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Groundwater Modeling at Pantex and Recommendations of the Technical Advisory Group

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Serious Texans Against Nuclear Dumping (STAND), Inc.

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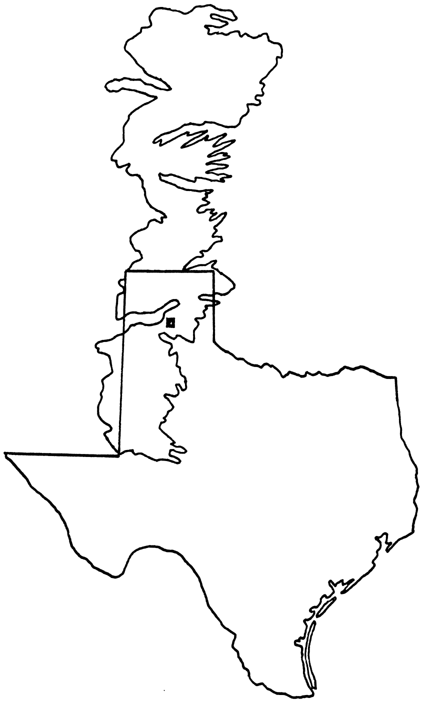
September 2002



STAND
Technical Report 2002 – 1

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Groundwater Modeling at Pantex and Recommendations of the Technical Advisory Group

prepared for

STAND

by

George Rice, Groundwater Hydrologist

September 2002

Executive Summary

The Department of Energy (DOE) Pantex Plant is developing models to simulate groundwater flow and contaminant transport. A Technical Advisory Group (TAG) was formed to examine groundwater modeling issues at Pantex, review available models, and recommend those models it felt were appropriate to the situations at Pantex.

This report discusses: (1) groundwater models; (2) modeling issues and requirements in general and at Pantex; (3) the TAG and its recommendations; and (4) the reliability of model results.

Computer models simulate groundwater flow and the movement of contaminants. They are used for a wide variety of purposes, including predicting the effects of pumpage, estimating contaminant migration rates, estimating cleanup times, and designing monitoring networks. The validity of model results depends on a large number of factors such as accurate site-specific information and an understanding of the range of geologic conditions in the subsurface.

Pantex is contaminated with a wide variety of hazardous materials, and contaminant flowpaths are complex. Contaminants migrate from land surface, through the upper unsaturated zone, to the perched aquifer. They then may migrate through the lower unsaturated zone to the Ogallala Aquifer. Thus, models used at Pantex must be able to simulate

- saturated and unsaturated flow in three dimensions,
- the simultaneous movement of multiple contaminants, and
- the chemical and physical processes that affect contaminant concentrations as they move through the subsurface.

The TAG recommended that separate models be developed for each of three areas:

- the Regional Ogallala Aquifer,
- the Burning Grounds and the City of Amarillo wellfield north of Pantex, and
- the southeast portion of Pantex (zones 11 and 12).

The TAG also recommended that model information, such as final input files, be made available to the public. Both of the primary groundwater flow models recommended by the TAG (MODFLOW and FEMWATER) are available at no cost.

DOE accepted the TAG's recommendations.

Model results are often presented to the public as if they are beyond question. However, model results are sometimes misleading or nonsensical. The public can, and should, question the reliability of model results. Interested citizens can raise the following questions:

- Are the assumptions incorporated into the model reasonable?
- Are all significant physical features included?
- Is the model based on site-specific data?
- Can the model predict the past? If not, with what confidence can it predict the future?
- Has a sensitivity study been done?
- Are the results believable?

Table of Contents

1.0 Introduction

The Department of Energy (DOE) is developing models to simulate groundwater flow and contaminant transport at Pantex. A Technical Advisory Group (TAG) was formed to examine modeling issues at Pantex, review available models, and recommend appropriate models[1].

This report discusses: (1) groundwater models, (2) modeling issues and requirements in general, and at Pantex, (3) the TAG and it's recommendations, and (4) the reliability of model results.

Endnotes appear in Section 8.0 and technical terms are defined in Appendix 2 – Glossary.

2.0 Groundwater Models

2.1 General

Models are simplified descriptions of complex natural systems. As used here, the term model means a computerized, mathematical[2] representation of a groundwater system. Models simulate groundwater flow or the movement of contaminants. They are used for a wide variety of purposes including:

- Evaluating groundwater availability
- Predicting the effects of pumpage on groundwater levels
- Estimating the time required for contaminants to reach a receptor
- Estimating contaminant concentrations at potential receptors
- Designing and evaluating aquifer cleanup systems
- Designing and evaluating contaminant containment systems
- Estimating the time required to meet cleanup goals
- Assessing past contaminant migration pathways
- Designing monitoring networks
- Delineating wellhead protection zones

There are a number of ways to classify models. The most common is to divide them into two types: ***groundwater flow models*** and ***contaminant transport models***.

Groundwater flow models simulate the flow of water through the subsurface. Flow may be simulated through saturated or unsaturated (vadose) materials. Models that are capable of simulating flow through unsaturated materials are more complex and require more data than models that simulate only saturated flow.

Contaminant transport models simulate the movement of contaminants through the subsurface. The simplest transport models simulate the movement of only a single contaminant (single component) and do not account for transformations that may occur along the flow path. More sophisticated transport models are capable of simultaneously simulating the movement of multiple contaminants (multi-component), and accounting for chemical transformations. These transformations may include radioactive and biological decay, reactions with other contaminants, and interactions with geologic materials. Sophisticated transport models are complex and require a great deal of data. Some transport models simulate both flow and transport. Others simulate only transport and must be used in conjunction with a flow model. Contaminant transport models are also called fate and transport models.

Models may also be classified as: two dimensional (2-D) or three dimensional (3-D), depending on whether they simulate processes in two or three space dimensions; single phase or multi-phase, depending on whether they simulate the flow of one (e.g., water) or more (e.g., water, gas, oil, solvents) fluids; and finite difference or finite element. Finite difference and finite element refer to the mathematical structure of models.

2.2 Processes that affect Contaminant Transport

Contaminants and other solutes being transported in groundwater are subject to a variety of processes that act to change their concentrations and reduce their migration rates. These processes include:

- **Dispersion** – the dilution of a contaminant due to spreading of the contaminant plume. An analogous process is the spreading (dispersion) of a plume of smoke from a smokestack.

