### DEVELOPMENT OF A SITE-WIDE SYSTEM ASSESSMENT CAPABILITY

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# ABSTRACT

The Hanford Site has initiated an effort to assess the cumulative long-term effects of Hanfordderived contaminants to the Columbia River and the region after the site closes. The assessment will include impacts to human and ecological health as well as the region's economy and cultures. To conduct this assessment, the site is in the process of developing the necessary tools and supporting data. The computational capability for performing an initial assessment is known as the System Assessment Capability (SAC Rev. 0).

SAC Rev. 0 is being applied during fiscal year 2001 to produce an initial assessment that is essentially a "proof-of-principle" that a probabilistic analysis of this scope and scale can be performed in a reasonable period of time and for a reasonable commitment of resources. However, initial results will also provide insight for the design of an improved capability, (e.g., SAC Rev 1) that can be used to support cleanup decisions that must be made in a regulatory environment. They should also provide an appreciation of sources of uncertainty and needed investment to first quantify and then reduce the uncertainty of results. At this time, aspects of history matching the SAC Rev. 0 models to uncertain Hanford Site events from 1944 to present are being studied. Initial indications are that a site-wide assessment of this scope and scale, when conducted in a time frame of interest to decision makers, is possible but will fully utilize computational resources available.

# **INTRODUCTION**

The Columbia River is a critical resource for the Pacific Northwest. The life style and economy of the region is intricately tied to the river, its resources, and the plants and animals the river supports. The river is also what drew the federal government to establish the Hanford Site for production of nuclear weapon materials. Past Hanford Site operations created a variety of complex waste streams from facilities, a large number of waste sites, and released a number of radioactive and hazardous chemical contaminants to the environment.

# THE SYSTEM ASSESSMENT CAPABILITY

A decade ago DOE required site-specific or waste-form-specific analyses such as performance assessments for active disposals, and remedial investigation / feasibility studies for past practice sites. In response to the Defense Nuclear Facility Safety Board Recommendation 94-2 (1), DOE Order 435.1 (2) now requires a site-wide assessment of the all-pathways dose for all radioactive wastes, and completed the first such analysis for the Hanford Site in 1998 (3). The Columbia River Comprehensive Impact Assessment (CRCIA) Part II document (4), written by representatives of federal and state regulatory agencies, stakeholders, and Tribal Nations,

provides guidance to the DOE regarding the design and completeness for an assessment of impacts to the Columbia River from Hanford. As a result, an effort has been undertaken to produce a cumulative assessment of Hanford-derived radioactive and hazardous chemical contaminants, and to perform this assessment for the Hanford Site and the Columbia River environments. The computational capability for performing the cumulative assessment is known as the System Assessment Capability, Revision 0, (SAC Rev 0). Using SAC, decisions for each cleanup and disposal action will be able to take into account the composite effect of other cleanup and disposal actions.

# SAC Risk and Impact

The SAC will include impacts to human and ecological health as well as the region's economy and cultures. In CRCIA Part II, the community suggested that a comprehensive examination of risk and impact should include quantification of risks to humans and the ecology, and of impacts to the economy and cultures, especially Native American cultures. Requirements under NEPA for the completion of environmental impact statements call for the inclusion of sections on public health risk, impacts to ecology, cost/benefit of alternate actions, cultural and archaeological resources, and environmental justice. However, performance assessments required by DOE Order 435.1 for active disposals include only analyses for dose impacts to the public, and similarly required composite analyses require evaluation of the all-pathways dose to the offsite public. Thus, acknowledging the desire of the community for a more complete assessment of risk and impact, the SAC examines four areas of risk; human health, ecological health, economy, and culture. It considers risk from both radionuclide and hazardous chemical contaminants.

Human and ecological health risk is quantified at points in the environment representing two overlapping sets; where the environment is contaminated and where specific species of interest inhabit the environment. In its initial development and testing of the concept, the SAC risk/impact assessment will focus on the near-shore or riparian zone and river environment with respect to the ecological species of interest.

The economic model will focus on the local and regional economy. Impacts upon the economy arising from a degraded quality of the water resource include consideration of the costs and impacts to agriculture, recreation, and water supplies for municipalities. The SAC analysis will not examine the cost/benefit of alternate disposals or remedial actions because such analyses are the responsibility of NEPA and RCRA/CERCLA documentation.

