7.4 Groundwater/Vadose Zone Integration Project Activities

D. G. Horton

Several activities were completed in 2001 to support the Groundwater/Vadose Zone Integration Project's System Assessment Capability modeling efforts. Data were gathered to describe the distribution of subsurface contamination for comparison with the results of numerical models describing contaminant distribution. Also, activities were completed that describe the features, events, and processes that are important for waste management and remediation efforts at the Hanford Site. This section discusses the activities of the vadose zone module of the System Assessment Capability.

7.4.1 Hanford Site Hydrogeologic Databases

D. G. Horton

The Characterization of Systems Task under the Groundwater/Vadose Zone Integration Project is responsible for establishing a consistent set of data, parameters, and conceptual models to support efforts to estimate the migration and impact of contaminants at the Hanford Site. As part of these efforts, the task assembled a series of catalogs in 2001 that identified the depth and breadth of existing geologic, hydrologic, and geochemical data. These catalogs are the first step in developing a comprehensive, useable, and scientifically defensible database of geologic, hydrologic, and geochemical data.

Fifty-five years of technical data gathering at the Hanford Site have resulted in data scattered among numerous databases, published and unpublished reports, and the technical files of individual contributors. The purpose of the catalogs was to identify these existing data, make an initial cursory assessment of the quality of the data, and gather the sources of the data in one place. Three catalogs were published and a fourth was drafted:

- *A Catalog of Geologic Data for the Hanford Site* (PNNL-13653)
- *A Catalog of Vadose Zone Hydraulic Properties for the Hanford Site* (PNNL-13672)
- *Data Catalog for Models Simulating Release of Contaminants from Hanford Site Waste Sources* (PNNL-13666)
- *Hanford Contaminant Distribution Coefficient Database and Users Guide* (PNNL-13895).

The geologic data report (PNNL-13653) includes 2,640 wells and boreholes in the 100 Areas, 200 Areas, and 300 Area from which some kind of geologic data exist. Nearly all of the wells (2,501) have some form of driller's log or geologist's log. Archived samples are available from 1,740 wells. Particle size distribution data are available from 1,124 of the wells, calcium carbonate content is available from 981 wells, and moisture content data from 423 locations. Most wells have data from numerous samples (e.g., 1.5-meter [5-foot] intervals throughout the well). In addition, some kind of geochemical data (excluding calcium carbonate content data) are available from 587 wells, physical property data (other than particle size distribution and moisture) are available for 269 wells, mineralogic information is available from 52 wells, and geochronology data from 23 wells. The report also contains an annotated bibliography of 158 references that contain the geologic data. This compilation of data sources is the most comprehensive made for the Hanford Site. It is believed that >90% of the available geologic data are represented.

The hydraulic property catalog (PNNL-13672) contains data sources from 182 boreholes and surface locations on the Hanford Site. For each sample location, there may be data from multiple depth intervals and many measurements taken at multiple time intervals. Table 7.4.1 shows the types of data available and their locations.

Table 7.4.1. Types, Abundances, and Locations of Laboratory and Field Hydraulic Data on the Hanford Site

Location (Area)	Sieve	Density	Moisture	Unsaturated Conductivity	Saturated Conductivity	Neutron	Storage	Drainage	Water Profile	Air Permeability
100	84	84	84	33	33	(a)	--	--	--	--
200-East	122	125	108	63	46	36	--	2	--	1
200-West	163	124	60	89	29	--	1	3	1	1
300	--	--	2	--	--	--	1	1	1	--
400	--	--	--	--	--	--	--	1	1	--
600	177	168	149	49	46	--	8	9	8	--
Total	468	501	423	234	154	36	10	16	11	2

(a) No data available.

The report summarizing release models (PNNL-13666) used in Hanford Site assessments published over the past 14 years (1987 to 2001)

- provides a summary of descriptions and uses of release models
- describes mathematical formulations that commonly have been used in recent years
- links release models to data on various waste sources found on the Hanford Site (i.e., saltcake, cement, soil-debris, reactor block, glass, and corrosion)
- provides sources of information and data used in the models.