- **Radioactive decay** – the disintegration of an atom to form other (daughter) products. The disintegration is accompanied by the release of energy (radiation).

- **Biodegradation (biologic decay)** – the transformation or destruction of organic contaminants (e.g., trichloroethylene [TCE], toluene) by microorganisms. This process may convert one contaminant into another. For example, TCE biodegrades to dichloroethylene (DCE), and DCE biodegrades to vinyl chloride.

- **Abiotic reactions** – the transformation or destruction of contaminants by chemical reactions that do not involve microorganisms. This includes the oxidation or reduction of metals, and the dehalogenation of organic contaminants.

- **Sorption** - a process that binds, usually temporarily, a contaminant to a mineral surface or to organic matter. This temporary binding acts to reduce (retard) the contaminant migration rate with respect to the groundwater. Some contaminants (e.g., nitrate) are not affected by sorption, and travel at the same speed as the groundwater. Others (e.g., most metals) are strongly affected by sorption and travel much more slowly than the groundwater. [Note: Under some circumstances, metals will combine (complex) with other solutes (ligands). The metal-ligand complex is often much more mobile than the uncomplexed metal.]

- **Precipitation** – the combination of solutes to form a solid material. This often happens to metals, as when dissolved lead and carbonate combine to form the mineral cerussite. Precipitation reactions are often not reversible, and the precipitated contaminant is permanently removed from the groundwater.

- **Volatilization/Vaporization** – the formation of gasses that may emerge from water as vapors. Many volatile organic contaminants (e.g., TCE, toluene) may vaporize and travel upward through the unsaturated zone.

Some contaminant transport models are capable of simulating only one or two of these processes. The most sophisticated models can simulate all of them (see Appendix 1).

2.3 Conceptual Models

The first, and perhaps most important step in producing a computerized model, is the development of a conceptual model. It is not a computer model. A conceptual model is the modeler’s concept of the groundwater system and the processes that control flow and contaminant transport. The computerized model is based on the conceptual model. If the conceptual model is based on incorrect assumptions or incomplete information, the computerized model will probably not produce reliable results.

A conceptual model for a groundwater flow model should describe all the significant features of the flow system and the relationships between them. These may include:

- Boundaries of the flow system
- Stratigraphy
- Aquifers and their hydraulic relationships to other geologic units
- Relationships between groundwater and surface water
- Groundwater levels
- Groundwater flow directions
- Groundwater sources (recharge)
- Groundwater sinks (e.g., wells, springs)

A conceptual model for a contaminant transport model should address the major contaminants and the processes that affect contaminant concentrations and migration rates. It should describe:

- Distributions of major contaminants
- Contaminant sources
- Contaminant sinks (e.g., extraction wells)
- Potential contaminant receptors
- Pathways from contaminant sources to receptors
- Processes that affect contaminant transport (e.g., biodegradation, sorption)

Figures 2.3-1 and 2.3-2 are examples of conceptual models. Figure 2.3-1 is a schematic representation of the major geologic units and contaminant pathways at Pantex. Figure 2.3-2 is a description of the relationships between contaminant sources and potential receptors at the Pantex Burning Ground.

