proportional to the gradient. The advective change in the x direction is a multiple of the gradient and the velocity. Rendered in words, the equation would read thus: the change in solute concentration C over time t is equal to [the hydrodynamic dispersion coefficient D times the concentration gradient] minus [the velocity v times the concentration gradient]. The effect for each dimension in space is summed in the two major terms.

Again, we do not expect the lay person to solve these equations, but they hold the concepts that provide the technical basis for modeling the transport and fate of contaminants in groundwater.

It is important to remember that this is a simplified formulation. It does not incorporate the effect of solutes reacting with the porous medium, nor the effect of radioactive decay or biological attenuation. The assumptions behind this relationship are: 1) the substrate, or area below ground, is saturated, 2) the flow is steady, 3) Darcy's Law is applicable, 4) the medium is homogeneous, and 5) the coefficients of dispersion do not vary in space. More complicated formulations with additional terms are capable of showing different effects and can dramatically improve modeling accuracy.

In simplest terms, a blob of concentrated solute (e.g., salt or a contaminant) will spread as it moves in the subsurface. It spreads, or disperses, in both longitudinal and transverse directions relative to the main flow direction; it usually stretches out more along the flow path than across it. Some parts of the solute plume move faster than the average velocity of the groundwater seepage, and some slower. This concept is fairly simple, but actual contaminant behavior gets far more complicated. A Michigan State University website (http://www.egr.msu.edu/igw/) has fine contaminant plume visualizations that show these effects on the time distribution of a point source solute.

2.3 CONTAMINANT MOBILITY

Another key concept in groundwater modeling is the mobility of contaminants that may be encountered. The velocity at which contaminants move through earth surface materials is a function of the physical and chemical properties of the contaminant, of the vehicle (usually water), and of the earth materials themselves. Much caution is required in making predictions or inferences from these properties, because there is a wide range of behavior. Contaminants can be adsorbed on, or bonded to the surfaces of, solids, particularly organic molecules. This slows the contaminant plume relative to the movement of the water itself, and spreads it out. If the contaminant is introduced as a blob, it will not remain a blob. Sorption characteristics are expressed as a ratio (Kd) of the amount of a solute to be found in sorbed form on solids, to the amount in dissolved form in water. The higher this ratio, or the Kd value, the lower the mobility of the solute or contaminant, and the slower it will move through the subsurface. In other words, a low value of Kd indicates a relatively mobile solute, and a high value of Kd indicates a relatively immobile one.

Applying the right Kd value for a given groundwater model in a specific situation is an important and often controversial exercise, even within the technical community working on the matter. There is a vast literature (e.g., Environmental Protection Agency, 1999; Grathwohl, 1998) containing empirically derived Kd values under a myriad of conditions, but cautions remain and surprises are possible. Some of the factors that can make reference sorption values meaningless are pH, cation exchange capacity, oxidation-reduction potential of the soil, nonlinearities as the solute concentration increases, presence of other species competing for sorption sites, and colloidal behavior. Radionuclides can sorb onto colloidal particles, which are actually small solids (from 1 to 10 nm) that can move with the water mass. Radioactive decay also produces daughter products. Unlike sorption of radionu-

Table 3. Contaminants of Concern in the Post-Closure Management of Nuclear Processing Facilities

High K_d, Low Mobility	Half-Life	Emission Characteristic
^{241}Am	432 yr.	γ (gamma)
^{60}Co	5.3 yr.	γ, β (gamma, beta)
^{137}Cs	30.1 yr.	γ
^{208}Pb	(stable)	n/a
^{239}Pu	2.4E4 yr.	α (alpha)
Moderate Mobility		
^{90}Sr	29.1.1 yr.	β
Low K_d, Low Mobility		
Cr(VI)	(stable)	–
^{3}H (most mobile radionuclide in groundwater at the Hanford site)	12.3 yr.	β
^{129}I	1.6E7 yr.	x, β
N	stable	n/a
^{237}Np	2.1E6 yr.	α, γ
Se	stable	–
^{99}Tc	2.1E5 yr.	β
^{238}U	4.5E9 yr.	α
CCl_4	stable	–

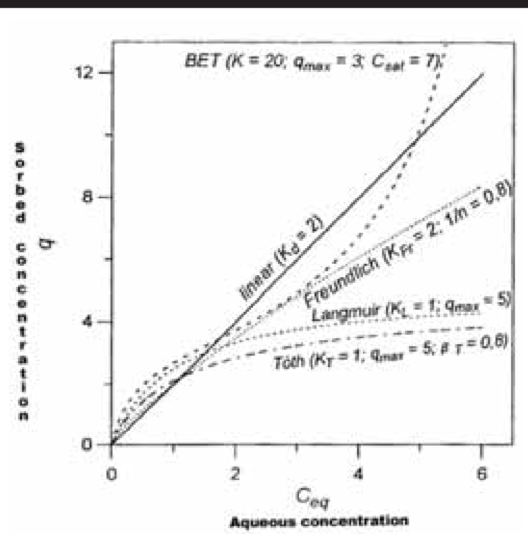
A useful description of the assayability and risk factors associated with the radionuclides in this list can be obtained in U.S. Department of Energy (1998). A list of the 25 chemicals and 46 radionuclides in the Best Basis Inventory may be found in U.S. Department of Energy, 2005, pp. 2–68. Source of mobility ranking: Hanford Contaminant Distribution Coefficient Database and Users Guide, PNNL-13895, Rev. 1 (PNNL 2003a), cited in DQO WMP-28945, Draft A.

clides to immobile rock matrix, radionuclides sorbed onto colloids can sometimes move more quickly than dissolved forms (Ho et al., 1995). The role of sorption behavior in specific contaminant analyses will be further discussed in Section 6.

A rough guide to the relative mobility of common contaminant radionuclides can be useful if the exceptions to it are kept in mind. Table 3 provides such a guide, and also shows half-lives and predominant emission characteristics. Half-life is a measure of how long-lived a radionuclide is; the type of radiation determines whether the ionizing energy can penetrate air, water, earth, steel, biological tissue, etc., and what kind of instrumentation is required to detect it.

This long explanation is intended to give the reader an appreciation of the fact that sorption models are potentially useful but somewhat dangerous; i.e., they are more likely than not to be wrong in any specific situation, and their use has many pitfalls. Often for computational simplicity, a linear relationship between sorbed and aqueous states is assumed even though Kd values are observed to change. The graphical presentation of Grathwohl (1998, p. 20) in Figure 2 shows the difference between linear and nonlinear sorption isotherms:

Figure 2. Sorption Isotherms



Source: Grathwohl, 1998.

The linear sorption isotherm is widely used because it is a simpler computation than the others, and in some situations it causes no difficulty. In complex hydrogeologic and chemical situations, however, caution is warranted. TRW (2000) acknowledges that "the transport of some contaminants…[is] subject to more complex transport phenomena, and other processes for which the linear sorption isotherm approach is inadequate may be affecting contaminant mobility." TRW then notes, "Restriction: For any application of the consolidated site-wide groundwater model, justification of the linear isotherm approach (linear equilibrium adsorption model) to represent the process of adsorption for specific contaminants will be necessary."

The distribution of chemical species or molecular forms among their various physical states—vapor, liquid, sorbed, and solid—is a key determinant of how they move in soils and the vadose zone. Each species behaves in its own characteristic way. To track these behaviors, there are numerous "distribution models" that produce contaminant concentrations based on limited inputs. Some models are nonlinear, some linear (see Figure 2). If one applies a linear model to a chemical that does not exhibit linear response, the predicted relationship can be seriously wrong in some parts of the range of values. RESRAD (for "residual radiation") is a linear model (Yu et al., 2001) that has been adopted as standard for remediation analyses. EPA (1999) warns: "It is important to note that soil scientists and geochemists knowledgeable of sorption processes in natural environments have long known that generic or default partition coefficient values found in the literature can result in significant errors when used to predict the absolute impacts of contaminant migration or site-remediation options. Accordingly, one of the major recommendations of this report is that for site-specific calculations, *partition coefficient [Kd] values measured at site-specific conditions are absolutely essential*" [emphasis in original]. The Kd values reported in the literature for any given contaminant may vary by as much as six orders of magnitude. Further, minute changes in the assumed value for Kd can produce huge changes in the resulting concentrations and travel times. The EPA (1999, p. 107) warns against the tempting but widespread practice of using values that have been obtained from "peer-reviewed" literature and not from the site itself.

3.0 Why Model?

The foregoing discussion laid out the rudiments of groundwater behavior. This section will take up various considerations related to modeling that behavior. There are many persuasive reasons for applying groundwater modeling techniques, not the least of which is that they are the best tools our society has to understand the long-term implications of radioactive and chemical contamination and what they mean for public health and the environment. Modeling is also a key tool for making appropriate decisions in cleaning up contaminated sites. To forgo modeling in present-day hydrogeology practice is to turn one's back on the extremely powerful and versatile tools that have been developed in the past 20 years.

3.1 ADVANTAGES OF MODELING

Rather than take for granted the various benefits of models, it is useful to review them.

■ Modeling can serve to some degree as a substitute for field data. If there are enough field data to establish trends or patterns, model simulations can fill gaps in the existing data.

■ Modeling in pursuit of some kinds of answers is cheaper than field data, which can be very expensive, especially when radioactive wastes are involved.

■ Modeling can be used to extrapolate beyond observational data into time and space domains that are inaccessible (past, future, off-site locations).

■ Obtaining real data may be invasive. Monitoring wells can create preferential contaminant flow pathways and cross-contaminate uncontaminated strata; most monitoring of well construction entails removal of wellbore materials, which may be presumed to be contaminated.

■ Modeling can help the hydrogeologist narrow choices of which additional data to collect.

■ Modeling usually includes sensitivity analysis. The model lets the practitioner understand the interactions and causation among parameters and the effects of varying parameter values, and explore the relative influence of different input parameters on the results (Neuman and Wierenga, 234/158).

■ Modeling is often used to evaluate the effects of remediation measures in advance of applying them in the field.

■ Various hypothetical questions can be answered at least provisionally by model exercises: How long will it take for contaminant x to reach point y? How long will it take for contaminant x to degrade to no-hazard status by radioactive decay, natural attenuation, and so on?

■ Modeling can illuminate anomalies. Contaminants are often associated with each other, and if only one turns up in a sampling regimen, one is prompted to ask where the others went. This may lead the investigator to look for a contaminant plume (EPA, 1993).

■ Models are capable of manipulating large quantities of data and applying complicated calculations. Using computers is the only way solutions can be made efficient.

■ Models can serve as effective communication tools. Modern modeling tools are well developed in the representation of graphical and spatial data. Simple model implementations that are based entirely on reasonable but synthetic or hypothetical data can serve as a valuable heuristic device, to show the effect of assuming different values for important parameters such as hydraulic conductivity. Models make it easy to play what-if games with considerable flexibility.

3.2 PITFALLS OF MODELING

While acknowledging the powerful importance of groundwater modeling, we should also examine the serious pitfalls in the practice of modeling groundwater contamination. The following come to mind:

■ Because modeling can serve as a substitute for field data, it is tempting to resort to the use of models with thin, inappropriate, or nonexistent data to support the model's conclusions and subsequent decisions that can affect public health and the environment for generations to come. The results can often be ridiculous, dangerous, or worse.

■ There is ample opportunity for delusion of the audience (including the modeler) with the appearance of reality that comes out of the model.

■ Models take on a life of their own, and resistance builds toward developing an alternate reality that may be closer to the truth. Money is spent, institutional positions become fixed, and those who have the largest stake do not want to hear a different story.