Socio-cultural impacts have ambiguous measures at the present time. To date, the agreed upon cultural impact metric is the land surface area underlain by groundwater contaminated at or above a selected contamination level. Thus, visualization of this metric is achieved by plotting the land surface projection of the groundwater contaminant plume above the selected concentration (cultural threshold), and tabulating the surface area as a function of time. Of course, the surface area is a function of the contaminants and selected cultural threshold concentrations.

### SAC Requirements and Design

To conduct this assessment, the project is in the process of developing the necessary tools and supporting data. The assembly of the SAC Rev 0 computational package was preceded by discussions with the regulator, stakeholder and Tribal Nation community about the desired analysis. This was followed by an effort conducted by the project staff to state SAC Rev 0 software requirements. These requirements are based in part on a) the analysis desired by the community, b) the baseline setting to be analyzed as an initial assessment, and c) the software, computational resources, and time frame available to produce the initial capability and assessment. These software requirements, the initial assessment statement, and the software design are documented (5), and have undergone a technical peer review and a management review.

The general design architecture shown in Figure 1 illustrates the decision to separate the inventory and environmental analysis on the left from the risk and impacts analysis on the right. SAC Rev 0 will focus on the subsurface environment and river pathways for long-term contaminant migration. Note that SAC Rev 0 will not include atmospheric transport and terrestrial ecology. The need for these capabilities will be evaluated in the future and they may be added to revisions to the SAC.

Modules and linkages that comprise the SAC Rev. 0 are shown in Figure 1. The software package is probabilistic and designed to implement a Monte Carlo analysis. Results of the probabilistic realizations of the environment are stored in the Environmental Concentration Data Accumulator (ECDA) file and are accessed by each of the risk and impact modules. The stored environmental response data can be thought of as a suite of snapshots saved in a form that can be used and reused in repeated risk/impact simulations where the risk/impact models and parameters are varied. A software structural architecture that separates environmental and risk modules was adopted because of the very high cost of performing environmental simulations and the relatively low cost of risk/impact simulation.

While the software was being assembled, the software requirements and software design were used as the basis for assembling model parameters and distributions. Data sets were assembled for all modules of the analysis. Inventory data were assembled from databases containing disposal records, simulations of future waste treatment and disposal, and estimates of total production in Hanford reactors. Release, vadose zone, groundwater, and river data were assembled from prior analyses and data collected during site-specific characterization and routine monitoring projects. Data for risk and impact models have been assembled from existing models and databases. Parameters to be treated as uncertain are listed in the software design report (5).

#### SAC (Rev 0) Systems Code





Fig. 1. Top-Level SAC Architecture, Modules, and Data Interfaces

### AN INITIAL ASSESSMENT - A PROOF-OF-PRINCIPLE DEMONSTRATION

The two primary purposes of the initial assessment, which employs the SAC Rev 0 tool, are a) to demonstrate that a probabilistic assessment on the scale of the Hanford Site and the scope of all residual materials is possible, and b) to define improvements needed to establish SAC Rev 1 as a regulatory decision assisting capability. To keep pace with advances in our understanding of Hanford Site wastes and their migration, and our knowledge of advancing numerical methods, it is recognized that iterative improvement and adaptation of the SAC design will be required. Thus, each application of the tool will have the objective of defining needed improvements. Through a process of improvement and adaptation, an enduring analysis capability will be created and maintained.

The initial assessment using SAC Rev 0 is a site-wide assessment. The Hanford Site lies within the semi-arid Pasco Basin of the Columbia Plateau in southeast Washington State. The site occupies approximately 1,450 km<sup>2</sup> (560 mi<sup>2</sup>) north of the city of Richland, Washington. About 6% of the land has been disturbed and has been actively used by the Department of Energy and its predecessors. The Columbia River flows eastward through the northern part of the Hanford Site and then turns south, forming part of the eastern boundary. The Yakima River flows near a

portion of the southern boundary of the Hanford Site before it joins the Columbia River south of the city of Richland. While bounded by one of the major rivers of North America, Hanford is a dry area, known for its sandy soil, basalt ridges, and shrub-steppe vegetation. A complete description of the Hanford Site can be found in an annual report on the environment (6). Details about Hanford Site groundwater can be found in the annual monitoring report (7). Unconfined and confined aquifers underlie the Hanford Site. In general, the unconfined aquifer flows from the higher elevation of Rattlesnake Mountain and the central plateau toward the Columbia River. This is the most likely path of long-term contaminant transport.