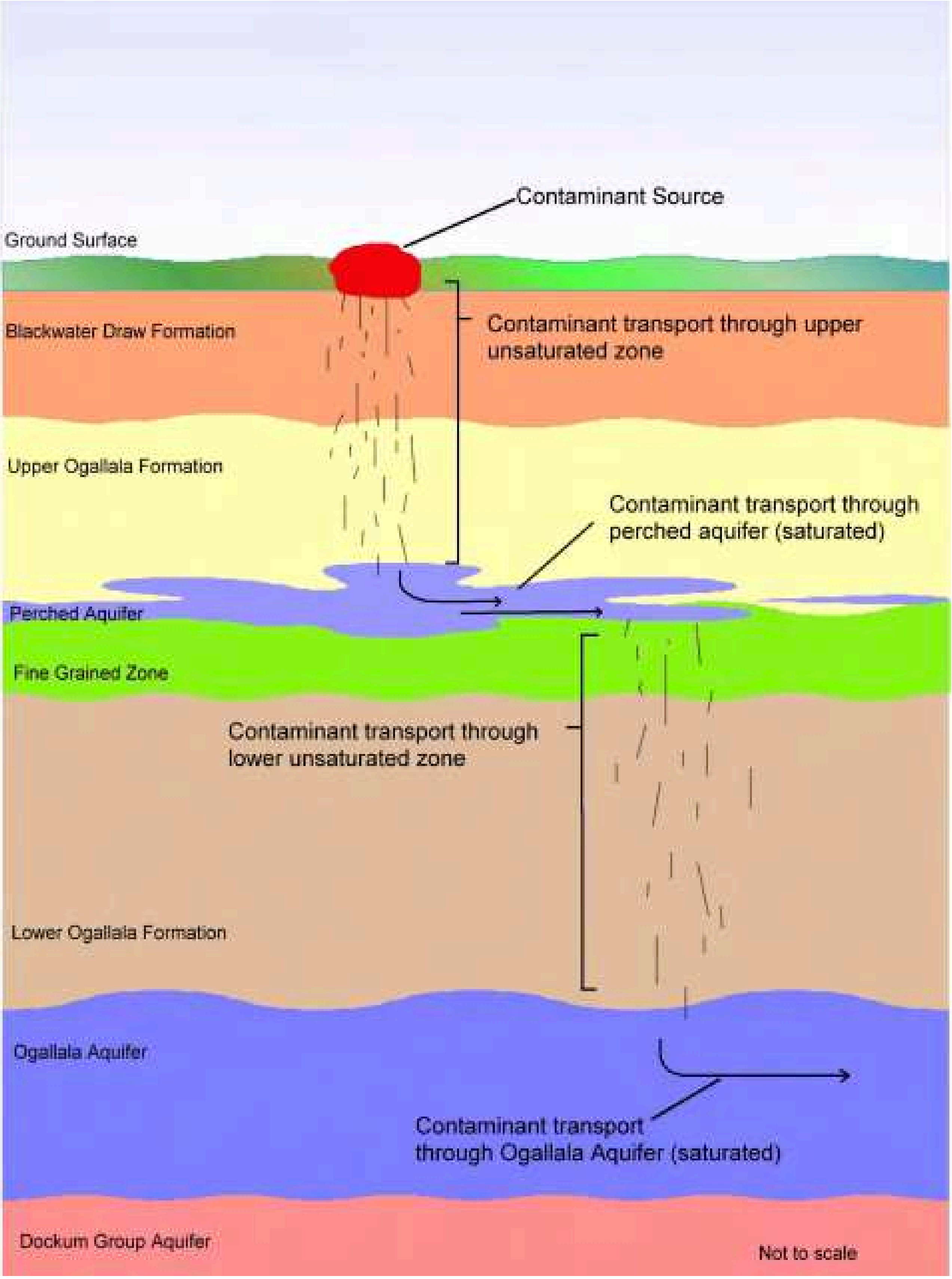

Figure 2.3-1 Conceptual Model-1
Geologic Units and Contaminant Pathways at Pantex
(Adapted from DOE, 2001)

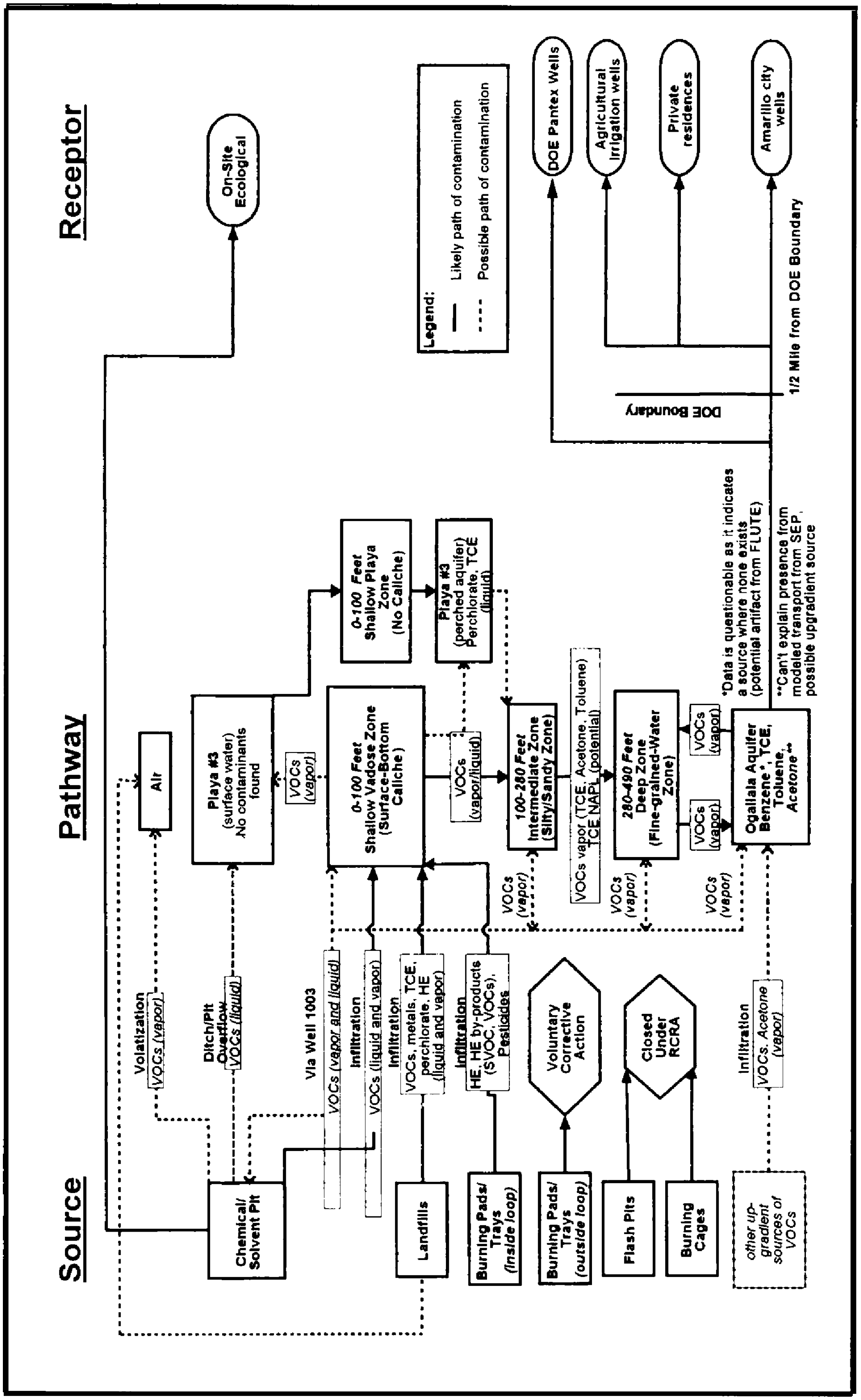

Figure 2.3-2 Conceptual Model-2
Relationships Between Sources and Receptors at Pantex Burning Ground
(Adapted from Draft in BWXT, 2001)

2.4 Data Requirements

Groundwater models require site-specific data and information concerning the flow system and contaminants. More sophisticated models(e.g., unsaturated flow models) require data in addition to that required by less sophisticated models.

Data and information required by groundwater flow models include:

- Flow system boundaries
- Depths and thicknesses of each geologic unit
- For each geologic unit:
  - Groundwater elevations or pressures (hydraulic head)
  - Recharge locations and rates
  - Discharge locations and rates
  - Hydraulic conductivities
  - Effective porosities
  - Storage coefficients
  - Hydraulic conductivity/saturation relationships (for unsaturated materials)

Additional data required by contaminant transport models may include:

- Initial distributions and concentrations of contaminants
- Locations of contaminant sources
- For each geologic unit in which transport is simulated:
  - Fluid chemistry, including concentrations of major solutes, pH, and oxidation-reduction potential
  - Dispersion coefficients
  - Bulk densities
  - Fraction of organic carbon
- For each simulated contaminant:
  - Partition coefficient
  - Biodegradation rate

3.0 Groundwater and Contamination at Pantex

There are three aquifers and two unsaturated zones at Pantex (Figure 2.3-1). The upper unsaturated zone extends from ground surface to the water table of the perched aquifer (depth ranges from 260 feet to 290 feet[3] below ground surface). The average saturated thickness of the perched aquifer is approximately 14 feet, and the maximum thickness is approximately 75 feet[4]. However, the perched aquifer is absent in some areas (e.g., Burning Grounds, See Stoller, 2001, figure 2-15). Where it is absent, a single unsaturated zone extends from ground surface to the water table of the Ogallala Aquifer. The lower unsaturated zone extends from the bottom of the perched aquifer to the water table of the Ogallala Aquifer (depth ranges from 350 feet to 425 feet below ground surface[5]). The saturated thickness of the Ogallala ranges from less than 25 feet to more than 400 feet[6]. The Dockum Group Aquifer immediately underlies the Ogallala[7].