■ It is extremely difficult for the layperson to comprehend the complexities of the modeling process and output. These complexities are not accessible to a wide audience unless the modeler has bent over backward to make them so.

4.0 What Do Groundwater Models Look Like?

There is no typical model of groundwater behavior. The variety is limited only by the modeler's imagination. The present-day groundwater modeling scene is international in character and very dynamic, with many smart people always thinking of new ways to skin old cats. To describe this scene is to deal with a mobile target, and to offer at best an unsatisfying, static picture at a single point in time. One does not find any comprehensive, up-to-date catalogs. If such a thing existed, it would have thousands of entries and would change on a weekly basis. Every issue of the technical journals has some new idea or refinement. What all this effort has in common is the search for a workable, practical abstraction from reality that lets the modeler understand that reality.

Neuman and Wierenga (2003, p. 21) observe, in a benchmark paper for the Nuclear Regulatory Commission,

> Whereas numerical simulation codes are often referred to as "models," we avoid such usage of the term on the understanding that they are tools rather than models. To transform simulation codes into models, one must apply them to particular hydrogeologic circumstances that represent either a hypothetical or a real setting.…A hydrogeologic model thus consists of a conceptual and a mathematical component… [and] relatively little attention has been devoted to the conceptual component.…In most mathematical models of subsurface flow and transport, the conceptual framework is tacitly assumed to be *given, accurate and unique. All three premises are challenged* by the strategy in this report (emphasis supplied).

A key EPA report lists 76 chemical reaction models that are discussed in the literature. Commenting on the number of available models, it says, "Typically the more general and comprehensive a geochemical code is, the more difficult and costly it is to use. Another factor may be that scientists are inherently reluctant to use any computer code that they and their immediate coworkers have not written" (EPA, 1999, p. 113). Given the kinds of people working with groundwater models and the environment in which they work, it is not surprising that model evolution would be divergent rather than convergent and would favor increasing diversity.

4.1 KINDS OF GROUNDWATER MODELS

Taking a more inclusive and commonly accepted definition of models than Neuman would permit, we can list some types of models that interested citizens will encounter as they explore these issues.

Physical: Henry Darcy's permeameter is the prime example for hydrogeologists (See Figure 1).

Simplistic: Among these is the Calculated Fixed Radius model, a simple equation that can be solved on the back of an envelope.

Conceptual: A conceptual model is based on what is known of the geologic setting: rock, clay, sand, flat, steep, dry, saturated. One conceptual model description takes 22 pages, in the report on the Hanford site-wide groundwater model (TRW, 2000).

Analytical: These consist of mathematical equations that attempt to behave like nature. They are often based on partial differential equations. Darcy's Law is among the simplest analytical models.

Analog and electrical: These models are based on similarities between the flow of water in porous media and the flow of electricity in a conductor. Electrical models consist of networks of resistors and capacitors to represent an aquifer (Fetter, 2001, p. 515).

Numerical: Spatially distributed parameter values such as hydraulic conductivity vary in space over a model domain. They define a time domain long enough to represent a problem of interest and define a space domain that reflects the heterogeneity of the problem. The model makes an overlay grid or net, with characteristics assigned to thousands of nodes or cells. Obviously a computer is needed to do all the calculations.

Stochastic: Fetter observes that the mathematics of statistical models is daunting to those not conversant

Table 4. Wellhead Delineation Models

CFR	Calculated Fixed Radius. Based on withdrawal rate, aquifer saturated thickness, modeling period, and estimated porosity. Assumes identical aquifer characteristics in all directions, and symmetrical radial flow toward the wellbore.
Conceptual	Qualitative description of soils, geology, and probable direction of flow based on topography and understanding of surficial geology.
Analytical	Example: WHPA (EPA, 1993b). Two-dimensional steady-state model for delineating capture zones for wells.
Numerical	Example: MODFLOW. Flexible grid structure. Input parameters estimated for all grid cells. Replicates heads. Requires calibration to observed head values, validation with independent data set (see Appendix B for details).

A common groundwater problem is the need to define the capture zone, or tributary area of land surface, that contributes recharge to a well. This problem is a necessary step in delineating a wellhead protection zone for the management of potential contaminant sources on the surface. It is the first step in groundwater source protection. The examples in this table span a wide range of complexity, cost, and accuracy of result.

with it, but the field is growing fast. Stochastic models are founded on the notion that there is a probability distribution to parameters of interest, such as hydraulic conductivity; deterministic models concentrate on single values for those parameters.

■ Fractured vs. porous media: Models differ as to the type of physical environment they attempt to illuminate. Geologists differentiate two big families and reach a fork in the road when they have to choose between flow in fractured rocks and flow in porous media (See Diodato, 1994).

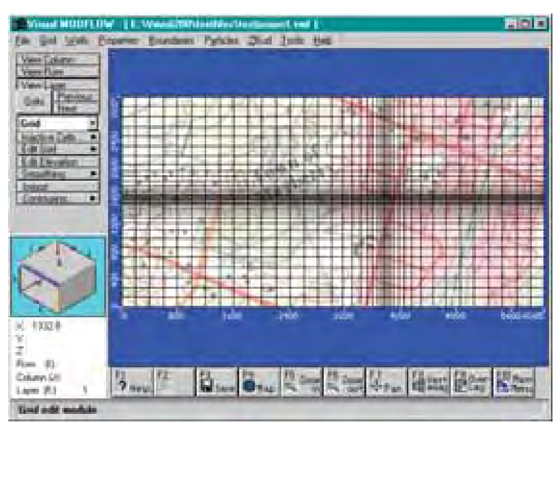
■ Saturated zone vs. vadose zone models: Water and its solutes do not behave the same way in saturated media as they do in dry or partly saturated media. Here is another fork in the road.

■ Solution methods: Among numerical models, there are a variety of solution methods, two of which are finite difference and finite element designs. The subject goes beyond the current treatment; see Fetter, 2001, chapter 13 for an introduction.

Each of these model types is conceived to deal with some aspect of groundwater behavior. The first question the investigator has to define is “What specific behavior are we trying to understand?” Delineation of a wellhead capture zone, or zone of contribution, is a common groundwater modeling problem. The available solutions offer a good example of a range of model complexity. Table 4 shows a progressively more rigorous set of modeling approaches to the basic question of where the water supplying a particular well comes from.

Computer-based numerical models typically define a model domain and discretize it by dividing it into a waffle-shaped grid. The model solves a set of equations for each cell, or node, in the grid. Figure 3 shows an illustration from Visual MODFLOW. The curious connoisseur of technical documents coming out of the Department of Energy will encounter references to the groundwater or vadose zone models that supported the work. Appendix B shows a small selection of common ones.

Figure 3. Visual MODFLOW



Source: Visual MODFLOW produced image from Waterloo Hydrogeologic inc. - A Schlumberger Company.

4.2 SOURCES OF GROUNDWATER MODELS

Many computer-based groundwater and vadose zone modeling programs are available over the Internet. These sources also provide access to online technical literature, demonstrations, and applications of groundwater models. Many of the actual operating programs are open source and available without charge. A selection appears below.

- The EPA website http://www.epa.gov/ada/csmos/models.html has some 30 models listed, with downloadable versions of the software.
- A U.S. Geological Survey website has descriptions and downloads of approximately 35 models or sub-models (http://water.usgs.gov/software/ground_water.html).
- The U.S. Department of Energy maintains an Energy Science and Technology Software Center where certain government-developed software programs can be obtained (http://www.osti.gov/estsc/index.jsp).
- The Colorado School of Mines hosts the International Groundwater Modeling Center (IGWC), which has software/model reviews by practitioners (http://www.mines.edu/igwmc/).
- The University of California Cooperative Extension Groundwater Hydrology Program at the Davis campus sponsors basic and applied research in hydrogeology, and operates an extension program supporting all levels of government with educational and technical resources. The "materials" page has dozens of links differentiated by subject area, e.g., vadose zone modeling, groundwater modeling, chemical databases (http://groundwater.ucdavis.edu/gwmodelingcourse.htm).

4.3 SEQUENCE OF MODELING STEPS

Despite the wide variation among models, each requires a sequence of generic steps. The International Atomic Energy Agency (2002) outlines, in the context of the proposed Yucca Mountain geologic repository for high-level radioactive waste and spent nuclear fuel, a sequence of steps to develop and prove up a conceptual hydrogeologic model of the area:

1. Determination of the boundaries of the system
2. Description of the major lithologic facies in the domain, with their geometry, major properties, measured heads, etc.
3. Estimation of the recharge and discharge fluxes
4. Development of a numerical model of the complex system
5. Calibration of the model using all existing data
6. Sensitivity studies. It is implied that if some of these steps are left out without strong justification, there is a weakness in the process. Zheng and Bennett (2002) are more emphatic: No mathematical model can resurrect a faulty conceptual model—for example, a conceptual model that hypothesizes two aquifers instead of one, or vice versa.

The challenge of producing useful model results is daunting because of the complexity of behavior and environments one wants to model: volatile organics, fuels, explosives, metals, LNAPLs (light nonaqueous phase liquids), DNAPLs (dense nonaqueous phase liquids), bioremediation depending on microbial activity, fractured bedrock. It is no wonder that there is an occasional expression of doubt that useful results can be achieved (EPA, 1993).

5.0 Common Modeling Concepts

As one dives into the literature of groundwater modeling, or perhaps into a technical work on a specific application of it, several concepts are likely to rise to the surface with the assumption that the reader knows what is being discussed. It is useful to provide an introduction to these related ideas: "calibration," "contouring," "kriging," "uncertainty," "Monte Carlo simulation," and "inverse modeling." Site-specific applications of these concepts will be described in the case studies below.

5.1 CALIBRATION, VERIFICATION, AND VALIDATION

Calibration is the process of adjusting the input parameters of a model until the model reflects to some acceptable degree of accuracy the physical situation it is intended to represent. Calibration of a groundwater model begins with initial estimates of boundary conditions and parameters—for example, hydraulic conductivity, porosity, etc.—and proceeds to adjustment of the parameters to bring the model into satisfactory agreement with observed data, such as hydraulic heads. Verification of a model consists of applying it to a set of input data separate from the set used for calibration. If the model as calibrated can reproduce a new set of observations, it may deserve acceptance as a satisfactory representation of reality. Validation means that the model has been shown after the fact to be capable of accurately predicting future conditions.

5.2 CONTOURING AND KRIGING

Contour mapping of contaminant distribution, or mapped lines of equal values, is often used to portray contaminant plumes. It behooves the reader to ask how the contours were generated, and what assumptions are hidden from view. Were the contours based on observation, or were they generated by a model using synthetic (manufactured) data? Kriging is a common geostatistical estimation technique used for contouring. It was developed to predict gold concentrations in the mines of South Africa. It takes randomly spaced data on a geologic condition of interest and interpolates it to produce values between the sampled locations. It then smooths the lines according to user preferences. For instance, given a series of points with known mineral concentrations, kriging can estimate concentrations at points with no observations. It does so through linear least squares estimation. One important point for the reader here is that *it makes a lot of difference to the result whether there are enough reliable data points, and which ones are used in the analysis*. We will return to this point later.

A key assumption in a kriging exercise is the choice of variogram model, which is the engine of the operation; the variogram controls how the model deals with heterogeneity in the model domain, and specifies the statistical model that describes the data to be contoured, analyzed, etc. For example, two sample locations along a buried stream channel will experience a greater degree of similarity than two locations the same distance apart across the channel. Further explanation of kriging is provided by Golden Software (2002):

> The development of a variogram model for a data set requires the understanding and application of advanced statistical concepts and tools; this is the science of variogram modeling. In addition, the development of an appropriate variogram model for a data set requires knowledge of the tricks, traps, pitfalls, and approximations inherent in fitting a theoretical model to real world data: this is the art of variogram modeling. Skill with the science and the art are both necessary for success.