From its creation in 1943 until recently, Hanford facilities were dedicated to the production of plutonium for national defense and management of the resulting waste (8, 9, 10). During its nearly 40-year mission to produce special nuclear materials, the Hanford Site has

- fabricated reactor fuel in the 300 Area,
- performed research and development in the 300 Area,
- operated nine production reactors in the 100 Areas,
- operated five chemical separation facilities in the 200 Areas, and
- fabricated plutonium components for nuclear weapons in 200 West Area.

This work created over 2,600 waste sites on the Hanford Site (11). The severity of contamination ranges from contaminated tumbleweeds to high-level radioactive and hazardous chemical waste stored in underground tanks. The majority of the waste was stored or disposed within the 100, 200, and 300 Areas. However, some waste was deposited outside these operational areas, e.g.,

- Gable Mountain Pond,
- Waste disposal caissons adjacent to Energy Northwest property, (e.g., 618-11 burial ground),
- 300 North burial ground, and
- Environmental Restoration Disposal Facility.

In addition, US Ecology, Inc., operates a commercial low-level waste disposal site located southwest of the 200 East Area. Many of the approximately 2600 sites identified in Waste Information Database System (WIDS) (11) have been included to ensure a complete listing of all potential waste sites. An initial screening has identified approximately 1000 sites that involve either radioactive or hazardous chemical wastes or a combination of them.

While the initial assessment is a proof-of-principle exercise, an effort is being made to create an assessment that provides meaningful insight into some of the larger issues associated with waste disposal and remedial actions planned for the Hanford Site. These issues include the relative significance of radioactive versus hazardous chemical contaminants, central plateau versus river corridor waste sites, and past-practice versus present-day waste sites.

### Initial Assessment – Major Assumptions

A number of simplifying assumptions have been made in the development of this initial assessment. Examples of these assumptions include the following:

- The physical domain of the Hanford Site and Columbia River downstream to McNary Dam is sufficient to evaluate the proposed capability.
- A duration of analysis ending 1000 years after an assumed Hanford Site closure date of 2050 is sufficient to evaluate the proposed capability.
- DOE will proceed with the cleanup described by the Tri-Party Agreement, RODs, interim RODs, and current multi-year work plans.
- The terrestrial ecological and atmospheric transport pathways are relatively minor contributors under current cleanup plans that isolate waste in the subsurface, and hence, minimize future atmospheric release and terrestrial environmental contamination.
- The vadose zone, groundwater, and river pathways are the dominant transport pathways for the migration of contaminants to the accessible environment, man, and the river ecosystem.
- The ecology, economy, and climate of the region surrounding the Hanford Site will remain stable and unchanged for the period of the analysis.
- Contributions to background from the Hanford Site aquifer to the Columbia River are negligible compared to contributions from the upstream watershed.

These and other assumptions are discussed below.

Spatial Domain. The initial cumulative assessment will address the region of the Columbia River from Vernita bridge to McNary Dam and the Hanford Site from Rattlesnake Mountain to the Columbia River. The current Hanford Site is included in the analysis domain. Thus, it will be possible to examine risks and impacts associated with future boundaries interior to the present day boundary of the Hanford Site, i.e., the Columbia River. The portion of the river to be analyzed was selected because higher concentrations of contaminants have been detected in Columbia River water and sediments above McNary Dam than downstream. The river reach between Priest Rapids Dam and Vernita bridge is not simulated because sediment does not deposit and resuspend (because of the relatively high velocity of the river in this channel), and there is no biota component that changes contaminant concentrations. All contaminants from the Hanford Site unconfined groundwater enter the river below Vernita bridge. Thus, river flow and contaminant concentration boundary conditions from above Priest Rapids are applied at Vernita bridge in the model.