The links allow users to quickly locate the specific release model information and data sources they need to apply the models to future site assessments.

The fourth report (PNNL-13895) contains distribution coefficient data for the sorption of several species on Hanford Site sediments. It is believed that ~90% of existing distribution coefficients are represented in the database. Table 7.4.2 lists the species for which data are compiled. Included with the distribution coefficients are pertinent experimental data such as the experimental method, equilibration time, initial concentrations in solution, solution/solid ratio, and source reference. In addition to these data, more detailed information about the solution composition and the composition and characteristics of the sediment are given in two appendices of PNNL-13895.

Table 7.4.2. Distribution Coefficients Included in the Geochemical Compilation

Species	Americium (Am^{3+})	Cobalt (Co^{2+})	Cesium (Cs^{+})	Nickel (Ni^{23+})	Lead (Pb^{2+})	Plutonium (Pu)	Strontium (Sr^{2+})
Number of Data	60	74	126	50	48	87	220
Species	**Chromate (CrO_4^{2-})**	**Iodine (I^-)**	**Nitrate (NO_3^-)**	**Neptunyl Ion (NpO^{2+})**	**Selenite Ion (SeO_4^{2-})**	**Pertechnetate Ion (TcO_4^-)**	**Uranyl Ion (UO_2^{2+})**
Number of Data	20	61	12	84	49	83	76

7.4.2 Initial Assessment Using the System Assessment Capability – Preliminary Vadose Zone Results

D. G. Horton and G. V. Last

An initial assessment is being conducted with the System Assessment Capability that simulates the transport of 10 different radionuclide and chemical contaminants released from 890 wastes sites, over a time frame of about 1100 years from 1944 through 3050. (The System Assessment Capability is the initial set of tools and data to determine the impact of the Hanford Site on the nearby environment.) During 2001, an initial assessment was performed to demonstrate proof-of-principle for the capability. The following discussion focuses on some preliminary results from vadose zone simulations conducted at the end of fiscal year 2001.

Three major efforts were associated with the vadose zone portion of the initial System Assessment Capability assessment: data gathering, history matching, and the initial simulations. This section summarizes each of these efforts.

Data Gathering. Data were compiled to support vadose zone modeling as part of the initial assessment performed using the System Assessment Capability. The data defined the physical and geochemical parameters for the vadose simulations conducted as part of the initial assessment.

Thirteen aggregate areas were defined based on geographically contiguous areas with relatively homogeneous hydrogeologic characteristics. Each of the six 100 Areas were designated as separate aggregate areas; the 200 Areas were divided into six aggregate areas based on differences in hydrogeologic characteristics; and a single aggregate area was defined for the 300 and 400 Areas.

Generalized geologic sequences were defined for each of the 13 aggregate areas. The sequences were based on existing information from driller's logs, geologist's logs, geophysical logs, and published interpretive depths of hydrogeologic units. Estimated average strata thicknesses were used for the generalized columns.

Hydraulic property data were assigned to each layer in each geologic sequence. From these data, residual saturation and effective porosity were estimated. Data were taken from WHC-EP-0883, HNF-4769, RPP-2696, and SAND98-2880.

Six types of waste chemistry were defined for use in the Composite Analysis (PNNL-11800). (The Composite Analysis is a radiological assessment to estimate dose to hypothetical future members of the public from low-level waste disposal and all other sources of radioactive contamination at the Hanford Site.) These waste chemistry types describe chemically distinct waste streams that affect the sorption of contaminants.

These same waste chemistry types were adapted for use in the initial assessment of the System Assessment Capability to assign distribution coefficients to each geologic layer in each of the 13 geologic sequences. The distribution coefficients describe the mobility of each specific contaminant in the vadose zone environment.

Finally, recharge rates were estimated for all surface conditions under consideration for the initial assessment of the System Assessment Capability. These conditions include four different barrier designs, degraded barriers, natural conditions, and unique conditions created by human activity.