The field of geostatistics is a realm of its own. See the website of the European Commission's Institute for Environment and Sustainability (http://www.aigeostats.org/). It has useful answers to common questions, references, and a forum.

5.3 TREATMENT OF UNCERTAINTY

How to handle various kinds of uncertainty is an abiding question in any model application. It deserves explicit discussion by the modeler and clearly defined measures to account for it. Kriging affords an example of uncertainty, in that uncertainty increases with increasing distance between an extrapolated location and an observed data point.

The groundwater analyst is typically interested in subsurface characteristics such as hydraulic conductivity (see section 2.1.1 above). Hydraulic conductivity, as one example, cannot be measured directly, so the analyst has to use other characteristics that can be measured and relate them in some quantitative way—with a correlation coefficient, for instance—to the parameter of interest. Porosity, or percent void space, is commonly used in this fashion. If the correlation is perfect, the coefficient is 1.0; if it is not so good, it could be, say, 0.5. In the latter case, basing an estimate of hydraulic conductivity on porosity increases the uncertainty of the estimate.

Groundwater modeling has abundant sources of uncertainty irrespective of the sophistication of the model or the analyst involved. Thus a recognition of the model's limitations is important to an understanding of the model's potential contribution to policymaking and cleanup decisions.

5.4 MONTE CARLO METHOD

The term "Monte Carlo method" (suggested by John von Neumann and S.M. Ulam in the 1940s; Ulam's uncle was a gambler) refers to the simulation of processes using random numbers. In Monte Carlo methods, a computer uses random-number simulation techniques to mimic a statistical population. In the STATISTICA Monte Carlo procedure, the computer constructs the population according to the user's prescription; then, for each Monte Carlo replication, it simulates a random sample from the population, analyzes it, and stores the results. After many replications the stored results will mimic the sampling distribution of the statistic. Monte Carlo techniques can provide information about sampling distributions when exact theory for the sampling distribution is not available—e.g., is it Gaussian, or symmetrically bell-shaped? (See http://www.statsoft.com/textbook/stathome.html.) The purpose of the tool is risk assessment, i.e., to tell you how far wrong you could be.

5.5 INVERSE MODELING

Inverse modeling is a frequently encountered concept for which elegant definitions are elusive. A selection of the best ones is offered here. Some other terms used interchangeably are "parameter estimation," "auto-calibration," and "history matching." It has been observed that if you are trying to match an historical data record, the implication is that you have sound, adequate data to match (Dawson, 2006).

One description says that "solution of an inverse problem entails determining unknown causes based on observation of their effects. This is in contrast to the corresponding direct problem, whose solution involves finding effects based on a complete description of their causes" (Alifanov, quoted by Woodbury, 1995; http://www.me.ua.edu/inverse/whatis.html).

Another definition comes from Los Alamos National Laboratory:

> Most mathematical models of fluid flow are of the "forward" type; that is, the relevant properties of the aquifer or reservoir are assumed known, as well as the initial and boundary conditions. A model then predicts the resultant flow. This is typically the approach taken in sensitivity studies, which are quite useful, and can show what the most important features or processes are likely to be for a site.
>
> However, in the field, we generally do not know the full spatial distribution of important properties such as permeability and saturations. Instead, we may have sparse and noisy measurements of pressure, flow rates and concentration at a set of wells, and an incomplete knowledge of the subsurface geology, obtained from cores and seismic soundings. From this information, we need to resolve the spatial distribution of properties such as permeability and saturation and concentration to adequately assess the aquifer or reservoir. Interpretations of this kind typically constitute what are called inverse problems. Finding solutions of inverse problems is a particularly difficult task because of the nonuniqueness difficulties that arise. Nonuniqeness means in effect that the true solution cannot be selected from among a large set of possible solutions without further constraints imposed. This undesirable behavior is due to noise in the measurements, and insufficient number of measurements.
>
> Many areas of geophysics, including atmospheric science, oceanography, geomagnetism and remote electromagnetic sensing, as well as

> hydrology and reservoir engineering, have developed methods for solving inverse problems. All the methods attempt to remove nonuniqueness by using a priori information as constraints. These constraints generally involve imposing smoothness on the unknown solution or its derivatives, or positivity, or maximum entropy or some other very general property (Travis, 2006).

Another useful description, from a geologist's point of view:

> Inverse modeling consists of attempting to understand physical systems by making inferences from data about those systems. Since nearly all data are subject to some uncertainty, these inferences are usually statistical. Further, since one can only record finitely many (noisy) data and since physical systems are usually modeled by continuum equations (at least geophysical ones are) no geophysical inverse problems are really uniquely solvable: if there is a single model that fits the data there will be an infinity of them. (A model is a parameterization of the system, usually a function.) Our goal then is to characterize the set of models that fit the data and satisfy our prejudices.
>
> To make these inferences quantitative one must answer three fundamental questions. How accurately are the data known? i.e., what does it mean to "fit" the data. How accurately can we model the response of the system? In other words, have we included all the physics in the model that contribute significantly to the data? Finally, what is known about the system independent of the data? This is called a priori information and is essential, since for any sufficiently fine parameterization of a system there will be unreasonable models that fit the data too. Prior information is the means by which we reject or downweight unreasonable models. (Adapted from Scales, 2006; http://mesoscopic.mines.edu/~jscales/gp605/what.html).

There are a variety of solution codes for applying inverse modeling to groundwater problems. Among them are MODFLOW PEST, PEST, UCODE, and iTOUGH. The latter was developed by Lawrence Berkeley Laboratory, which maintains an especially useful website with detailed explanations, examples, and a flow chart of the concepts of inverse modeling (http://esd.lbl.gov/ITOUGH2/). Rockware's GMS (groundwater modeling system) supports automated parameter estimation for the MODFLOW simulations. They outline the process as follows: 1) Build a base model with MODFLOW; 2) input observed data (point or flux data); 3) specify the model input parameters that the inverse model can adjust to make the model match the observations; and 4) let the inverse model run—it will adjust input parameters and run the MODFLOW simulation repeatedly until the best match between computed data and observed data is obtained (See http://www.rockware.com/). Groundwater Vistas is another graphical user interface and modeling platform that allows the user to calibrate on any combination of aquifer parameters including hydraulic conductivity, vertical conductance, boundary head, well flow rate, recharge, and evapotranspiration. A demonstration version of the program, and many other tools, can be downloaded from http://www.mt3d.org/software.htm.

Zheng and Bennett (2002) give an example of the use of inverse modeling to eliminate predictions of contaminant concentrations that do not satisfy chosen criteria, and thereby to narrow the range of predicted contaminant behavior (p. 363). These authors distinguish "trial-and-error" adjustment of numerical models and automated calibration but point out that "the terminology can be misleading because it implies that the entire calibration process is automated, while in fact it is rare that more than a part of it (e.g., the estimation of parameter values) is actually automated." They cite Neuman's distinction (1973) between direct and indirect techniques of automatic parameter identification:

> The direct approach requires sufficient data to define the hydraulic heads and/or solute concentrations and their spatial distribution throughout the domain of interest; model parameters to be adjusted are solved for as independent variables….The indirect approach does not require as extensive a database as the direct approach, and is based on minimization (or optimization) of a specified error (or objective) criterion. For most groundwater problems, the indirect solution process is carried out by repeatedly solving the forward equation, using a minimization routine to determine the updated parameter values, and iteratively updating the process until parameter values do not change much between iterations.…[T]he indirect approach is in essence an automated version of trial-and-error adjustment of parameter values (Zheng/Bennett, p. 330).

Any tool can be misused and misapplied, even a shovel. Inverse models are no exception, and one may encounter objections to some applications that they amount to no more than turning knobs until the model appears to match a suite of observational data. It is worth heeding the oft-heard warnings about nonunique solutions—that there may be many parameter combinations that cause the model to fit the data, but some of them might make no sense at all.

5.6 INPUT DATA

What is the source of the data in the model being evaluated? Did the data come from field observations, or are they really output values from another model? What kind of data quality process was undertaken ahead of the collection effort? Are the data appropriate as to source and type for the process being modeled? What uncertainties are inherent in the data? These are fundamental questions that are useful for the citizen interested in understanding a model's basis and how that model may relate to decisions about the cleanup of a particular groundwater site. An example: The surface soil burden of gamma-emitting radionuclides can be assessed with aircraft-borne gross gamma sensors. Or it can be assessed with a handheld sensor and matching GPS locations. The difference strongly affects the uncertainty and reliability of the resulting model conclusions. Site-specific data are all-important.

5.7 SENSITIVITY ANALYSIS

The purpose of sensitivity analysis is to understand how changes in one variable in a groundwater problem affect other variables. There are formal measures of this sensitivity that produce a numerical sensitivity coefficient (Zheng and Bennett, 2002). These authors recommend performing sensitivity analysis both before and after calibration of a model. The first round gives insight into how the model responds to key parameters. The second round gives quantitative measures of the model's sensitivity to those parameters. If a model is sensitive to a parameter that has a lot of uncertainty associated with it, the model will not furnish highly reliable predictions.

5.8 INDEPENDENT REVIEW

In appraising an application of modeling, it is useful to ask questions such as: What kind of independent peer review has the model generally, or the specific implementation of it, been subjected to? By peer review, we mean independent expert team review. There are numerous examples of sites where the basic hydrogeologic work has been carried out by DOE and then evaluated by a formal peer review panel of competent independent practitioners. It is worthwhile to find out whether any peer review has been carried out on the work product in question, and to argue for it if it has not.

In a sense the adversarial hearing process is intended to function somewhat like a peer review, but because of severe resource limitations it is seldom possible for interveners or members of the public to mount any presence on an appropriate scale. Terms of reference for independent peer reviews are readily available and should be consulted. One example is offered in the terms of reference for the independent review of the Yucca Mountain site by the International Atomic Energy Agency (http://www.nea.fr/html/rwm/reports/2002/nea3682yucca.pdf).

5.9 KEYS TO SUCCESSFUL MODEL APPLICATIONS

Zheng and Bennett (2002) offer a succinct summary of guidance for modelers and others interested in the successful application of groundwater modeling:

■ The importance of establishing a purpose for modeling cannot be overemphasized. Most of the decisions required during the model application process depend on the goals of the exercise, and without a clear and well-defined purpose, inefficiency or failure is inevitable.

■ One must develop a clear conceptual model of the study site *based on all available information*. Because of the general paucity of data and the problem of nonuniqueness, the conceptual framework formulated in the early stage of a modeling study frequently constrains the numerical model to a large extent. While this is not necessarily desirable, it is often unavoidable.

■ It is vitally important to have a good understanding of the basic concepts and numerical techniques underlying a contaminant transport model. Without this understanding, a groundwater simulation code can be used only as a "black box," and this clearly limits intelligent application of the model.

■ One should *avoid overkill in the complexity of a numerical model*. As pointed out by Mercer (1989), the temptation to apply the most sophisticated computational tool to a problem is difficult to resist. As a consequence, a common mistake in numerical simulation is to try to construct a numerical model that is more complex than required by the study goals or supported by the available data. It is important to keep in mind that a model, by definition, is a simplified approximation to the real world. *A simple model, as long as it captures the essence of the problem, is always preferred over a more complex one*. An overly complex model not only increases computational times and costs, but also introduces additional uncertainties if detailed data are not available (Hunt and Zheng, 1998).