Temporal Domain. The period of analysis is from 1944 until 1000 years after site closure, which is assumed to occur in 2050 AD. One thousand years is the regulatory (decision) period following site closure defined in DOE Order 435.1 and is of interest for that reason alone. It will be important that the SAC Rev 1 capability is able to provide estimates of system performance well beyond the regulatory period, perhaps 10,000 years or more beyond site closure. Because we lack knowledge about the present day location and concentration of contaminants, we choose to simulate from 1944 forward. Analysis from 1944 to present provides an opportunity to history match with field observations of contaminant movement. Analysis from present day until site

closure (e.g., 2050) requires a clear understanding of DOE planned actions for remediation of the Site. Simulation of the 1000 years following closure informs decision-makers of environmental response, and risk, dose, and impacts arising from planned disposal and remedial actions.

Climate and River Structures. A major assumption behind this initial assessment is that the current regional and local climate remains unchanged for the period of analysis. Furthermore, it is assumed that major engineering structures in the region (e.g., Grand Coulee Dam) will be maintained for the long term. At this time, the SAC model does not address alternate future climate change (e.g., global climate change, glacial flooding) or potential events (e.g., failure or removal of the reservoir system).

Background Contaminants, Risks and Impacts. The initial assessment will attempt to distinguish Hanford Site and upstream river sources of impact by simulating two cases and examining the difference between them. One case will examine the risk and impact caused by contaminant background concentrations entering the Hanford reach in Columbia River water from above Priest Rapids Dam, the Yakima River, the Snake River, and the Walla Walla River. The second case will examine the risk and impact resulting from contaminants derived from Hanford Site operations plus the background contaminants. The difference between the two cases will enable a first order evaluation of Hanford Site risk and impact as distinguished from background risk and impact.

Contaminants to be Analyzed. Through a process involving regulators, stakeholders, and Tribal Nation representatives, the SAC team selected seven radionuclides and three hazardous chemicals as the first set of contaminants whose transport and fate through the vadose zone, groundwater, and Columbia River are modeled in the initial assessment. The radionuclides are tritium, technetium-99, iodine-129, uranium-238, strontium-90, cesium-137, and plutonium-239/240. The three hazardous chemicals are total uranium (i.e., as a toxin to the kidney), carbon tetrachloride, and hexavalent chromium. Within this set are contaminants that move at different rates through the subsurface environment. Thus, by creating a capability to simulate this suite of contaminants, one ensures applicability to Hanford contaminants of different mobility.

# HISTORY MATCHING - ISSUES WITH SIMULATING 50 YEARS OF OPERATION

Model verification and validation are often performed to build confidence that long-term simulations are reasonable predictors of what may occur. These steps allow analysts, regulators, the public and other users to assess the utility of model results. The technical elements that comprise the SAC Rev 0 capability have each been verified to simulate as designed. Verification has been accomplished by comparing model results against analytical model results and/or hand calculations. Validation is a term from high-level waste repository programs. Validation is a process carried out by comparison of model predictions with independent field observations and experimental measurements. A model is not considered validated until sufficient testing has been performed to ensure an acceptable level of predictive accuracy (12). This has led to years of field experiment work to develop relevant field-scale data sets under controlled situations for the high-level waste disposal programs around the world. Definition of "an acceptable level of predictive accuracy" is subjective and may vary depending on the specific problem being addressed and simulated.

For SAC Rev 0, a philosophy of history matching models to available field data has been adopted. Hence, the proof-of-principle exercise will not wait for extensive field observations to perform exhaustive validation. Extensive validation data sets may be prohibitively expensive and full validation of a site-wide model of a site as complex as the Hanford Site may not be feasible. Accordingly, where available, independent data sets are being used first to calibrate models to a typical event, and then to make a blind comparison to a second data set that captures a similar disposal or discharge event. Thus, for SAC Rev 0, the models will be history matched to existing and admittedly limited data. It will not be validated against complete data sets designed to represent all current and future events.

The system assessment capability is composed of technical elements or modules with widely differing potential for history matching. A two-phased approach has been taken to history match SAC, Rev 0. First, individual technical elements are history matched and calibrated to events documented within their respective domains. These simulations are deterministic and history match criteria involve simple comparisons of model predictions at points in space to field observations. Second, following completion of individual history matching efforts, the complete SAC Rev 0 tool is applied to simulate the migration and fate of tritium and technetium-99. The second phase is a probabilistic application of the tool. Analysis of second phase results will reveal the ability of the stochastic tool to simulate the migration of mobile contaminants from inventory through risk. Both contaminants have established plumes in the groundwater system. Tritium is roughly twice as abundant in Columbia River water below the Hanford Site as it is above. Tritium and technetium-99 were selected for the overall history match because they provide field data to confirm the modeling capability.