Vadose Zone History Matching. The purpose of the history matching effort was to compare test model predictions with field observations. Eight facilities were selected for System Assessment Capability history matching (Table 7.4.3). These facilities were selected because they represented

- facilities from different aggregate areas
- facilities with a range in discharge from low volume (216-B-46 crib) to high volume (216-A-8 crib)
- facilities that received chemically different waste steams
- facilities that received at least one of the selected constituents of interest (cesium-137, technetium-99, carbon tetrachloride, plutonium-239/240, and tritium)
- facilities for which historical subsurface contaminant distributions through time were available.

Each facility was assigned an array of attributes that included one of the 13 geologic sequences with assigned hydrologic and chemical properties, the volume of waste discharged, and the surface area receiving the discharge.

Four types of data were used to describe the historical distribution of contamination in the vadose zone: borehole spectral gamma-ray logs, laboratory data obtained from soil samples collected during drilling,

Table 7.4.3. Test Cases for Vadose Zone History Matching

Facility	Constituent	Year Simulated	Facility Area Multiplier	Simulation ID Number
216-A-8 crib	^{137}Cs	1995	1x	1
			2x	2
	^{99}Tc	1945-2050	1x	3
	^{3}H	1945-2050	1x	4
216-B-5 reverse well	^{137}Cs	1979	1x	5
			5x	6
			50x	7
216-B-46 crib	^{137}Cs	1991	1x	8
			0.5x	9
		1996	1x	10
	^{99}Tc	1945-2050	1x	11
	^{3}H	1945-2050	1x	12
241-T-106 tank	^{137}Cs	2000	1x	13
			0.5x	14
216-Z-1A tile field	$^{239/240}Pu$	1998	1x	15
			2x	16
		2050	1x	17
			2x	18
		3000	1x	19
			2x	20
	Carbon tetrachloride	1992	1x	21
		2050	1x	22
216-Z-12 crib	$^{239/240}Pu$	1998	1x	23
		2050	1x	24
216-U-10 pond	Water	1940-2045	1x	25
			2x	26
			3x	27
216-U-12 crib	^{137}Cs	1991	1x	28
			2x	29

gross gamma-ray logs, and groundwater chemistry data. Three criteria were developed with which to judge the success of the System Assessment Capability simulations. The criteria were

- Does the simulated result place the center of mass of the contaminant distribution within the same hydrogeologic unit as the measured center of mass for the same time period? If yes then,
- Does the simulated center of mass fall within ±2 meters (±6.5 feet) of the measured center of mass for plutonium-239 or within ±3 meters (±10 feet) of the measured center of mass for cesium-137?
- For highly mobile constituents (e.g., carbon tetrachloride, technetium-99, tritium), the success criterion was whether the simulation matched the time of first arrival of a surrogate constituent at the water table within ±2 years.

Table 7.4.3 lists the 29 cases tested. Table 7.4.4 shows the results of each history match test. Figure 7.4.1 shows an example history matching result. The figure shows a comparison of two simulated cesium-137 distributions with the measured concentrations for the 216-A-8 crib in the 200-East Area.

The two simulations include (1) a 1x simulation that used the facility dimensions to define the wetted

Table 7.4.4. Results of Vadose Zone History Matching[a]

Facility	ID	Stratigraphic (or First Arrived) Criteria	Simulated Stratigraphy (or) First Arrival)	Center of Mass Criteria (depth in m)	Simulated Center of Mass (depth in m)
216-A-8 crib	1	Hanford gravel	*Hanford sand*	7.8	*11.2*
	2		Hanford gravel		8.2
	3	Not determined	*2017*		
	4	Not determined	*1956*		
216-B-5 reverse well	5	Ringold Formation	*Hanford formation/ Plio-Pleistocene*	Not determined	Not determined
	6				
	7				
216-B-46 crib	8	Hanford gravel	Hanford gravel	8.3	*5.1*
	9				5.3
	10			12.3	*5.1*
	11	(1956)	(1956)		
	12	(1956)	(1956)		
241-T-106 tank	13	Hanford gravel	*Hanford gravel*	13.2	12.0
	14				12.1
216-Z-1A tile field	15	Backfill	Hanford gravel	5.2	8.2
	16				7.5
	17		NA[b]		NA
	18		NA		NA
	19		NA		NA
	20		NA		NA
	21	(1963)	*CCL4 did not reach groundwater by 2050*		
	22				
216-Z-12 crib	23	Hanford gravel	*Backfill*	7.2	5.8
	24		NA		NA
216-U-10 pond	25	Simulations for 216-U-10 pond were done only to assure that the model worked for a pond disposal site			
	26				
	27				
216-U-12 crib	28	Hanford coarse	Hanford coarse	7.3	7.1
	29				6.0