■ One should know the uncertainties and limitations associated with model results. The danger of blindly trusting the results of a numerical model has been eloquently pointed out by many authors (e.g., Anderson, 1983; NRC, 1990). While model calibration, sensitivity, and uncertainty analysis as described in Zheng and Bennett chapters 12 and 13 can be applied formally to address uncertainties in model results, often the problems and errors in the results can be avoided and detected by using common sense and a few simple calculations.

The following "Ten Hydrogeologic Commandments" appeared in the *Newsletter From the Directorate of Hydrogeology*, Department of Water Affairs and Forestry, Republic of South Africa, in 1998. For the convenience of the lay reader, an explication of each commandment is offered in italics (emphasis added):

1. Thou shall not assume isotropy, homogeneity, or uniform gradient without field evidence. *These conditions very rarely apply; anisotropy [differing void geometry in all directions], heterogeneity, and varying gradient are the norm*.
2. Thou shall not assume wells or streams to penetrate fully or flow systems to be two dimensional. *These are common assumptions of the model builder, often violated in reality*.
3. Thou shall not use regional data to make site-specific judgments. *Regional data are very generalized and probably consist of a lot of averages. One cannot assume they apply in any specific location*.
4. Thou shall not use color graphics to enhance lousy science. *Needs no explanation*.
5. Thou shall not employ geostatistics to obfuscate poor interpretations or weak conclusions. *This refers to the temptation to overcomplicate a problem*.
6. Thou shall not rely on stochastic methods to disguise insufficient field data. *If there are insufficient data to sustain a judgment, no amount of statistical gymnastics will help*.
7. Thou shall not place geochemical interpretations above hydraulic interpretations.
8. Thou shall never regard geophysics as the truth. *"Truth" is supremely evasive*.
9. Thou shall never use a contouring program to make a watertable map. *The map will always be wrong*.
10. Thou shall never use more than three significant digits. *Don't misrepresent by false precision what we know or how well we know it*.

6.0 Case Study: Hanford, Washington

This section attempts to portray the complex environment in which the technical exercise of groundwater modeling takes place at one of the nation's largest nuclear facilities. This environment is shaped by several factors: the complex physical conditions of the Hanford site, the culture of people and organizations, the government agencies and the contract operator arrangement, and the attendant bureaucracy and management issues.

The Hanford complex was built on a 586-square-mile site on a bend in the Columbia River in Washington State. It was established in 1943, when the nation was in a rush to build the first atomic bomb under the Manhattan Project. Generations of weapons, nuclear research, and power reactors have been built, operated, and in some cases dismantled on the site. Early waste-management practices were cavalier by today's standards. One report proclaimed that "the Hanford Atomic Products Operation…lies in a region admirably suited to the disposal to ground of large volumes of liquid wastes" (Parker, 1954). The contamination has occurred over 60 years, dangers were not understood, care was not taken, haste was the order of the day, and gargantuan radioactive and chemical pollution problems resulted. Much of the dangerous material did not stay put in its initial parking place, but leached and moved in the natural materials of the earth. The result is that the Hanford site is the most densely contaminated site in the United States. The U.S. Department of Energy is heir to the whole mess.

6.1 COMPLEXITY OF THE HANFORD HYDROGEOLOGIC ENVIRONMENT

The geologic character of south-central Washington has been shaped by a long history of flooding, first by lava flows and then by water from huge failing ice dams. In between there was a long period of crustal deformation and folding, resulting in the creation of a structural depression now known as the Pasco Basin between the Horse Heaven Hills and the Saddle Mountains. It partly filled with crustal sediments carried by the ancestral Columbia River and associated lakes. Much later Pleistocene ice-dam lakes in the Clark Fork basin of Montana impounded huge amounts of water that repeatedly breached their walls and rushed to the sea down the Columbia, scouring the land to bedrock in many places and leaving behind Olympian-size river features such as bars, dunes, current scars, terraces, and dry channels. In low-energy backwater areas the turbid waters left temporary lakes that dropped thick sequences of sands, silts, and clays. The confluence of the Columbia and Yakima rivers lies in the basin.

The generalized stratigraphic section, starting from the bottom with the oldest, consists of the following sequence: Columbia Plateau basalts, Miocene (6 to 17 million years old), 13,000 feet thick

- Uplift, folding, and dissection, later repeated, leaving a warped and undulating surface
- Ringold Formation, consisting of river sediments from the ancestral Columbia. The Ringold includes the conspicuous White Bluffs across the river from the Hanford site and has many subunits; at least seven lithofacies[1] have been distinguished.
- Cold Creek unit, an erosional surface with a paleosol, often characterized by a caliche layer. It sometimes behaves as an aquitard and causes lateral spreading of downward-percolating groundwater.
- Hanford Formation, consisting of sediments from the Pleistocene Lake Missoula floods. Flooding also left sequences of gravel, silt, sand, and clay behind to form the subsurface of the Hanford site.

The dry climate and extensive vadose zone result in a deep water table throughout much of the Columbia Basin. A convenient summary and appropriate references on the geology of the Hanford site can be found in DOE, 2006. For more general geology of the Inland Empire region of Washington and Oregon, see Bjornstad (2006) and Allen and Burns (1986).

In addition to the routine complexity, there is the occasional extraordinary situation, like that at 300-FF-5, a site close to the Columbia River. The vadose zone in this location is not well sampled or understood, but it appears to be the source of groundwater uranium, which has been detected there since 1957. There are daily flow reversals in

[1] lithofacies: variant of a rock formation; paleosol: ancient soil; caliche: hard calcium carbonate-rich layer; aquitard: slowly permeable layer.

the river due to diurnal changes in discharges from the upstream hydroelectric dam; these act like a pump and smear the uranium through much of the vadose zone. It takes a sampling time-step considerably shorter than the diurnal cycle to make it possible to discern the effect. To complicate it further, there are at least 21 aqueous complexes of uranium (Yabusaki, 2006). Alkalinity and calcium, the chemical constituents that most strongly affect sorption behavior, vary by a factor of three between the aquifer and the river.

6.2 IMPORTANCE OF THE VADOSE ZONE AT HANFORD

The deep vadose zone at the Hanford site has been poorly characterized despite decades of investigations (Faulk, 2006). Fluor Hanford, the current operational contractor, says plainly that organizational responsibility for vadose zone characterization and monitoring is unclear (DQO data quality objective summary report 200-BP-5 OU, WMP-28945, Draft A). The vadose zone at Hanford has been described by one informed visitor as a "no-man's-land" (Neuman, 2006a). The General Accounting Office/Government Accountability Office (1992, 1998) has been exhorting DOE for many years to effectively integrate the vadose and groundwater realms. Vadose zone properties have much to do with the development of preferential flow pathways. Soils with high levels of exchangeable sodium often show low permeability zones. Vadose zone modeling is different from modeling for saturated conditions; there is moisture in the vadose zone, but there is free air in the pore spaces as well.

The Hanford Waste Management Areas include 177 underground storage tanks for high-level radioactive waste. In the closure process for these areas, the Department of Energy has conceptualized three barriers that reflect a "defense in depth" philosophy. They include two engineered barriers, which consist of a surface cover and grouting of the actual tank structure; and a natural barrier, which consists of the vadose zone (DOE, 2006, p. ES-v). Past contaminant releases from the tanks and continuing remediation dominate the cleanup task, which can be visualized in the following table.

Table 5. Single Shell Tank Groundwater Impacts

Performance Objective	Maximum Contaminant Level[a]				Exposure Scenarios[b]		
	Beta-Photon 4 mrem/yr	Tc-99 900 pCi/L	I-129 1 pCi/L	Cr 0.10 mg/L	All-Pathways Farmer 15 mrem	Radiological ILCR Industrial 1.0E-4 to 1.0E-5	WAC 173-340 Hazard Index Method B 1.0
WMA	***Tank Residuals***						
S-SX	◇	◇	◇	◊	◇	◇	◊
T	◇	◇	◇	◇	◇	◇	◇
TX-TY	◊	◊	◇	◇	◇	◊	◇
U	◊	◊	◇	◇	◇	◊	◊
C	◇	◇	◇	◇	◇	◇	◇
B-BX-BY	◇	◇	◇	◇	◇	◇	◇
A-AX	◇	◇	◇	◇	◇	◇	◊
WMA	***Past Releases***						
S-SX	●	●	◊	●	◊	○	○
T	●	●	◊	●	◊	○	◊
TX-TY	●	●	◊	○	◇	◊	◊
U	●	●	◇	○	◇	◊	◊
C	◊	◊	◇	◊	◇	◊	◊
B-BX-BY	●	●	◇	○	◇	◊	◊
A-AX	●	●	◇	○	◇	◊	◊

Below Performance Objective:
◇ Greater than a factor of 10
◊ Less than a factor of 10

Above Performance Objective:
● Greater than a factor of 10
○ Less than a factor of 10

[a] Evaluated from year 2000 to 12032.
[b] Evaluated from year 2332 to 12032.
ILCR = incremental lifetime cancer risk

The black oval symbols indicate where past groundwater release impacts exceed maximum contaminant levels by more than a factor of 10. For all but one of the Waste Management Areas, 90 percent immobilization or removal of ^{99}Tc-contaminated soil from past releases was determined to be necessary to achieve groundwater performance objectives. Key parameters affecting contaminant migration in the vadose zone are thickness between waste and unconfined aquifer, hydraulic properties of major geologic strata (hydraulic conductivity, anisotropy, dispersion), initial moisture content, and distribution coefficients (K_d). All of these are poorly known. The first key factor for the unconfined aquifer is groundwater gradient; it is widely recognized that the gradient in the 200 E area is unknown, and is complicated by the dissipation of the recharge mound created by past disposal of cooling water.

It is worth noting that although tank leaks from C Farm are probably currently contaminating groundwater with ^{60}Co, ^{137}Cs, and ^{99}Tc (Hartman et al., 2006), the SST-PA (Single Shell Tank Performance Analysis), (Department of Energy, 2006) indicate that past leaks from C farm will not reach groundwater for 10,000 years. Nonetheless, the C Tank Farm is scheduled to be closed first.

6.3 THE STRUCTURE OF BUREAUCRACY AND DECISION MAKING

In a sprawling bureaucratic environment such as the Department of Energy cleanup program, there is a need to systematize how decisions are made, how the public can exercise its right to affect those decisions, what studies have to be done, how progress is measured and documented, and how the review process takes place. To accomplish all this, a standard progression of major tasks and work products has been developed by DOE. The sequence of activities and products is typically as follows:

- Data Quality Objectives (DQO) summary to identify and evaluate existing data, to better understand data gaps and uncertainties, and to define additional data requirements
- Remedial Investigation/Feasibility Study (RI/FS) process
- Performance Assessment (PA) to predict future contaminant migration under various conditions, from no action to alternative remedies
- Environmental Impact Statement (EIS) to assess the collective effects on human health and the environment of all remedial actions
- Entry of decisions in "Records of Decision" (ROD), which is published in the Federal Register

Institutionalized fixed assumptions are a feature of the decision-making culture in many large organizations. An example at Hanford is the deeply ingrained belief that although major contaminants might have escaped from storage tanks, they did not migrate more than a short distance in the vadose zone. For many years this assumption took on the status of accepted wisdom in the face of information to the contrary: It was documented as far back as 1954 that uranium was turning up in groundwater discharging to the river (Parker, 1954). The General Accounting Office (1998) pointed out that "over several decades DOE built its waste disposal strategy on the assumption that the vadose zone would prevent most wastes from migrating down to the groundwater, without setting up a program for determining whether its assumption was correct." Groundwater modeling at Hanford has been influenced by the assumption that most radionuclides do not migrate far once they have escaped from storage tanks. Blumenkrantz (2004) supports this assumption because "a similar waste site demonstrates decreasing radionuclide contamination with depth." A major Environmental Impact Statement (DOE, 1996) concluded that tank wastes in the vadose zone would take more than 100 years to reach groundwater.