# **Phase 1 – History Matching - Individual Modules**

As shown in Figure 1, the system assessment capability is comprised of individual environmental modules that are linked in a series; inventory, release, vadose zone, groundwater, and river. Each of the environmental modules has unique history match aspects; some have no opportunity to history match, others have a significant opportunity.

The risk modules are uncoupled from the environmental simulation and their history match cases are conducted as independent calculations. The human health and ecology risk modules were created and history matched as part of the CRCIA, Part I (13) study. The biota model, now incorporated into the river modules, was the only risk component history matched to field data in this study. The economic module is based on established algorithms, and the socio-cultural model relies entirely on the predicted groundwater contaminant plume. Neither requires history matching at this time.

History match efforts for the vadose zone, groundwater, river, and biota seek to use field observations to finalize conceptual models and model parameters. Each technical element, (i.e., vadose zone, groundwater), is being history matched independent of upstream and downstream models of the SAC. Each of these history match efforts, briefly described below, conducts simulations as a series of deterministic events.

Inventory. The inventory data used in the initial simulations were developed on a waste site basis. Release information, in the form of waste volume and concentration of contaminants in the waste volume, was developed for each waste site. All of the sites were added together to provide a Hanford combined release profile. This profile was generated on an annual basis. One of the history matching exercises was to evaluate how well the sum of inventory from all of the waste sites compared with independent estimates of the total inventory generated in Hanford Site production reactors.

Figure 2 displays a probability density function for the total technetium-99 produced on the Hanford Site. This density function of total production was generated using 100 stochastic realizations of waste disposition actions for each waste disposal site in the rollup of Hanford site inventory. Final disposition of this inventory would be partitioned into offsite disposal (high level waste glass), liquid disposal (past and future) onsite, solid disposal on site (exclusive of ILAW glass), and disposal of ILAW glass onsite. Table 1 provides average values from the 100 realizations of the inventory. Estimates of the total amount of technetium-99 produced on the Hanford Site have been developed in the past independent of this activity. The best estimate of total production of technetium-99 is 32,000 curies (14). The average values in Table 1 are consistent with this estimate. In addition, the probability plot shows that the rollup of inventory is consistent with the best estimate being accurate to within 10 to 20%.

During the early years of Hanford Site operation, reprocessing of irradiated fuel was limited to the production of B, D, and F reactors. Total production and hence total processing was limited to these fuels and the bismuth-phosphate process that was run in T-Plant and B-Plant. The inventory of waste discharged and disposed to ground from these plants during this era represents a relatively small fraction (e.g., 3%) of the total Hanford Site inventory. This historical estimate matches well with the simulation estimates of about 4% of the tecnetium-99 inventory being released to the ground in the form of liquid releases during this period and shortly afterward during uranium recovery operations in the mid to late 1950s (8).



Fig. 2. Stochastic estimate of the total technetium-99 produced at the Hanford Site.

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Realizations of Technetium-99 Inventory		
Final Disposition	Average	Average
	(Curies)	(Percent of Total)
Offsite Disposal	1099	3.4%
Liquid Releases Onsite	1284	4.0%
Solid Disposal Onsite	18955	58.6%
ILAW Glass Disposal Onsite	10993	34.0%
Total Produced at Hanford	32331	

Table I. Average Values from 100 Stochastic Realizations of Technetium-99 Inventory

This example shows that the technique of defining technetium-99 inventory at the Hanford Site on a waste-stream basis has the ability to match historical summary information. This approach, together with history matching to operational losses during specific operational eras, helps ensure that total inventory mass balance is achieved across the site.

Release. There is a complete absence of field data regarding the release of contaminants from waste disposal or discharge sites. Accordingly, history matching of release models is not achievable. During this phase of the history match effort, each of the release models was executed on the complete range of data available for the initial assessment. Thus, the release models were thoroughly verified on data sets relevant to Hanford Site wastes.

Vadose Zone. Vadose zone data sets are more abundant; however, they are few relative to the number of vadose zone contamination events at the Site, (e.g., ~1000). This is because few sites have undergone post-mortem excavation and evaluation, few sites outside the tank farms have been routinely dry-well logged to define moisture or contamination levels, and there is an absence of routine vadose zone monitoring data.