Groundwater flow directions in the perched aquifer vary depending on location[8]. Groundwater near the western plant boundary flows southeasterly, onto the plant. Groundwater in the eastern portion of the plant flows in all directions, with a significant amount flowing off-site to the east and southeast[9]. Groundwater in the Ogallala Aquifer flows from southwest to northeast[10]. Flow directions in the Dockum Group Aquifer are not known[11].

The saturated and unsaturated zones at Pantex are contaminated with a wide variety of hazardous materials including: solvents[12] (e.g., TCE, tetrachloroethylene [PCE]), metals[13] (e.g., chromium, lead), and explosives[14] (e.g., RDX, TNT).

The perched aquifer is contaminated with solvents, metals, and explosives[15]. The most widespread contaminant is RDX. The RDX plume in the southeastern portion of the plant (Zones 11 and 12) extends approximately 3.5 miles from north to south, and 2 miles from east to west. The RDX plume extends approximately one half mile beyond the eastern plant boundary[16].

The Ogallala Aquifer in the northern portion of the plant is contaminated with TCE and toluene[17]. Benzene and toluene have been found approximately one half mile north of the plant, near the City of Amarillo's well field[18]. High concentrations of metals (e.g., lead, thallium[19]) have also been found in the Ogallala beneath Pantex. However, because background concentrations have yet to be established, the origin of these metals has not been determined.

Information on contaminants in the Dockum Group Aquifer is not available.

Additional information on groundwater and contamination at Pantex can be found in: Battelle (1997), DOE (2000h), Rice (2001a), and Stoller (2001).

4.0 Modeling Requirements and Deficiencies at Pantex

At Pantex the DOE has used, or intends to use, models to[20]:

- Predict contaminant migration rates
- Predict contaminant concentrations at potential receptors
- Evaluate alternate cleanup system designs
- Design monitoring systems
- Identify contaminant sources

4.1 Model Requirements at Pantex

The choice of models to be used at Pantex should be based on the characteristics of the groundwater systems, the distribution of contaminants, and the types of contaminants present.

A wide variety of contaminants are present at Pantex. Water is transporting these contaminants from near ground surface, through the upper unsaturated zone, to the perched aquifer (see Figure 2.2-1). Upon reaching the perched aquifer, the bulk of the contaminants are probably transported laterally. Some of them, however, may migrate into the lower unsaturated zone, and toward the Ogallala Aquifer. At any point along their flowpaths the contaminants are subject to the processes that affect contaminant transport (see section 2.2).

In view of the above, the flow models used at Pantex should be able to simulate saturated and unsaturated flow in three dimensions. The transport models should simulate the simultaneous movement of multiple contaminants, and account for the transformations that occur along the flowpaths. It is possible that other liquids (e.g., DNAPLs) are also present in the subsurface at Pantex. If so, multi-phase models may be required. Either finite difference or finite element models may be used.

4.2 Conceptual Model Deficiencies and Data Gaps at Pantex

Several important features of the flow systems and the extent of contamination remain unknown at Pantex.

- The extent of contamination in the Ogallala Aquifer is unknown. Large areas on the Pantex plant contain no Ogallala wells. These include the northwest portion of the plant, the areas around playas 2 and 4, and the area between the Burning Grounds and the Pantex supply wells in the northeast corner of the plant[21].

- The extent of the perched aquifer in the northern and western portions of Pantex, and to the northeast of Pantex, is unknown. There are few or no monitor wells or borings in the perched aquifer in these areas[22].

- The lateral extent and hydraulic properties of the Dockum Group Aquifer at Pantex are unknown[23]. The direction of any groundwater flow between the Ogallala Aquifer and the Dockum Group is also unknown[24].

- Wastewater from the Pantex was discharged to Pantex Lake from 1942 until 1970[25]. DOE has not investigated the possibility that the wastes have contaminated groundwater near the lake.

Much of the site specific data required to develop defensible models of groundwater flow and contaminant transport at Pantex have not been collected. Parameters for which no data, or an insufficient amount of data, have been collected include:

- The hydraulic conductivity of Ogallala Aquifer
- The hydraulic properties of the Dockum Group Aquifer[26]
- Relationships between hydraulic conductivity and degree of saturation
- Parameters that control contaminant transport:
    - Dispersion coefficients
    - Bulk densities
    - Fraction of organic carbon
    - Partition coefficients
    - Biodegradation rates

DOE acknowledges the existence of data gaps and other problems in its characterization of groundwater and contamination at Pantex[27]. It is correcting some of these deficiencies.

5.0 The TAG

The TAG was formed by DOE's contractor, BWXT Pantex L.L.C., to make recommendations concerning groundwater models to be used at Pantex. TAG recommendations were based on a review of groundwater systems and modeling requirements at Pantex, and a review of available models. The TAG's recommendations were not binding, and final decisions were made by the DOE.

5.1 Membership and Schedule

The following TAG members attended at least one meeting:

Ray Brady	Panhandle Groundwater Conservation District
Michelle Bolwahnn	BWXT

Boyd Deaver, Chairman	BWXT
Larry Deschaine	SAIC
Russel Edge	DOE, Albuquerque
Dr. David Janecky	Los Alamos National Laboratory
Dr. Roger Peebles	Texas Center for Applied Technology (for TNRCC)
Dr. Ken Rainwater	Texas Tech University
George Rice	STAND
Dr. Bridget Scanlon	Texas Bureau of Economic Geology
Dr. Jeff Stovall	BWXT

The following also took part in or attended the meetings: Pam Allison (STAND), John Ford (Stoller), Tad Fox (SAIC), Tom Hicks (DOE), Shawn Leppert (Leppert Associates), Laura Pendlebury (DOE), Mike Space (Terradigm), Andrea Starnes (intern), Anna Stickrod (BWXT), and Dale Stout (BWXT).