(a) Criteria in *italics* are outside the acceptance criteria.
(b) NA = Not applicable; applies to simulations of future contaminant configurations.

column area beneath the crib and (2) a 2x simulation that used twice the facility dimensions to define the wetted column area. Adjustments to the wetted areas were an attempt to capture the lateral spreading that normally occurs in the vadose zone.

Comparing the concentrations measured in field data obtained in 1995 with the simulated concentrations for the 1x case showed that the bulk of contamination as measured in the field was at a depth of 7.8 meters (25.6 feet), whereas the simulated bulk of contamination was at a depth of 11.2 meters (37 feet). Also, the bulk of measured contamination was within the Hanford formation gravel sequence, whereas the simulated result was within the Hanford formation sand sequence. Thus, the simulation was outside both acceptance criteria.

Comparing the results for the 2x case showed that the simulated bulk of contamination was at a depth of 8.2 meters (27 feet) and within the Hanford formation gravel sequence. Thus, the 2x simulation was within the acceptance criteria.

Approximately 30% of the deterministic test cases initially failed to meet the acceptance criteria. However, modifications to the wetted column areas reduced the failure rate to <20%. Those test cases that continued to fall outside the acceptance criteria were associated primarily with either plutonium or carbon tetrachloride.

The reasons the plutonium test cases failed were due in part to the assigned generalized stratigraphy and associated hydraulic properties and in part to the