Data for specific facilities that have undergone post-mortem studies or dry well logging have been used to history match specific discharge events. In general, these efforts have been limited to sites that received a significant discharge volume or inventory or both, and as a result presented a case of interest or concern regarding the breakthrough of contamination to the aquifer or the development of a critical mass. Examples are plutonium cribs, 216-Z-1A and 216-Z-12, and the PUREX crib, 216-A-8. Results of the few vadose zone events history matched will be applied to broad classes of release, (i.e., adjustments made to history match a crib receiving a large discharge are applied to all cribs that received large discharges).

History matching was conducted for eight sites, including high volume cribs, low volume cribs, a high-level waste tank, a reverse well, and a pond. Simulations were also conducted using different column areas and for a number of contaminants ranging from highly mobile (e.g. technetium-99) to highly immobile (e.g. plutonium-239/240).

Figure 3 illustrates the simulation results for cesium-137 transport beneath the high volume 216-A-8 crib. The first simulation was conducted using the areal dimensions of the crib. The second simulation was conducted using twice the area, to help account for lateral spreading. Note that the second simulation produced a better fit with spectral-gamma logging data from a dry well located adjacent to the headend of the crib. Similar areal adjustments also appeared to work well for other high volume crib simulations. Thus, this general rule of doubling the area for high volume cribs will be applied to all high volume cribs.

Groundwater. History matching of the model of the unconfined aquifer is made possible by the abundance of water table observations for period of 1944 to present. This data set has been greatly improved over time by monitoring technology and numerous observation wells, and represents a transient long-term record that captures the water table response to discharges of cooling water, wastewater, and changes in surface infiltration. All water table elevation observations contribute to a single body of knowledge that applies to the aquifer.

Simulation of contaminant transport through the unconfined aquifer system at the Hanford Site has been performed using a relatively complex three-dimensional model composed of seven hydrogeologic units (3, 15). However, completing the stochastic simulations for SAC within a reasonable time required a faster model. The history- matching process, therefore, involved two steps: 1) comparing historical plume movement to simulations with the full three-dimensional model and 2) comparing the full model results with simpler models including three-dimensional two-unit, three-dimensional one-unit, and two-dimensional models. For the three-dimensional cases, each unit is divided into several "transport layers" so that the contaminant is not spread over the entire unit thickness.



Fig. 3. Plot of cesium-137 predictions for the 216-A-8 high volume crib.

An early tritium plume, which originated in the central Hanford Site and traveled approximately 20 km to the Columbia River, and a later tritium plume from the same area were used for the history matching exercise. The first plume resulted from wastewater discharged between 1955 and 1972. Unfortunately, because tritium was not routinely measured in wastewater or groundwater until about 1974, the source term and early movement of this plume are unknown.

However, groundwater measurements taken in 1974 established an initial condition for simulation of this plume. Transport modeling was performed to predict the plume movement through 1998. Because of uncertainty in the plume thickness, five separate simulations were run with different initial vertical distributions of tritium. The case with tritium distributed over the upper 20 m of the aquifer, but not in mud-dominated sediments, gave the best results. The later tritium plume was discharged to the vadose zone during 1983 to 1987. Tritium source information is available for this plume, which was simulated from the source input to its 1998 distribution. Simulations with the simplified transport models are underway.

River. The Columbia River has a short-term response relative to the subsurface environment, especially to mobile contaminants that disperse in the river water and do not adsorb on sediment. Thus, short-term but relatively thorough field observations related to well quantified releases can yield sufficient data for limited history matching of transport events. Two such events have been used to perform history matching of the Columbia River model; reactor cooling water discharges during the reactor operation era, and releases from groundwater plumes in the recent past.

The River Flow and Transport Model, MASS2 (16), provides the capability to calculate the flow, sediment transport, and contaminant transport in the Columbia River system. MASS2 is a two-dimensional depth-averaged model that simulates the lateral (bank-to-bank) variation of flow and contaminants. MASS2 includes the capability to simulate sediment transport, sediment-contaminant interaction (using Kd's), sediment-sorbed contaminant transport, and contaminant transport within the riverbed sediment layer. The simulated contaminant concentrations from the MASS2 model were compared to measurements for two separate time periods; 1964-1966 when radionuclides including chromium-51 and zinc-65 were directly discharged to the river from once-through cooled plutonium production reactors and 1992-1996 when contaminants including tritium and uranium enter the river from groundwater sources and upstream inputs. The results of these comparisons are shown in Figure 4. These results illustrate the ability of model predictions to lie within the range of field observations.