Institutional memory and consistency of cleanup approach are elusive at Hanford. A keenly interested observer, Washington governor and former state attorney general Christine Gregoire observed in 2006, "It has been 17 years since I signed the TriParty Agreement for the federal cleanup of Hanford with the Energy Department and the Environmental Protection Agency. Since that time we have had three presidents of the United States, 11 secretaries or acting secretaries of energy, five prime contractors for the Waste Treatment Plant, and three different business models for designing and building the treatment plant."

6.4 MODELING HARDWARE REQUIREMENTS AND THEIR APPLICABILITY AT HANFORD

Over the past 20 years the development of personal desktop and laptop computers has proceeded apace. The processing speeds, memory, and storage of today's machines were hardly conceivable when most of today's practitioners started their professional careers. Many computational programs such as MODFLOW can be run on a readily available UNIX workstation or even a laptop.

A few other programs require more hardware. We have learned (above) that there are discontinuities between vadose zone and groundwater specialists at Hanford in the way they view contaminants; there is a discontinuity in their approach to model design as well. MODFLOW, albeit in a special one-off dedicated version, is now the officially sanctioned tool for groundwater flow modeling at Hanford. STOMP is the chosen tool for the vadose zone. Because of numerical dispersion effects, the STOMP implementations at Hanford have been discretized at 600,000 to 700,000 grid cells. The computational effort to perform one realization of this model requires two 48-hour run periods on the MPP2 (Massively Parallel Processing System 2; see details at http://mscf.emsl.pnl.gov/hardware/config_mpp2.shtml). This computer complex is housed at the Wiley Environmental Molecular Sciences Laboratory (EMSL), operated by the Department of Energy at Pacific Northwest National Laboratory (PNNL) in Richland, Washington. The system deploys the horsepower of 1,960 parallel Itanium2 processors and can operate at a speed of 11 x 10^{15} floating point operations per second. Use of the facility is open to the general science community, but it is hardly available on a walk-in basis. Jobs require a competitive application and review process (Yabusaki, 2006). It is not the system for performing multiple runs in the same day for sensitivity analysis purposes because of the extreme computer and human resource requirements.

Little effort has apparently been made to optimize the STOMP code for parallel operation, so it is inefficient. The solver takes most of the time. The August 2006 Review Panel members asked the users, what if you had a much less expensive model that had the same physics built into it? Wouldn't you get quicker answers and be able to bracket the results with more runs? How do you know that a complex model is generating any better results than a simpler one would? (Neuman, 2006).

It appears that the cumbersome nature of massive processing arrays may have contributed to DOE's decision to change from CFEST to MODFLOW. The most important justification for abandoning the CFEST model and going to MODFLOW was that the latter (at least in its off-the-shelf version) is accessible to most practitioners in the hydrogeologic community.

CFEST is not the only code that has had to confront the platform issue. Pruess (2004) says that "most applications of the TOUGH codes are currently being run on Unix workstations and on PCs. For the nuclear waste storage investigations at Yucca Mountain, the LBNL [Lawrence Berkeley] group is routinely running three-dimensional problems with more than 100,000 grid blocks on PCs. A massively parallel version of TOUGH2 has also been developed and has been used for problems with more than 2 million grid blocks."

There are some cumbersome aspects to the practice of groundwater modeling at Hanford that make it slow, expensive, inflexible, and inaccessible to all but the practitioners on the inside. In the world of modern computer development, these limitations could be surmounted.

6.5 ADEQUACY OF INPUT DATA

The importance of sound, consistent, high-quality observational data on the right parameters cannot be overemphasized. One can develop a useful model that makes sense out of good data, but there is no point in trying to come up with data that satisfies a preconceived model. There have been numerous controversies at Hanford over questions concerning data collection. Some examples:

- Is the borehole decommissioning program proceeding too quickly to allow existing boreholes to furnish data with modern logging techniques that would strengthen site characterization?
- Have economical drilling methods been fully explored, applied, and adapted to the Hanford situation? How does one proceed with a waste characterization when important boreholes stop just below a tank base or waste mass and do not show contaminated material in the deeper vadose zone or the groundwater?
- What happens when the analyst confronts troubling data that do not fit the model? On what grounds does one omit data from the analysis?

The academic research community has produced extensive thinking on this subject of data sufficiency. Assuming one sincerely wants to know what is going on, more reliable site characterization data are needed, not less (Neuman, 2006). This emphasis came up repeatedly during the three days of discussions among members of the Central Plateau Review Panel in August 2006[2].

New technology in the instrumentation field has played a large part throughout U.S. nuclear facilities, but the development process does not happen overnight. The most recent high-resolution resistivity (HRR) instrument design has been championed as a potential source of valuable data, but it is not being subjected to baseline comparison before being deployed. Geomatrix (2005) made

[2] This review panel had a formal schedule that envisioned production of draft and final reports by the end of October 2006. As of February 2007, it appears that it will yet be some months before the release of the review panel's final report.

a detailed evaluation of the surface HRR technique and concluded that it is not mature.

S.M. Stoller Corp. is the geophysical logging contractor at Hanford and is therefore due some credibility on the subject. The findings and recommendations in the company's annual report (2005) offer a commentary on the logging and data-gathering operation:

- For all of 2005, there was effectively no routine monitoring in the single-shell tank farms.
- Resources have been directed away from routine monitoring to tank waste retrieval operations, with the result that many holes have not been monitored since 2003. This was in spite of very low logging productivity—an average of 0.1 well per day, with extreme levels of downtime: two days of availability in three months.
- The only way to determine whether an increase in contamination is related to tank waste retrieval operations is to do routine monitoring around the tanks; this is not being done.
- A spectral gamma log is the best unequivocal indication of a tank leak.
- The vadose zone monitoring should be consolidated under one contractor. It was split, and nobody is looking to see whether the data from different contractors are comparable.
- Neutron moisture logging instruments are a useful technology, but their use at Hanford has not been subjected to rigorous procedural and calibration controls. Continued reliance on neutron moisture measurements as the primary means of leak detection is not recommended because no long-term baseline of neutron moisture measurements has been established, and it is impossible to determine whether small increases are related to waste retrieval operations or simply to normal seasonal fluctuations.

The General Accounting Office (1993) thought that cheaper drilling methods should be adopted. Although its report mentioned seven or eight different methods, it did not mention the pile-driven casing method advocated by Grand Junction Office engineers (Brodeur, 2006).

Estimates of curie content of leaks could be made using the empirical characterization data instead of basing those estimates on gross assumptions of the contamination distribution such as what the CH2M Hill vadose zone integration team has recently done as reported in Field and Jones (2005).

6.6 EVOLUTION OF THE HANFORD SITE-WIDE GROUNDWATER MODEL

The Hanford site has experienced a shifting policy over consistency and standardization of groundwater modeling tools: model code, input parameters, databases, and assumptions. A miscellaneous collection of disparate and overlapping groundwater models were in use at Hanford up to the late 1990s. By 1998, modeling activities had converged on two main models, but it was decided to consolidate them and their functions under a single site-wide model. A lengthy document tracks the decision process (U.S. Department of Energy, 2000). There was an extensive multiyear process, a public involvement program, and an outside peer review panel. The DOE response to Congress does not acknowledge the existence of a previous site-wide groundwater model, though its development has consumed vast resources at Hanford. DOE (2000) published a 250-page report titled "Selection and Review of a Site-Wide Groundwater Model at the Hanford Site." This report went into voluminous detail about the options and their relative merits and recommended the selection of the CFEST code as the site-wide platform. The recommendation was acted upon, and the CFEST model was built. In 2006, however, DOE abandoned the CFEST model and is making a transition to MODFLOW. It is not clear what the process was that resulted in the selection of MODFLOW in 2005–06. This much is clear: MODFLOW was hardly worth a mention in the 2000 site-wide model selection process (DOE, 2000). It does not appear that any such selection process was applied to the MODFLOW choice in 2006 as was applied to CFEST in 2000.

Questions occur to the interested observer: Why were off-the-shelf USGS models such as MODFLOW not used? (It was mentioned only in passing, with no analytical comparison, in the report.) Which other models could have done the job, and why was a proprietary model based on CFEST chosen instead? If it took a huge document and a multiyear process to bypass MODFLOW in 2000, what did it take to adopt it as the preferred model in 2006? Why, when the 2000 study noted the need for integration of tools for vadose and saturated zones, did it not do anything to improve that connection?

The last question persists today. The implementation of CFEST in 2000 and after did not deal with the vadose zone, nor does the 2006 implementation of the MODFLOW model. The August 2006 Review Panel made the important observation that the vadose zone is a sink for contaminants leaking from shallow sources and the surface; but it is the all-important contaminant source term for the groundwater here.

6.7 MANAGEMENT OF MODELING AT HANFORD

Hanford has attracted the notice of the U.S. Congress. The Joint House–Senate Appropriations Committee directed the Department of Energy as follows:

> **Technology Development and Deployment**
> The conference agreement provides $30,065,000. The conferees are concerned about DOE's efforts to protect contaminants from reaching the Columbia River. Technology used in several remedies is not performing satisfactorily, and there is a lack of new technologies to address contamination issues. The conferees provide $10,000,000 for analyzing contaminant migration to the Columbia River, and for the introduction of new technology approaches to solving contamination migration issues. The conferees understand that the various program groups managing the groundwater and vadose zone cleanup program are fragmented, and not well coordinated. The conferees direct the Department to report to the House and Senate Committees on Appropriations on the organization and operations of these groups, and how they will be better coordinated, within 60 days of enactment of this Act. (U.S. House of Representatives 109th Congress 1st Session, Report 109275. Appropriations For Energy And Water Development. Conference Report To Accompany H.R. 2419, P. 172).

This foray came from the subcommittee chair and apparently was not precipitated by outside lobbying, leaks, or special-interest presence.

The secretary of energy responded to this directive with a letter and report that summarized background, progress, current organization, and proposed changes (Rispoli, 2006). The proposed changes consist in part of the following:

> DOE will consolidate the approach to modeling and risk assessment on the site to provide a forcing function to ensure integration of assessments.…DOE will establish a single set of conceptual models and computer codes.…[T]he new Tank Closure and Waste Management EIS for the Hanford site will develop a site-wide groundwater model.…RL and ORP will use common databases and parameter assumptions for site risk assessments. Key databases and parameter assumptions will be placed under DOE configuration control (FY 2006). The Groundwater Remediation Project, with participation from ORP, will provide the central clearinghouse for all models, parameters, and assumptions used by Hanford risk assessments.… DOE will centralize and strengthen the responsibility for groundwater and vadose zone cleanup under the Groundwater Remediation Project.

An observer with a regulatory perspective (EPA) described the situation by noting that "the Department [of Energy] is wrapped around the axle on this issue of which tool to use. They have an edict that you can't use anything but MODFLOW. It's not which tool you use, but what you put into the tool that matters" (Faulk, 2006).

This sequence of developments gives rise to some concerns about what is resulting from it. Centralized control of modeling tools, parameters, input data, and methods will likely result in an artificial straitjacket for the practitioners of groundwater and vadose zone modeling. The huge commitment of money and time spent on false starts in developing preferred models has created a distraction. The various flow model solution codes are largely equivalent, so the choice among them is not as important as the integrity of the data that go into the chosen model. If the control over key aspects of the modeling effort is to be centralized in a brain trust, it matters who those individuals are. They should be adept, by reason of training and experience, at applying the tools whose use they are controlling.