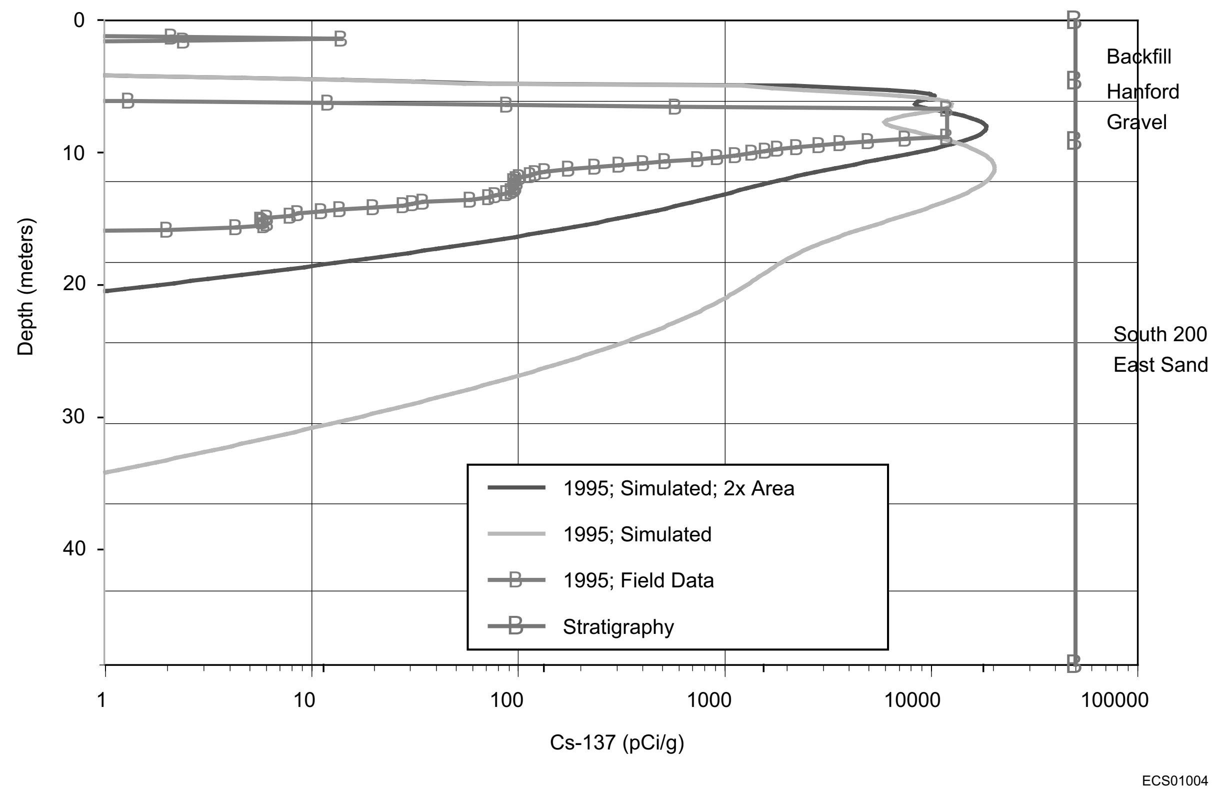

Figure 7.4.1. Cesium-137 History Matching Results for the 216-A-8 Crib

simplified algorithms used to simulate plutonium transport. In reality, plutonium in the effluent stream was probably present as both a plutonium dioxide particulate that was filtered from the effluent by the sediment directly beneath the facilities and as an organometallic complex which transported plutonium deeper in the system (RHO-ST-17), neither of which was accounted for in the simulation.

The carbon tetrachloride simulations failed because they considered only aqueous phase transport and not organic (non-aqueous) phase transport.

The overall results of the history matching exercise indicated that the System Assessment Capability computer codes were ready for the overall history match and initial assessment.

Initial Results of the System Assessment Capability. The migration of contaminants through the vadose zone was simulated with the Subsurface Transport Over Multiple Phases (STOMP) computer code (PNNL-11217; PNL-8637). The original 890 waste sites were reduced to 719 sites by aggregating nearby solid waste or low volume liquid disposal sites.

Four vadose zone template models were prepared for each of the 13 aggregate areas. These corresponded to sites representing surface liquid disposal, shallow land liquid disposal (cribs and trenches), buried waste tank disposal, and reverse well disposal of contaminants. A total of 67 base templates were prepared. By distributing copies of the base templates, 719 site templates were created, each of which was then modified within the System Assessment Capability model by inserting randomly selected values from the range of possible values for hydrologic and geochemical properties to create the final set of input files for simulation.

Preliminary results from the initial assessment are available for 25 simulations of 9 contaminants at 719 vadose zone release locations, or a total of 161,775 individual simulations. Direct analysis of individual results was impractical, so a way was developed that allowed evaluation of accumulated results in various ways. The results were examined at a variety of levels from individual contaminants at an individual waste disposal site to total releases from the Hanford Site as a whole. The results also indicated where improvements to the initial assessment were needed and provided insight in understanding Hanford Site issues.

At one level, the total Hanford Site releases from the vadose zone to groundwater were summed over all 719 sites by year, by constituent, and by simulation. An example of this is shown in Figure 7.4.2 that illustrates the total Hanford Site releases by constituent. This figure indicates that nearly all releases from the vadose zone to the groundwater occurred prior to ~1990, except for carbon tetrachloride and hexavalent chromium, which will continue to be released for some time into the future.

Another analysis determined the mass balance and vadose zone releases to groundwater by disposal facility type and by operational area. For example, Figure 7.4.3 illustrates the releases of tritium from the vadose zone to groundwater from the various types of disposal facilities. The results indicate that nearly all releases are from cribs and that they occurred before ~1995.

Use of Process Relationship Diagrams to Develop Conceptual Models

G. V. Last, V. J. Rohay, F. J. Schelling, and L. Soler

This section reproduces the abstract of the report PNNL-SA-34515 that describes the strengths and limitations of process relation diagrams. The actual master process relationship diagram and two test case diagrams are presented in the original report. They are not reproduced here because of the complexity of the diagrams.