The TAG held four meetings:
August 2, 2001 - Pantex Plant
August 30 and 31 - San Antonio, TX
November 27, 2001 – Austin, TX
February 4, 2002 – Pantex Plant

5.2 Model Review and Recommendations

The TAG reviewed 19 groundwater flow and contaminant transport models. A brief description of each model is given in Appendix 1.

The TAG recommended a graded approach to modeling. Under this approach, relatively less complex models would be used initially. More complex models and model options would be used only as necessary to address issues that require more sophisticated features (e.g., multiphase flow).

The TAG recommended the development of separate models for each of three areas.

- Regional Ogallala Aquifer. This area will be modeled with a saturated flow model. The boundaries of this model may extend miles beyond the Pantex plant.
- Burning Ground and off-site areas to the north of the plant, including the City of Amarillo well field. This area will be modeled with a groundwater flow and transport model. The model will encompass the perched aquifer and Ogallala aquifer, as well as the unsaturated zones. The model will be linked to the regional Ogallala Aquifer model.
- Zones 11 and 12 on the southeast portion of the Plant, and the contaminated areas to the south and east of the plant. This area will also be modeled with a groundwater flow and transport model. The model will encompass the perched aquifer and Ogallala aquifer, as well as the unsaturated zones. The model will be linked to the regional Ogallala Aquifer model.

The Dockum Group Aquifer may also be included the models, depending on the results of future investigations. The TAG's model recommendations are presented in table 5.2-1.

In the future, the models for each area may be integrated into a single, comprehensive model. The TAG also recommended the use of computerized tools to aid in determining the extent of contamination (plume delineation) and to optimize the design of cleanup systems.

The TAG also recommended using the GMS graphical user interface (GUI). GUIs are computer programs that aid model design and create maps of model results. Other GUIs such as ArgusONE and Groundwater Vistas may be used if necessary[28].

Table 5.2-1, TAG Model Recommendations

Area	Regional Ogallala	Burning Ground	Zones 11 and 12
Groundwater Flow Model	MODFLOW (finite difference)	FEMWATER (finite element)	FEMWATER (finite element)
Bioreactive Contaminant Transport Model	SEAM3D & BioRedox	SA_MAPS FEHM	SA_MAPS FEHM
Geochemical Contaminant Transport Model (metals)	OS3D		
Option for Complex Contaminant Transport Modeling	None	HBGC123D	HBGC123D
Plume Delineation	PlumeFinder	PlumeFinder	PlumeFinder
Optimization Tools	MODOFC & SOMOS	OA Method	OA Method

Note: FEHM can be used to model the transport of both bioreactive contaminants (e.g., TCE) and metals.

5.3 Public Access to Information

The TAG recommended that model information, such as final input files, be made available to the public[29]. Both of the primary groundwater flow models recommended by the TAG (MODFLOW, FEMWATER) are available at no cost.

DOE accepted the TAG's recommendations. A detailed description of the TAG's recommendations is presented in BWXT (2002). The TAG will meet annually to review the progress of the modeling.

6.0 Assessing Model Reliability

The results of groundwater flow and contaminant transport modeling are often presented to the public as if they were the products of an objective scientific process that are beyond question. However, there is no reason to assume that a computer model produces reliable results. Some models produce results that are reliable and useful. Others produce results that are misleading or nonsensical. It is often difficult to determine whether model results are reliable, even for experts. But, one need not be an expert to ask relevant questions. The public can, and should, question the reliability of model results. The following sections present questions that can be asked, and issues that can be examined, to help assess model reliability.

6.1 Conceptual Model

Computerized models are based on conceptual models (see section 2.3). If the conceptual model is not correct, the computerized model will probably not produce reliable results. The documents that describe model results should include a thorough description of the conceptual model. Questions that should be asked of the conceptual model include: (1) Are the assumptions incorporated into the model explicitly identified, and are they reasonable? (2) Are all significant physical features included? (3) Are the major processes that affect contaminant transport included?

Problems associated with the conceptual model for Pantex are described in section 4.2.

6.2 Data

Models require input data, i.e., the values of the parameters that control groundwater flow and contaminant transport. The values of these parameters may vary over wide ranges. For example, according to the scientific literature, the hydraulic conductivity of sandy aquifers ranges from less than one foot per day, to more than 1000 feet per day[30]. Thus, reliable model results require site specific data. When site specific data are not available, modelers may: (1) collect the necessary data, or (2) rely on values reported in the literature, or (3) guess.

Modelers may ignore site specific data even when it is available. They may also use parameter values that are at, or beyond, the extremes of literature values. In some cases, this may be legitimate. However, ignoring data and using extreme values is often a sign of problems, such as a seriously flawed conceptual model, or an attempt to force the model to produce a desired result.

The lack of site specific data at Pantex is discussed in section 4.2.

6.3 Reasonable Results

Models are usually used to predict future conditions or to evaluate alternate scenarios. Thus, we often cannot say with certainty whether the results are correct. However, we can determine whether model results appear to be reasonable.

Occasionally, results are clearly nonsensical. For example; modeling done for the San Antonio Water System predicted that water levels in an aquifer would rise over a 50 year period, even as pumping was substantially increased over the 50 years[31].

Most cases aren’t as clear as the example above. Predictions may seem farfetched, but we cannot ‘prove’ them wrong. Modeling done for DOE[32] – before TCE was discovered in the Ogallala Aquifer at the Burning Grounds – predicted it would take between 135 and 1580 years for TCE to travel from Pantex to the City of Amarillo’s Ogallala well field. A dubious result such as this should lead us to question the model assumptions behind it. In this case, the modeler used a very large retardation coefficient for TCE[33].

6.4 Verification (History Matching)

Models should be tested to determine whether they can reproduce conditions known to exist in the past (e.g., water levels, contaminant distributions). This testing is called model verification, or history matching. If a model cannot reproduce past conditions, we cannot have much confidence in its ability to predict future conditions.