Regarding the desirability of standardized protocols at Hanford, the Nuclear Regulatory Commission has a view somewhat different from that of the Department of Energy. In a key report section titled "Why Formulate Multiple Conceptual Site Models?" researchers working for NRC say,

> Hydrogeologic systems are open and complex and the corresponding knowledge base is invariably incomplete and imprecise. Therefore, such systems almost always lend themselves to multiple conceptualizations and the postulation of several alternative hypotheses. It is therefore im-

portant to explore varied conceptual frameworks and assumptions through a comprehensive evaluation of a broad range of regional and site data, their translation into coherent and internally consistent conceptual models or hypotheses, and an in-depth examination of these hypotheses in light of the available knowledge base. The more experts with a wider range of earth and environmental specialties are given access to the knowledge base, the larger and more varied are the alternative site descriptions they may identify (Neuman and Wierenga, 2003).

The appropriate response when one is confronted by a disagreement between model prediction and observed data can be illustrated in the cleanup of the Rocky Flats Nuclear Weapons Facility. In the early 1990s and before, soluble transport models were applied to explain the distribution of plutonium at the site. Data collected in the wet spring of 1995 could not be explained by those models. Through the work of an outside advisory group, alternative models based on erosion and sediment transport processes were adopted and led the Department of Energy and the community to a remediation plan that has been successfully implemented (Clark et al., 2006). It is clear that throwing away the data that did not fit the original model would not have led to a successful conclusion.

Encouragement of multiple approaches and a diversity of solutions is well established in other important high-stake decision arenas. To understand future climate scenarios, many general circulation models have been developed around the world. Recognizing the value of diversity of solutions, a Coupled Model Intercomparison Project has been undertaken by Lawrence Livermore Laboratory. A cooperative appraisal of 11 different general circulation model simulations was performed using a comparable set of initial conditions. The simulations pointed out a number of areas where the different model results agreed, as well as where they disagreed (Phillips et al., 2006).

6.8 MODELING AND MONITORING PRACTICE AT HANFORD—SOME EXAMPLES

As this paper observed at the outset, it is impossible to separate the practice of groundwater or vadose zone modeling from the observational data that feed it. Very often a conversation will start over an aspect of the modeling exercise, but it soon becomes apparent that the model does not matter to the ultimate conclusion as much as what goes into it. This connection is starkly illustrated by some examples in the following section. The context is important to keep in mind. Hanford now has 53 million gallons of high-level radioactive waste, much of which is stored in 149 single shell tanks; 67 of these have been officially recognized as leakers. As an example, the B-BX-BY Waste Management Area covers 116 acres and contains 36 single shell tanks that still contain 1.5 million curies of radioactive waste. Of the 36 tanks, 19 are acknowledged leakers. The area has 198 leak detection wells and approximately 90 other boreholes for monitoring conditions in the subsurface (Department of Energy, 2006).

6.8.1 Typical Issues in Which Groundwater Data and Modeling Play a Part

Most of the major modeling-related policy questions at Hanford have to do with waste management, either historical or prospective. Some examples are the following:

■ The present Tank Closure and Waste Management Environmental Impact Statement was conceived to replace the prior effort to prepare a tank closure EIS. The Washington State Department of Ecology sued the Department of Energy for failing to adequately consider cumulative impacts to groundwater in the Hanford Solid Waste EIS (February 2004). In the January 2006 settlement, Energy agreed to expand the scope of the Tank Closure EIS and include an adequate analysis of the cumulative impacts to groundwater from all contamination sources in Hanford's Central Plateau (including the 200 East and 200 West areas. See Federal Register February 2, 2006). Groundwater and vadose zone modeling will help answer questions about impacts from various closure strategies.

■ Energy's proposed decisions to leave remaining waste in the single shell tanks and to leave the tank leaks in the ground will be based on model results and on the forthcoming EIS. Modeling plays a large part in the discussion of how much and how fast the leaked contaminant plumes will migrate and what they will affect. What is an acceptable level of "leave-behind" contamination in the cleanup process? The scoping document for this question is the Federal Register February 2, 2006 (Vol. 71, No. 22: 5655–5660), which states "a reasonable tank waste retrieval range is comprised of three levels: 90 percent, 99 percent, and 99.9 percent. The 99 percent retrieval is the goal established by the Tri-Party Agreement (Milestone M4500).

■ A huge question at this writing is whether the Hanford site should receive new shipments of nuclear weapons wastes, spent fuel from commercial power reactors, or nuclear waste imported from outside the United States under the Bush administration's proposed Global Nuclear Energy Partnership.

6.8.2 The Data Are as Important as the Model

It is difficult to overemphasize the importance of the integrity of input data to the various modeling exercises throughout the Department of Energy complex. Ultimate decisions depend strongly on the original data.

6.8.2.1 B Reactor Waste Tank Site

The B and C reactors, the original plutonium production reactors, commenced operation in 1943. The B reactor was located approximately 3,000 feet south of the Columbia River. Radioactive and chemical wastes were dumped into retention basins or open-bottom trenches between the reactors and the river. Cleanup of the surface operable units (100-BC-1 and -2) was primarily handled as an Interim Remedial Measure (IRM). It was decided to use limited field investigations (LFI) as a basis for the IRM approach. The exercise consisted of doing an analysis to decide whether the operable unit (a bureaucratically defined subarea of a waste site) met a Remedial Action Goal, which was the maximum contaminant level for drinking water applied to the groundwater below the site. The exercise was recorded in several documents known as cleanup verification packages.

The 116-B-5 retention basin consisted of a pair of concrete and steel tanks that received single-pass cooling water from the B reactor, which went into production in 1944. The tanks had a long leak history before they were eventually demolished and the site graded and covered with clean soil. In 1999 a cleanup verification package (CVP) was carried out to show compliance with cleanup standards (Blumenkrantz, 2004). Monitoring data were available for hundreds of surface points in the footprint of the old tanks but were not available at a depth where escaped contaminants could be expected. The same was true of the CVP for the 116-B-1 trench. The hundreds of samples from exact locations over a very large surface area at least showed a spatially differentiated picture of the distribution of contamination on the surface. Instead of being contoured to show where likely hot spots might be identified, the precise location-specific data were homogenized into an average for the entire site. Obviously the surface sample data do not show the distribution of contamination in the deep zone. The report obfuscates the situation by taking a ratio of the shallowest to the deepest observation layers and extrapolating it to depth.

Statistical methods offer many ways to extract information out of data; in this situation, the analysts manipulated their data in such a way as to eliminate any useful information that might have emerged. The apparent objective in the 100 area was not to characterize the distribution of contaminants in the area, but rather to produce a "rule-beater" calculation that showed the place to meet the remedial action objectives. By contrast, according to the 2002 Monitoring Report, "The groundwater monitoring objective is to describe the nature and extent of contamination." The CVP process is analogous to averaging the contaminant load of the entire Hanford site and dividing it by the entire 580-square-mile area and concluding that the average contaminant levels are not so bad.

The centerpiece of the finding that the site will not violate drinking water standards is the RESRAD model. The question of sorption coefficient or Kd value for the 116-C-5 site is reduced to a single value for each contaminant species. The RESRAD calculation model assumes a homogeneous and isotropic subsurface domain with respect to porosity, density, and hydraulic conductivity—conditions that are met nowhere in the Hanford formation sediments. Each radionuclide is assigned a distribution coefficient, or Kd value. For a specified distribution coefficient, the RESRAD model calculates, using a simple linear equation, the release to the groundwater of a specified quantity of uniformly distributed contaminant within the uniform block of soil. The predicted effect on groundwater is governed by the specification of the contaminant source term and the selection of the distribution coefficient.

DOE guidance says that the linear isotherm is satisfactory for most places at Hanford, with exceptions: "However, in some situations the linear adsorption model will not be appropriate, such as where large changes in chemical conditions occur (i.e., underneath a leaking high-level waste tank)." The importance of using a qualified geochemist for selecting appropriate Kd values was repeatedly emphasized (Cantrell, 2003).

6.8.2.2 Other Problems with the 100-BC Cleanup Analysis

Technecium-99 is identified as one of the contaminants of potential concern in the interim Remedial Investigation/ Feasibility Study. It was not included in the 1978 baseline contaminant survey, possibly because of limitations on analytical capabilities and budget constraints. For some reason it was apparently dropped as a contaminant of concern in the 1998 version of the sampling and analysis plan (DOE, 2001) and has not been monitored since. As a relatively mobile radionuclide, it could be expected to help define the extent of the contaminant plume at the site.

The 116-C-1 trench was used as an overflow site when contaminated water from a fuel cladding failure had to be disposed of. Monitoring data for ^{90}Sr show repeated spike concentrations up to 160 pCi/l (pico-curies, or 10^{-12} curies, per liter), which have not been explained or followed up. The 2002 groundwater monitoring report (Hartman, 2003) shows a plot of the data but covers up the problem in the accompanying text by not specifically identifying the likely source, and referring to the three-fold spikes as "variable or declining."

Another feature of the basis for decisions on interim remediation is the use of "analogous sites." No site-specific data are required, because data can be imported from another site that is assumed to be geologically and chemically comparable. At Hanford, this is at best a highly debatable assumption. On top of that, there can be doubts about the accuracy of the data from the comparison site that make it problematical for itself; never mind extrapolating it elsewhere (Brodeur and de Bruler, 2005).

The cleanup verification package for the 116-B-1 trench (Blumenkrantz, 2004) uses the contaminant concentration data from the excavation floor to represent the deep zone. The 1978 monitoring data show that the depth of maximum concentration is below the 15-foot depth of excavation. The radionuclides that show increasing concentrations with depth include ^{90}Sr, ^{239}Pu, ^{240}Pu, ^{60}Co, ^{154}Eu, and ^{137}Cs.

6.8.2.3 TY Tank Farm

The TY Tank Farm is located in the north-central portion of the 200 West Area. It contains six single shell tanks constructed in 1951 and 1952. The TY Tank Farm was built to provide supplemental tank space for the uranium recovery process. The Department of Energy acknowledges five of the six TY tanks as leakers; there is clear evidence that the sixth is also a leaker, but the DOE does not acknowledge it as such. An account of the TY Tank Farm leaks consists of disparate bits of unreconciled information and conclusions. A major factor appears to be simple wishful thinking as to the current or likely future extent of the contamination.

"The only man-made radionuclide detected in this borehole [520211] was Cs-137.…The maximum Cs-137 concentration was 54 pCi/g at 43 ft. K-40 concentrations increase at about 45 ft and increase again at about 50 ft. The Th-232 and U-238 concentrations begin to increase at about 90 ft.…It can not be ruled out the contamination originated from a leak in tank TY102" (GJO Tank Summary Data Report for Tank TY102, March 1997).

TY-103 (Borehole 520306): "A zone of relatively high concentrations of Co60 was detected continuously from 54 to 100 ft (the total depth logged). The concentrations of Co60 within this zone increase with depth, demonstrating that the Co60 contamination is relatively mobile and has migrated a relatively long distance (at least 45 ft) from the contaminant source. Because this borehole terminates at 100 ft, the downward extent of the Co60 contamination is unknown" (GJO Tank Summary Data Report for Tank TY103, May 1997). *In other words, this plume has been persuasively shown to exist, but nobody knows how far it extends or what its maximum concentration is.*

^{99}Tc levels ten to fifteen times the drinking water standard were observed in the groundwater east of Waste Management Area TX-TY. The most likely source for most of this material is tank waste from the Waste Management Area (Hartman et al., 2003, p. 2.8-19).