The Characterization of Systems Task under the Groundwater/Vadose Zone Integration Project tested the application of features, events, and processes methodology (Nuclear Energy Agency 2000) for documenting the technical knowledge about the Hanford Site and application of that knowledge for performing impact/risk assessments. As part of that effort, the Characterization of Systems Task is evaluating the use of process relationship diagrams to document the relationships between features, events, and processes and to assist development, communication, and translation of conceptual models (i.e., what is known and not known about a particular environmental problem) into simplified implementation models that can be numerically simulated. A master process relationship diagram was created to describe the most relevant high-level processes and conditions affecting contaminant transport at the Hanford Site.

This diagram graphically represents the logical structure of how the environmental system works and identifies the important processes and their interrelationships. This master diagram was from domain-specific (e.g., vadose zone-specific) diagrams prepared independently for various components (technical

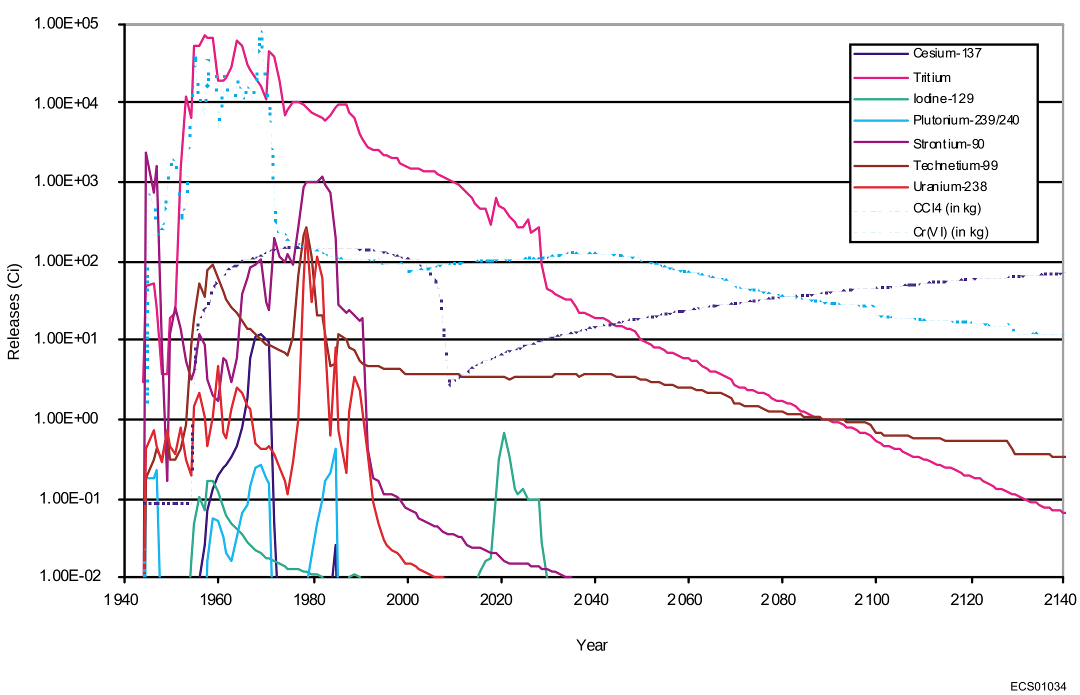

Figure 7.4.2. System Assessment Capability Simulation of Total Hanford Annual Releases from the Vadose Zone to Groundwater by Constituent