6.5 Sensitivity Study

There is always some uncertainty associated with model input data (e.g., hydraulic conductivity, retardation coefficients). There is not a single ‘correct’ value for most parameters. Instead, there is a range of ‘reasonable’ values. A sensitivity study is a series of model simulations in which parameter values are varied over their reasonable ranges, and the effect on model results is examined.

For example, a study might examine the sensitivity of predicted cleanup times to variations in retardation coefficients. If predicted cleanup times varied between 10 to 20 years, or 40 to 80 years – this may be acceptable from the point of view of model sensitivity. However, if the predicted cleanup times ranged from 5 to 200 years, then the model results are too sensitive to reasonable variations in input data. Model sensitivity may be reduced by collecting additional site specific data. The additional data may reduce the reasonable range of values for input parameters.

A sensitivity study should be part of every modeling project. Model results should not be presented as a single ‘answer’, e.g., cleanup will be completed in 17 years. Rather, model results should be presented as a range of reasonable predictions that are derived from a sensitivity study, e.g., cleanup will probably be completed in 12 to 22 years.

6.6 Predicted *vs* Actual Conditions (Performance Monitoring)

As time goes by, model predictions should be compared to the conditions that actually develop. For example, after three years, actual conditions should be compared to the conditions the model predicted would exist after three years. Models may need to be adjusted to correct differences between predicted and actual conditions.

7.0 References

Amarillo Globe-News, August 4, 2001.

Battelle, 1997; *Three-Dimensional (3-D) Groundwater Flow Model and Contaminant Transport Model for U.S. Department of Energy Pantex Plant*, Draft Final Report, prepared by Battelle Columbus Operations, March 17, 1997.

BWXT 2001; *Path Forward Recommendations for Groundwater Modeling at the DOE Pantex Plant,* Presentation to TAG dated October 26, 2001 (presented November 27, 2001).

BWXT, 2002; *Final Report, Recommendations of the 2001 Groundwater Modeling Technical Advisory Group for the Pantex Plant*, January 2002.

DOE, 1998a; *Environmental Information Document*, October 1998.

DOE, 1998b; *Safety Information Document,* October 1998.

DOE, 2000a; *Pantex Plant Burning Ground Monitoring Data Analysis Report for 1999*, April 2000 (citation uncertain).

DOE, 2000c; *Pantex Plant Burning Ground Monitoring Data Analysis Report for Second Quarter 2000 (April through June)*, September 2000.

DOE, 2000d; *Protecting the Ogallala Aquifer, Recommendations for Characterization of Trichloroethylene at the Pantex Burning Grounds, Final Report to the Secretary of Energy,* May 5, 2000.

DOE, 2000f; *Protecting the Ogallala Aquifer II, Recommendations for Characterization and Remediation of the Southeastern Plume at the Pantex Plant*, June 9, 2000.

DOE, 2000h; *Groundwater Program Management Action Process (GPMAP),* June 2000.

DOE 2001; Meeting Notes, Public Presentation, April 2, 2001.

Freeze, R.A., and Cherry, J.A., 1979; *Groundwater,* Prentice-Hall Inc., Englewood Cliffs, NJ, 604 pp.

IT Corporation, 2000; *Interim Corrective Measures Design: On-Site Stabilization and Treatment of the Pantex Perched Aquifer in the Zone 12 Area by Groundwater Extraction, GAC Filtration, and Chemical Precipitation*, Design Basis Document, Prepared by IT Corporation and S.M. Stoller Corporation, August 2000.

Rice, G., 2001a; *Evaluation of Groundwater Characterization and Modeling at the Pantex Plant*, STAND Technical Report 2001-1, June 2001.

Rice, G., 2001b; *Evaluation of HDR/SAWS Modeling of the Carrizo-Wilcox Aquifer in Lee, Bastrop, and Milam Counties, Texas.*

Stoller, S.M. Corporation, 2001; Final FY 2000 Summary and Progress Report for Groundwater Investigations at DOE Pantex Plant, January 29, 2001.

8.0 Endnotes

[1] BWXT, 2002.
[2] A brief review of model mathematics is presented in BWXT 2002, Appendix B.
[3] DOE, 2000f, page 1.
[4] Stoller, 2001, figure 2-15.
[5] Battelle, 1997, page 10.
[6] BWXT, 2002, Figure 2.16.
[7] Battelle, 1997, page 13.
[8] DOE, 2000h, page C-1; and Rice, 2001a, page 5.
[9] Battelle, 1997, page 41, figure 4-10.
[10] Rice, 2001a, figure 4.
[11] Battelle, 1997, page 13.
[12] DOE, 2000d, page 6; DOE 2000f, page 1; and Stoller, 2001, pages 1-54 and 1-83.
[13] DOE, 1998a, page 16-10; and DOE, 1998b, Appendix B; and Stoller, 2001, pp. 1-26, 1-43, and 1-69.
[14] DOE, 1998b, Appendix B; and Stoller, 2001, page 1-39.
[15] IT, 2000, page 3-1; and DOE 2000f, page 1.
[16] Stoller, 2001, figure 4-1.
[17] DOE, 2000a, page 17; and DOE, 2000c, pages 19 and 29.
[18] Amarillo Globe-News, August 4, 2001. Contaminants found within 200 yards of city well 623.
[19] Rice, 2001a, table 1.
[20] BWXT, 2002, pages 18 and 23.
[21] BWXT, 2002, Figure 2.15; and Stoller, 2001, figure 1-19.
[22] BWXT, 2002, Figures 2.8 and 2.9; and Stoller, 2001, figure 1-19.
[23] Battelle, 1997, page 13.
[24] DOE, 2000h, page C-9.
[25] DOE, 1998a, page 5-5.
[26] DOE, 2000h, page C-9.
[27] Stoller, 2001, chapter 6.
[28] BWXT, 2002, pages 49 and 50.
[29] BWXT, 2002, page 52.
[30] Freeze and Cherry, 1979, page 29.
[31] Rice, 2001b.
[32] IT, 2000, Appendix B, *Pantex Fate and Transport Modeling in Support of Groundwater Treatment System Expansion, Analysis of 1,2-DCA and TCE Outside of 25-Year Capture Zone,* July 23, 1999, Table 2, well 06-44-307.
[33] IT, 2000, Appendix B, *Pantex Fate and Transport Modeling in Support of Groundwater Treatment System Expansion, Analysis of 1,2-DCA and TCE Outside of 25-Year Capture Zone,* July 23, 1999, Table 1.