During May 2002, monitoring in borehole 52-03-06 in the TY Tank Farm detected a prominent gamma activity peak between depths of 16.8 and 17 m that was not present during the baseline spectral gamma logging in 1996 (Hartman et al., 2003, p. 3.2-2).

"A total of 9 boreholes located around tanks TY-103, -104, -105, and -106 were monitored during FY 2003. Borehole 52-03-06 showed an increase in ^{137}Cs concentration between 55 and 58 ft during the initial monitoring event on 5/2/02. Subsequent monitoring events have not shown additional increases in ^{137}Cs concentrations. Borehole 52-06-05 continues to show evidence of increasing ^{60}Co concentrations between 130 and 147 ft. Borehole 52-06-07 showed evidence of possible increases between 200 to 225 ft (Appendix B)" (Hanford Tank Farms Vadose Zone Monitoring Project Annual Monitoring

Report for Fiscal Year 2003. GJO–2004–554–TAC).

"Routine monitoring was not performed in TY Tank Farm during FY 2004" (Hanford Tank Farms Vadose Zone Monitoring Project Annual Monitoring Report for Fiscal Year 2004). DOE–EM/GJ777–2004. No annual monitoring report has been published for FY 2005.

"Tanks TY-102 and TY-106 have indications of leaks with no drywell data to support these conjectures" (from Single Shell Tank Performance Analysis, p. 2-130, DOE 2005).

"Most of the single shell tanks and tank farms remain essentially unmonitored. In particular, the Department obtained data indicating a fifty-fold increase in contamination below two tanks in the TY Tank Farm in 2002, but took no action to install ongoing leak detection capabilities outside the tanks, or to use existing boreholes to monitor such an alarming increase" (Wyden et al., 2006).

The Department of Energy has concluded on the basis of the HTWOS model (Hanford Tank Waste Operation Simulator), which is designed to track tank residual waste, that there has been no past release from TY-102. The inventory of tank residuals was based on model estimates rather than on actual measurements. The map showing the TY Tank Farm does not identify 102 as a "suspected/confirmed leaking single shell tank" (SSTPA, p. 2-133; Fig. 2-50).

The TY farm has deep contamination already in groundwater, which is ignored by the site characterization; the proper instrumentation for mapping the extent of the contaminant plumes (high-resolution spectral gamma logging) has been bypassed in favor of low-resolution instrumentation of marginal utility (Brodeur, 2006).

These conflicting statements are difficult to organize into a conclusion, but one might run this way: We know there are contaminant plumes in specific tank farms; we know the concentrations increase steadily as one moves toward the bottom of the boreholes, which indicates that they may keep on increasing below that; we have seen recent disturbing increases in subsurface contaminant distribution; we have not followed up on these plumes to delineate their size, content, and location; we have ceased routine tank farm monitoring; we do not know where the contaminants are distributed; and on this edifice of questionable information, we are building a tank closure plan and contemplate receiving new waste shipments to add to the old.

6.8.2.4 BX Tank Farm

The BX Tank Farm was constructed from 1946 to 1948. The tanks in the farm received high-level waste from essentially all major chemical processing plants at the Hanford site from 1945 through the late 1970s (Knepp, 2002). A spill during a tank overfill episode took place in 1951 at Tank BX-102. The spill contained an estimated 10 tons of uranium. Between 1993 and 2000 a uranium groundwater plume developed with a horizontal extent of about 2,500 feet from the farm. A tortuous path of events culminated in two reports that disagreed with the notion that uranium is immobile in the vadose zone. The reports found that the plume came from the 1951 leak and was on its way to the groundwater and eventually the Columbia River (Sobczyk, 2005). The first of these reports (S.M. Stoller Corp., 2004) was heavily criticized in an unpublished memo (Myers et al., 2004) and suppressed. The second was published outside the Department of Energy. The Myers memo was a death by a thousand infinitesimal quibbles, criticisms that could be applied to legions of published reports of far less significance, rather than an analysis of the substance of the report. The flavor of the dispute, and telling insights into the culture of waste management at Hanford, can be gathered from the summary below. A much more detailed chronology of the situation is offered by Sobczyk (undated).

After uranium concentrations exceeded the drinking water maximum contaminant level in a key monitoring well some 100 meters east of the BX farm in April 1994, groundwater sampling was discontinued for three years. Between 1994 and 2002, average uranium concentrations in two wells to the northwest of the BX farm increased from 9.2 to 180 µg/L, and from barely detectable to over 300 µg/L. There was abundant other data showing that uranium concentrations in the vadose zone and the groundwater were increasing (Sobczyk, 2005). At this writing, vadose zone monitoring appears to have been discontinued again: "Routine monitoring was not performed in BX Tank Farm during the 3rd quarter of FY 2005.… The date of the last routine monitoring event in BX Farm was 10/6/2003" (S.M. Stoller Corp., 2005).

The conclusion reached by Knepp (2002) and others that uranium in groundwater will not exceed the MCL if further recharge events are prevented is based on the most convenient conceptual model: that it was a flood that drove the plume. It points to an obvious, simple solution: Put a raincoat over it and it will stop moving. The more problematical conceptual model attributes the plume to the BX-102 spill. An additional complication is that when uranium reaches the perched water in the Cold Creek unit, it is transported laterally at an increased rate over relatively large distances. The initial conditions for the risk model placed the distribution of uranium 30.5 m (100 ft) above groundwater. The uranium contamination in the vadose zone located only 3.7 m (12 ft) above groundwater at 299-E33-41 was not included in the model. Lateral flux in the vadose zone across the model boundary at the BX Tank Farm fence line was not modeled. The model does not account for the increasing concentrations of uranium observed within 9.1 m (30 ft) of groundwater at borehole 299-E33-41 between 1991 and 1997.

The picture that emerges is one of denying the evidence, sandbagging an inconvenient report, and drilling eight new monitoring wells—at a probable cost of $2.5 million—upgradient of the problem (Sobczyk, 2005). If one hand-picks the data and omits hot wells and the wells outside the fence, one can manage the resulting picture to suit preconceived needs. It is not necessarily advantageous to go get the data, because what they show might not be a desirable picture. Then, in the absence of adequate, sound data, you try to model your way out of it. The modeling and analysis exercise does not fit the data, so the data must be wrong. Control the allowed tools, so kriging can't be applied in any unexpected ways. Eliminate alternative conceptual models as "technically inadequate."

One might ask, how does all this information affect the choice of remediation strategy? It would obviously be simpler to assume that the uranium will stay put if we just keep the rain off it than it would be to set up a pump-and-treat system to attempt to recover it.

The Department of Energy response to information from Sobczyk that it or its contractors did not want to deal with was the following: Presented with an honest and sincere controversy, sandbag the report so no one else can evaluate it; prevent its publication. The original report, the CH2M-Hanford critique of the report, and the author's response to the critique should all be out in the open to be judged on their merits by all comers. DOE's Single Shell Tank Performance Assessment says, "A conceptual model for each contaminant migration pathway was developed for each WMA [waste management area], incorporating all available *and relevant* site-specific data" (DOE 2006 p. ES-vi; emphasis added). The Department's treatment of the BX Tank Farm requires a highly constrained definition of what is relevant.

7.0 Conclusions

Certain issues emerge from the exercise of writing this report. The conclusions below attempt to point the reader to the important questions arising out of the foregoing material, offering lines of inquiry to establish a frame of reference for a first assessment of a situation in which groundwater modeling has been involved.

■ What are the presuppositions that invisibly frame the discussion arising out of a groundwater modeling situation? What is the body of accepted knowledge, the things that "everybody knows"?

■ What constraints are there on the development of alternative conceptual models—those that offer different explanations for observed geologic or hydrologic features?

■ What are the qualifications and experience of the "experts" who are involved? In what disciplines are they trained? How are their experience and backgrounds related to the question at hand?

■ What form of peer review, or review by independent experts, has gone into the effort? How technically competent and independent are the regulatory agencies with jurisdiction over the situation by virtue of RCRA (Resource Conservation and Recovery Act of 1976) or CERCLA? These would typically be the state environmental and health agencies, the Environmental Protection Agency, and possibly the Nuclear Regulatory Commission.

8.0 Recommendations

The foregoing discussion and analysis leads to a number of clearly desirable remedies for the ways in which groundwater modeling is carried out in the radioactive waste management enterprise. It would be most useful to undertake the following actions:

- Explore why the decades-long sequence of inquiries by the General Accounting Office have had no apparent effect on the way business is done at Hanford. Many of the criticisms in earlier reports are repeated in later ones and are as valid today as when they were first written.
- Review the centralized control over modeling codes, conceptual descriptions, input parameter values, etc. The control over the solution codes is probably not as potentially great a source of mischief as the control over input data, assumptions, etc., which can lead to serious misapprehensions—e.g., "Everybody knows" that the uranium from a leaky waste tank migrates a few feet and then stays put.
- Require accessible posting for any and all dissident critiques of Hanford operations. Like reports and information developed by the Department of Energy and its contractors, dissident reports ought to stand or fall on their own merits. Hiding them from public view and refusing to acknowledge their existence simply becomes part of a larger strategy to hide problems. Any sincere criticism, dissenting reports, information from whistle-blowers, etc., should be made publicly available on a readily accessible Department of Energy or TriParty website or, failing that, an NRDC website.

The peer review process itself should undergo a review. The basis for the requirement of peer review panels is buried in the abstruse provisions of gargantuan contracts. There is no systematic provision for how members of the public should or should not be given notice of a review panel, communicate with peer review panel members, or hear their opinions. There is no accountability for implementation of review panel recommendations; after the time and expense of conducting a review panel, there is nothing to stop the Department from reverting to customary business as usual. There is no continuity between one review panel and the next on a given or related subject; one panel may not even be aware of the existence of a previous one. There does not appear to be an explicit provision that would prevent the appointment of peer review panel members who would be a rubber stamp for Department practices.

There is the potential for expanding the Nuclear Regulatory Commission's (NRC) jurisdiction and review role over Department of Energy operations. NRC was designed to have more of a regulatory outlook than Energy. Increasing its role in Energy operations might at least offer the marginal and perhaps questionable benefit of competing bureaucracies. What is truly needed is to break up DOE groupthink and institutional ossification.

The role of the few intrepid individuals who have worked inside the Department of Energy complex and have made public deeply held reservations about their work is an extremely important one. There is a very thin thread of competent information that connects us, the public, to the world inside the Department of Energy and its contractors. It is impossible for an outsider, even a highly trained and persistent one, to penetrate the arcane practices and predigested public conclusions that come out of the nuclear weapons establishment. Only a trained and experienced individual who has worked on the inside has the requisite insight to know what is happening and its significance. This means the public and its leaders are dependent on what our government chooses to tell us, or on the dissenting voices of those who are both brave enough to speak out and well-enough informed to be taken seriously. This should not be interpreted as meaning that the insider turned dissident is entitled to any more credibility than anyone else; but he or she should be given a fair hearing, their concerns followed up, and their technical insights subjected to customary scrutiny.

If it were not for a handful of whistle-blowers at Hanford, many questions of public and environmental safety would lie buried from view. Their function, and the basic civil right that allows them to be heard, are an indispensable part of effective management of Department of Energy facilities. They are a rare counterbalance to the dangers of orthodox groupthink that characterizes all large organizations. Their role and position should be guarded zealously.

9.0 Appendices

APPENDIX A

From: pwilling@telcomplus.net [mailto:pwilling@telcomplus.net]
Sent: Monday, July 31, 2006 11:05 AM
To: Spane, Frank A
Subject: Inquiry on groundwater data usage

Dear Mr. Spane,

As you suggested, I am following up our telephone conversation with an e-mail to try to arrange a meeting with you and others involved in the groundwater modeling enterprise at Hanford. I have also communicated with Mike Thompson, Doug Hildebrand, and Jeff Harvey from Public Affairs.