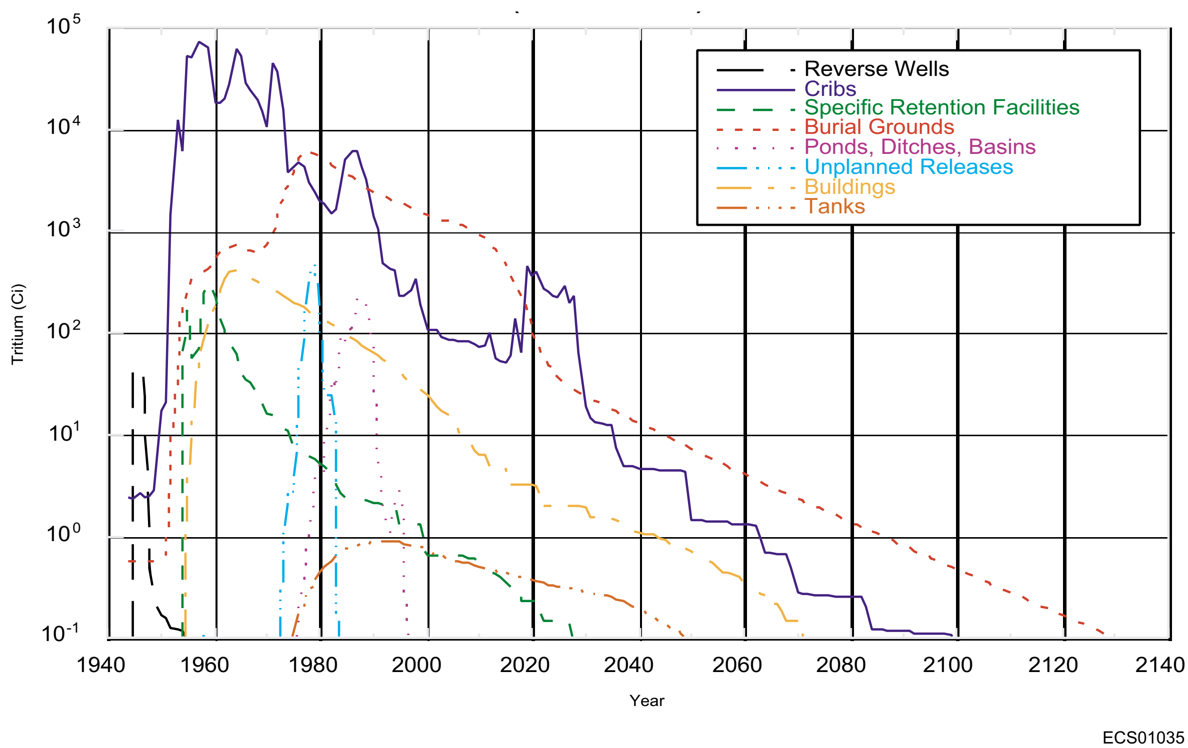

Figure 7.4.3. System Assessment Capability Simulation of Total Hanford Annual Releases of Tritium from the Vadose Zone to Groundwater by Waste Facility Types

elements) of the system (i.e., inventory, release, vadose zone, groundwater, river, and risk). The diagram was necessarily simplified by focusing on processes, keeping it at a high level, and by not including details of the risk elements. The preparation of this master diagram was intended only as an example or template for the development of problem-specific diagrams.

The master process relationship diagram then was used to analyze two different types of problems from two related operable units. The first problem attempted to identify the dominant, and to some extent the subordinate, processes controlling the fate and transport of all contaminants released from the 200-PW-1 Operable Unit. (The 200-PW-1 Operable Unit is a group of related waste sites in the 200-East and 200-West Areas that received similar uranium-rich process waste.) The second problem attempted to examine different conceptual models for the 200-ZP-1 Operable Unit, a group of related waste sites in the 200-West Area that received carbon tetrachloride wastes, concerning high carbon tetrachloride concentration in groundwater beneath the Plutonium Finishing Plant, and in doing so, to assist site selection and data collection strategies for a proposed borehole that would test these various conceptual models.

These limited efforts suggest that development and application of process relationship diagrams is a useful approach with the flexibility to facilitate the development and documentation of conceptual models for many types of environmental problems. This approach also can provide a consistent framework and method to facilitate the completeness of those conceptual models. One of its greatest values is to facilitate discussion among the principal project scientists.

However, these diagrams can become very complex and can be difficult for audiences to visualize. It is often difficult to show on one diagram all the necessary levels of detail and important features, conditions, and attributes that affect the processes. Thus, several different diagrams at different levels of detail may be needed to represent a given problem. The use of a master process relationship diagram is not intended as a stand-alone tool, but instead should be used in a facilitated process, in combination with other methods (e.g., graphical illustrations, text, influence matrices, calculations), to fully analyze and document the conceptual models.