Appendix 1 – Models Reviewed by the TAG

The following models were reviewed by the TAG. Additional information on each model can be found in BWTX (2002) and at the website addresses provided below.

BioRedox-MT3DMS
3-D contaminant transport. Multi-component dispersion, sorption, chemical transformations, and biodegradation-redox reactions. Biodegradation mechanisms include oxidation, co-metabolism, and reductive dehalogenation. Also capable of simulating NAPL dissolution. Must be used in conjunction with a groundwater flow model.
Website: http://www.enssi.com/P4-0-BioRedoxMain.htm

FEFLOW (Finite Element subsurface FLOW system)
3-D groundwater flow, heat flow, and contaminant transport. Saturated and unsaturated flow. Capable of simulating single component dispersion, sorption, and chemical reactions.
Website: http://www.wasy.de/english/produkte/feflow/index.html

FEHM (Finite Element Heat and Mass transfer)
3-D groundwater flow, heat flow, and contaminant transport. Saturated and unsaturated flow. Multiphase (gas, water, and oil), multi-component, flow through porous and fractured media.
Website: http://www.ees5.lanl.gov/fehm

FEMWATER
3-D groundwater flow and contaminant transport. Saturated and unsaturated flow. Capable of simulating dispersion, adsorption, decay, and biodegradation.

HBGC123D (HydroBioGeoChem123D)
3-D contaminant transport and heat transfer in saturated and unsaturated materials. Capable of simulating multi-component dispersion, sorption, chemical and microbiological reactions. Accounts for reaction kinetics. Must be used in conjunction with a groundwater flow model.
Website: http://hbgc.esd.ornl.gov

MAGNAS
3-D groundwater flow and contaminant transport. Saturated and unsaturated flow. Multiphase flow (water, air, and NAPL). Capable of simulating dispersion, sorption, volatilization, and mineral dissolution and precipitation.
Website http://www.hgl.com/software/MAGNAS.cfm

MODFLOW
3-D groundwater flow. Website: http://water.usgs.gov/software/modflow-2000.html

MODFLOW-SURFACT
3-D groundwater flow and contaminant transport. Saturated and unsaturated flow. Multi-component flow capable of simulating dispersion, sorption, decay, and biodegradation.
Website: http://www.hgl.com/software/M-SURFACT.cfm

MT3DMS (Modular Transport 3-D Multi-Species)
3-D contaminant transport. Single component dispersion, sorption, and chemical reactions. Must be used in conjunction with a groundwater flow model.
Website: http://hydro.geo.ua.edu/mt3d

NAPL Simulator
3-D contaminant transport in the saturated and unsaturated zones. Capable of simulating multiphase flow (water, NAPL, gas) and transport of a single solute.
Website: http://www.epa.gov/ada/csmos/models/napl.html

NUFT (Nonisothermal Unsaturated-Saturated Flow and Transport model)
A suite of 3-D groundwater flow and contaminant transport models. Saturated and unsaturated flow. Multiphase and multi-component.

OS3D (Operator Splitting 3-Dimensional reactive transport, also known as CRUNCH)
3-D contaminant transport. Multi-component dispersion, mineral dissolution and precipitation reactions. Must be used in conjunction with a groundwater flow model.
Website: http://www.earthsci.unibe.ch/tutorial/os3d.htm

Princeton Transport Code
3-D groundwater flow and contaminant transport. Saturated and unsaturated flow. Multi-component flow capable of simulating dispersion and sorption.
Website: http://ftp.argusone.com/pub/PTC_Files/Ptc-hbk.pdf

RT3D (Reactive Transport in 3-Dimensions)
3-D contaminant transport in saturated materials. Multi-component sorption, chemical reactions, and biodegradation. Must be used in conjunction with a groundwater flow model. Website: http://bioprocess.pnl.gov/rt3d.htm

SA_MAPS (Stream-Aquifer Management and Planning Simulator)
3-D groundwater flow and contaminant transport. Saturated and unsaturated flow. Multiphase flow (water, oil, and gas). Capable of simulating dispersion, diffusion, sorption, and biodegradation kinetics. SA MAPS is a family of codes that includes: **BioF&T3D**, **BioSlurp**, **BioSVE**, **MARS**, **MOFAT**, **MOVER**, **OILVOL**, and **SOILPARA**.
Website: http://www.rasint.com/software.html

SEAM3D (Sequential Electron Acceptor Model, 3 Dimensional)
3-D contaminant transport. Multi-component dispersion, sorption, and biodegradation. Must be used in conjunction with a groundwater flow model.
Website: http://gms.watermodeling.org/html/seam3d.html

TRACR3D
3-D groundwater flow and contaminant transport. Saturated and unsaturated flow of air and water in porous or fractured media. Multi-component flow capable of simulating sorbtion and biokinetics.
Website: http://www.ees5.lanl.gov/porous_media.html

TOUGH2 (Transport Of Unsaturated Groundwater and Heat, Version 2.0)
3-D groundwater flow, heat flow, and contaminant transport. Saturated and unsaturated flow in porous and fractured media. Multiphase flow (water, air, NAPLs, and volatile organic compounds (VOCs)), mineral dissolution and precipitation.
Website: http://www-esd.lbl.gov/TOUGH2/tough2v2.html

UTCHEM
3-D groundwater flow, heat flow, and contaminant transport. Saturated and unsaturated flow. Multiphase (water, gas, oil) and multi-component. Capable of simulating dispersion, sorption, biodegradation, and mineral dissolution and precipitation.
Websites: http://www.epa.gov/ada/csmos/models/utchem.html and http://www.pe.utexas.edu/CPGE/UTCHEM

Appendix 2 – Glossary

Aquifer: a saturated geologic formation capable of transmitting an economically significant quantity of water.