I have open times all day Wednesday, and Thursday up to about 2:00 p.m.

Thank you in advance for the opportunity to meet with you and your colleagues.

Sincerely,
Peter Willing
Peter Willing, Ph.D., Hydrogeologist
Water Resources Consulting LLC
1903 Broadway
Bellingham, Washington 98225 3237
360 734 1445

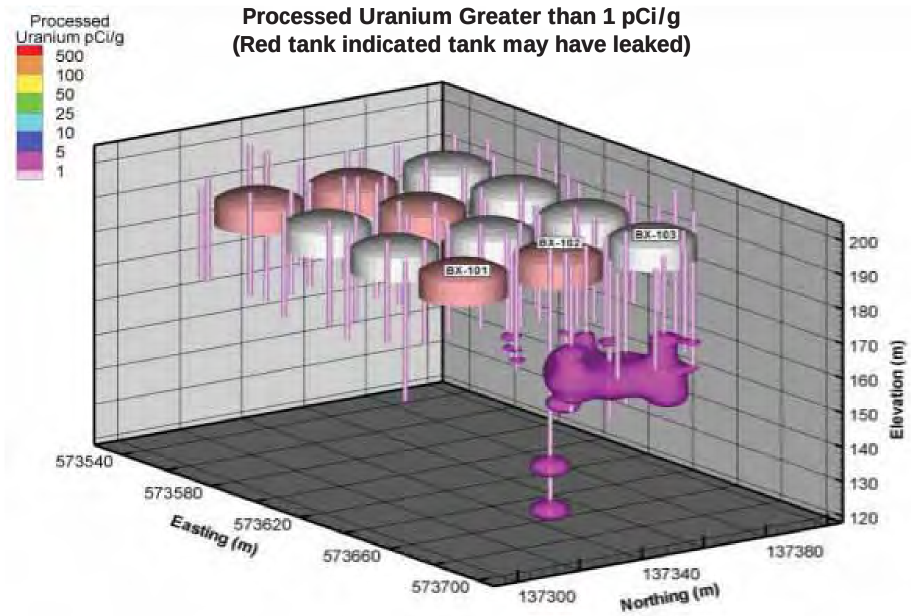
Subject: RE: Inquiry on groundwater data usage
From: “Spane, Frank A.” <frank.spane@pnl.gov>
Date: Mon, 31 Jul 2006 12:57:28 0700
To: pwilling@telcomplus.net
CC: “Harvey, Geoffrey L” <Geoffrey.Harvey@pnl.gov>, “Thompson, K M \(Mike\)” <K_M_Mike_Thompson@rl.gov>, “Hildebrand, R D \(Doug\)” <R_D_Doug_Hildebrand@rl.gov>, “Luttrell, Stuart P” <stuart.luttrell@pnl.gov>, “Gilmore, Tyler J” <tyler.gilmore@pnl.gov>

Pete:

Sorry to inform you that we’ll not be able to schedule a meeting this week. I have been informed by DOE Richland that they are currently discussing the matter of a meeting between you, myself, and other PNNL staff with DOE Headquarters. They haven’t received an answer yet from Headquarters on granting your requested meeting. Please coordinate your future meeting requests/inquiries directly to Mike Thompson (DOE RL). When I receive an approval from DOE/Mike Thompson, then we can proceed in scheduling a meeting to discuss your questions.

Regards.
Frank

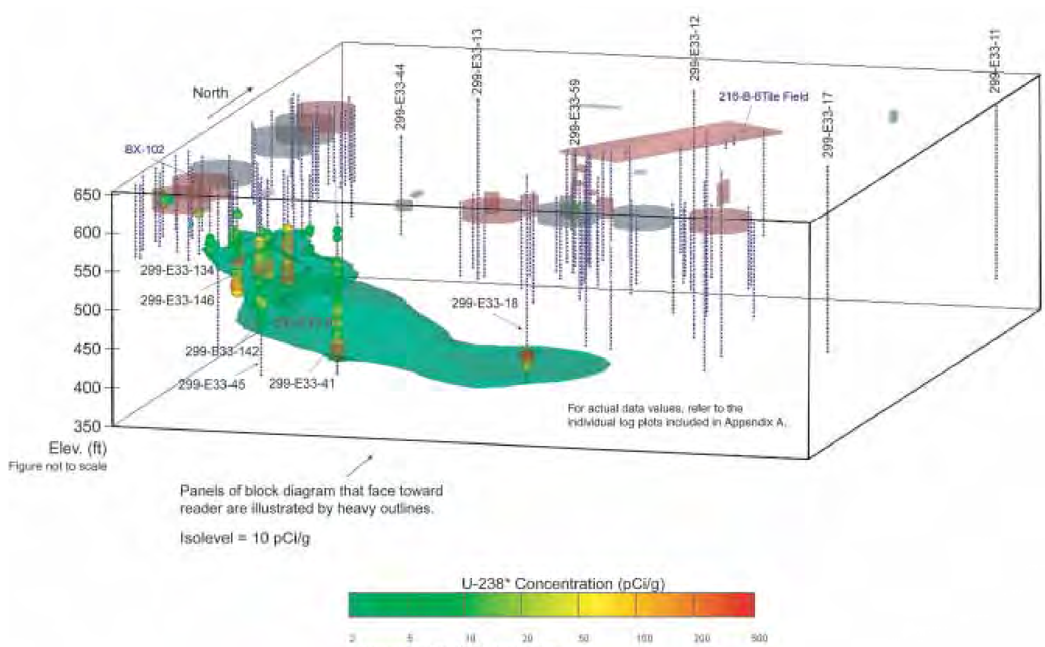
Figure 4. Visualization of BX-102 Uranium Plume



Krigged uranium-238 plumes indicating contamination below 120 feet in drywell. 21-02-04 are based on somewhat less reliable uranium-238 spectral gamma logging data. These data are less reliable because of interferences from the high levels of cesium-137 in the soil.

Source: Knepp, 2002 (under separate cover).

Figure 5. Visualization of BX-102 Uranium Plume



Source: Sobczyk, 2004 (under separate cover).

APPENDIX B

Selected numerical groundwater models that may be encountered by the active reader in the nuclear facility literature.

Model name	Purpose, application	dimen-sional-ity	Steady state or dynamic	Proprietary or open source	Developer of software	Technical reference	Solution method	Where encountered
VAM3DCG	Candidate code for site-wide model in 2000, Hanford	3-D	Dynamic	Proprietary, available for purchase from developers	Hydrogeologic, Inc., Herndon, Virginia			Selection and Review of a Site-Wide Groundwater Model at the Hanford Site, DOE/RL-2000-11, p. 110
PORFLOW	Simulation of flow, heat, salinity, and mass transport in multiphase, variably saturated, porous, or fractured media	2-D or 3-D	Transient or steady state	Proprietary, available for purchase from developers	Analytic & Computational Research, Inc.	ACRi, 1994. PORFLOW: A Software Tool for Multiphase Fluid Flow, Heat and Mass Transport in Fractured Porous Media Validation, Version 2.50	Finite difference	Selection and Review of a Site-Wide Groundwater Model at the Hanford Site, DOE/RL-2000-11; used at Savannah River, INEL, Yucca Mtn, Hanford, ANDRA (French national agency for management of radionuclides)
STOMP	"Subsurface Transport Over Multiple Phases" simulates subsurface flow and transport; designed for remediation of VOC and radwaste sites	1-, 2-, 3-D	Dynamic	Battelle Memorial Institute holds copyright	Pacific Northwest National Laboratory's Hydrology Group	http://stomp.pnl.gov/documentation/application.pdf	Finite difference; see document-ation	The official vadose zone model at Hanford
CFEST	"Coupled Fluid, Energy, and Solute Transport"—selected in 2000 for site-wide model, Hanford	3-D	Dynamic		CFEST Co., Irvine, California	http://www.cfest.com/cfestSITES.asp	Finite element	Selection and Review of a Site-Wide Groundwater Model at the Hanford Site, DOE/RL-2000-11
MODFLOW	Simulate saturated flow in porous media; confined, unconfined	3-D	Transient or steady state	Available from USGS	USGS	McDonald & Harbaugh, 1984	Finite difference, block centered	Ubiquitous—"the industry standard"
MT3D	Transport model for simulation of advection, dispersion, and chemical reactions in groundwater	3-D		Open source program and documentation available at http://www.epa.gov/ada/csmos/models/mt3d.html	Zheng Chunmiao	Zheng, 1990	Euler-Lagrange, method of character-istics	Fetter 530, cd accompanying text interfaces with MODFLOW
RT3D	Reactive transport	3-D		Open source	Clement; PNNL	http://bioprocess.pnl.gov/rt3d_hist.htm#hist; http://bioprocess.pnl.gov/rt3d.htm		
Spread-sheets	Many simple tasks can be done with spreadsheet tools	Either [2-, 3-D]	Either	http://nevada.usgs.gov/tech/excelforhydrology/index.htm.	various			Fetter 531; Mitchell; Keith J. Halford, Carson City, NV

APPENDIX B (CONT.)

Selected numerical groundwater models that may be encountered by the active reader in the nuclear facility literature.

Model name	Purpose, application	dimen-sional-ity	Steady state or dynamic	Proprietary or open source	Developer of software	Technical reference	Solution method	Where encountered
HYDRUS	A family of models for water flow and solute transport in unsaturated or variably saturated porous media	1-, 2-, 3-D	Dynamic	Proprietary; $1,800	U.S. Salinity Laboratory in cooperation with the International Groundwater Modeling Center	Applications and users' manuals at http://www. pc progress.cz/Fr_ Hydrus.htm	Finite element	John Selker, 2004. Review of D. Rassam, J. Simunek, and M.th. Van Genuchten, Modelling Variably Saturated Flow with HYDRUS 2D. Vadose Zone Journal, 3:725
FLOWPATH	Groundwater flow and contaminant transport modeling	2-D	Steady state	Proprietary, $600	Waterloo Hydrogeologic	Franz, T., and N. Guigner, 1992	Finite difference	Selection and Review of a Site-Wide Groundwater Model at the Hanford Site, DOE/ RL-2000-11, p. 200
PEST	Parameter estimation							
WHPA	Wellhead capture zone delineation	2-D	Steady state	http://www.epa. gov/ada/csmos/ models/whpa. html	EPA	EPA, 1993b	3 computa-tional modules	
MOC	Solute transport					Konikow and Bredehoeft, 1978	Advection-dispersion equation	Fetter, 1993, p. 101
TOUGH iTOUGH	Unsaturated groundwater and heat transport model	1-, 2-, 3-D	Either	Open source from U.S. DOE Energy Science and Technology Software Center, http://www esd. lbl.gov/TOUGH2/ tough2v2.html	Pruess, 1991; Lawrence Berkeley Lab	Pruess, 1991; LBL 29400. "TOUGH" stands for "transport of unsaturated groundwater and heat" and is also an allusion to the tuff formations at Yucca Mountain, which represented one of the chief application areas of the code at the time. Pruess, K., 2004. The TOUGH Codes—A Family of Simulation Tools for Multiphase Flow and Transport Processes in Permeable Media, Vadose Zone Journal, 3:738 746	Integral finite difference method	
RESRAD	Radiation exposure pathway model for evaluating human health risk at radionuclide-contaminated sites	1-D	Static	http://www.ead. anl.gov/project/ dsp_topicdetail. cfm?topicid=21	Yu, Argonne; 1989–2001			

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