Biodegradation (biologic decay): the destruction of organic contaminants (e.g., TCE, toluene) by microorganisms. This process may convert one contaminant into another, e.g., TCE biodegrades to DCE, which biodegrades to vinyl chloride.

Bulk density: the density of a material, usually soil or rock, including pore spaces. The in-place or undisturbed density. For example, the density of the minerals that make up a soil may be 170 pounds per cubic foot. But the bulk density of the soil; including pore spaces, organic matter, and minerals, may be 110 pounds per cubic foot.

Capillary fringe: a zone immediately above the water table. The water in this zone is held by capillary forces and cannot flow freely. Portions of the capillary fringe may be saturated.

Dehalogenation: the removal of a halogen atom (e.g., chloride, fluoride) from a molecule.

Discharge: the movement of water out of a groundwater system. Water may be discharged naturally through springs and evapotranspiration, or through man made structures such as wells and drains.

Dispersion: the dilution of a contaminant due to spreading of the contaminant plume. The spreading occurs in all directions; parallel to the flow (longitudinal dispersion) and perpendicular to flow (transverse dispersion). It is caused by variations in groundwater flow directions and speeds. An analogous processes is the spreading (dispersion) of a plume of smoke from a smokestack.

DNAPL: Dense Non-Aqueous Phase Liquid. Liquids that are more dense than water. Hence, they tend to sink to the bottom of aquifers. Most chlorinated solvents (e.g., TCE, DCE) are DNAPLs. DNAPLs are liquids, sometimes referred to as ‘pure product’. They should not be confused with solutes – contaminants that are dissolved in the groundwater.

Effective porosity (also see porosity): the amount of interconnected porosity available for the transmission of fluids. Effective porosity is expressed as a ratio or percentage. In most materials, effective porosity and total porosity are nearly equal. However, some materials, such as clays, have high total porosities but low effective porosities because the pore spaces are too narrow to allow water to flow freely. In other materials, such as volcanic rocks, the pore spaces may not be interconnected.

Graphical User Interface (GUI): a computer program; pre-processor and post-processor tools that allow modelers to automate some aspects of model design (e.g., grid generation, calibration), integrate optimization tools with models, and create maps of model results.

Hydraulic conductivity: a measure of the ability of a material allow water to flow through it. The higher the hydraulic conductivity of a material, the easier it is for water to flow through it. Hydraulic conductivity is expressed as length per unit time (e.g., feet per day, centimeters per second).

Hydraulic head: the elevation of water in a well. Groundwater flows from areas of higher hydraulic head to areas of lower hydraulic head. Hydraulic head is a measure of the energy of groundwater and is the sum of two components; elevation head, and pressure head.

LNAPL: Light Non-Aqueous Phase Liquid. Liquids that are less dense than water. Hence, they float on the water table. Common LNAPLs include oil, gasoline, and diesel fuel. LNAPLs are liquids, sometimes referred to as 'pure product'. They should not be confused with solutes – contaminants that are dissolved in the groundwater.

NAPL: Non-Aqueous Phase Liquid. General term that includes DNAPLs and LNAPLs. NAPLs are liquids, sometimes referred to as 'pure product'. They should not be confused with solutes – contaminants that are dissolved in the groundwater.

Organic: derived from plant or animal materials.

Organic carbon: carbon derived from organic sources (e.g., plant material). Distinguished from carbon derived from non-organic sources (e.g., atmospheric carbon dioxide, carbonate minerals). Organic carbon sorbs organic contaminants.

Oxidation: the addition of oxygen to an atom or molecule, or the removal of electrons from an atom or molecule.

Partition coefficient: a measure of the degree to which a solute is adsorbed. Solutes with higher partition coefficients (e.g. TCE) are more strongly adsorbed (i.e., bound to the solid material of the aquifer) and migrate more slowly (are more retarded) than contaminants with lower partition coefficients (e.g., vinyl chloride). For organic contaminants, the partition coefficient increases as the amount of solid organic carbon in an aquifer increases.

Porosity: a measure of void space in a material. The ratio of the volume of void spaces in a rock or sediment to the total volume of the rock or sediment. Voids may be spaces between sand grains, fractures, or solution cavities. In the saturated zone, the void spaces are completely filled with water. In the unsaturated zone, the voids are filled with water and air.

Precipitation: the combination of solutes to form a solid material. Metals often precipitate, as when dissolved iron and carbonate combine to form the mineral siderite. Precipitation reactions are often not reversible, and the precipitated contaminant is permanently removed from the groundwater.

Recharge: the entry of water into a groundwater system. Recharge often occurs along streambeds, along mountain fronts, and through the bottoms of playas.

Reduction: the addition of electrons to an atom or molecule.

Retardation: Due to sorption, most contaminants move more slowly than the groundwater which transports them. Their movement is said to be retarded with respect to the groundwater.

Retardation coefficient: a measure of retardation - the rate at which a solute travels through a groundwater system, compared to the velocity of the groundwater. The ratio of the groundwater velocity to the solute velocity. A solute with a retardation coefficient of 2 moves at ½ the velocity of the groundwater that is transporting it.

Saturated zone: a zone where the void spaces are completely filled with water or some other liquid.

Sensitivity study: a test of a model's response to changes in parameter values or assumptions (e.g., hydraulic conductivity, boundary conditions).

Sink, groundwater: see discharge.

Solute: a substance dissolved in a liquid.

Sorption: A process that binds, usually temporarily, a contaminant to a mineral surface or to organic matter. This temporary binding acts to reduce (retard) the contaminant migration rate with respect to the groundwater. Sorption is a general term used to encompass the processes of absorption and adsorption.

Source, groundwater: see recharge.

Storage coefficient: a measure of the ability of an aquifer to store and release water. The volume of water an aquifer releases from or takes into storage, per unit surface area of the aquifer, per unit change in hydraulic head.

Unsaturated zone: a zone where the void spaces are not completely filled with water or some other liquid.

Vadose zone: the unsaturated zone plus the capillary fringe immediately above the water table. The capillary fringe may be saturated.

Volatilization/Vaporization: the formation of gasses that may emerge from water as vapors.

2-D model: a model that simulates flow or contaminant transport in space two dimensions. The dimensions may be horizontal or vertical (cross section).

3-D model: a model that simulates flow or contaminant transport in three space dimensions.