Biota. Ecological risk is being estimated using the ecological chemical exposure model, ECEM. The model was developed for the CRCIA and estimates ecological exposures from metals, organics, and/or radionuclides to 52 riparian and aquatic species. ECEM is based on a food-web architecture that has been developed for the Columbia River and associated riparian zone. Exposures are estimated through water (surface water and porewater), soil/sediment exposure and foods. The results of the model include: 1) for the riparian species, equilibrium doses for ingestion, inhalation, and dermal routes, total radiological dose (where appropriate), and tissue concentrations for terrestrial receptors; and 2) for the aquatic species, effective water concentration and equilibrium tissue.

In order to ensure that ECEM best represents the ecosystem in the SAC study area, ECEM output was calibrated to historic biological monitoring data from the Hanford Site. The source of this historical data was the Hanford Environmental Information System (HEIS). Some of the programs that store data in the HEIS are PNNL's Groundwater Monitoring Program, PNNL's Surface Environmental Surveillance Project (SESP), and the Environmental Restoration Contractor's CERCLA remedial investigation/feasibility study programs. Many special studies also place their data in HEIS.



Fig. 4. Comparison of simulated and measured concentrations (Ci/m<sup>3</sup>) for a) zinc-65, b) chromium-51, c) tritium, and d) uranium at the Richland Pump House.

Biological data were available for seven of the SAC contaminants of interest (i.e., cesium-137, inorganic metallic chromium, plutonium-239/240, strontium-90, technitiumm-99, tritium, and uranium-238). No data were available for carbon tetrachloride and iodine-129. These data were further reduced to those aquatic and terrestrial species (periphyton, phytoplankton, marcophytes, aquatic insects, riparian vegetation, fish, birds, mammals) that could be reasonably matched to the SAC species of interest based on similar taxonomy and lifestyle attributes.

The historic biota averages were then compared to average body burdens (chromium [mg/kg]) and average radiation doses (radionuclides [pCi/kg]) generated by contaminant, species and river segment by ECEM. The comparison was made by calculating the quotient of ECEM and historic biota averages. Positive quotients expressed an overestimation by ECEM of the historic biota averages. Negative quotients expressed an underestimation by the ECEM of the historic biota averages. Quotients of  $0.0 \pm 15$  were considered acceptable. For contaminants and species with a quotient greater or less than  $\pm 15$ , the most sensitive ECEM parameter values (bioconcentration factors, chemical assimilation efficiencies/ingestion absorption factors, depuration rates, and soil/plant transfer factors) were increased or decreased accordingly. ECEM was subsequently rerun with the new parameter values and the resulting quotients were re-calculated. The new quotients were compared with the previous quotients to determine which parameter values still needed to be increased or decreased. This process was repeated until the majority of the quotients fell within the range of acceptance.

Computational Resource Requirements. Estimates for the analysis of an 800-site problem for the 1106-year period and ten analytes are based on preliminary findings of the individual history match efforts. The execution of inventory, release, and risk/impact modules of the SAC does not require significant resources. However, the computation time requirements for vadose zone, groundwater, and river simulations of the 100 realization Monte Carlo analysis are ~64 days, ~21 days, and ~15 days respectively. Thus, the total run time could be ~100 days. If the number of realizations is halved, the simulation time is halved. This still represents a substantial time requirement, and will challenge the patients of decision-makers. With the execution of the river module, the software architecture assigns each contaminant its own processor. Thus, the ten contaminants use ten Pentium III processors.

Memory requirements for the vadose zone and river modules are substantial because of the number of disposal and discharge sites in the vadose zone and the number of nodes and time steps in the river simulation. Memory requirements for the vadose zone and river are on the order of 140 gigabytes and 200 gigabytes respectively. While significant, resources of this magnitude are readily accessible.

# Phase 2 – History Matching – Overall SAC

Where Phase 1 is devoted to history matching and calibration of the suite of models that comprise the SAC, Rev 0, Phase 2 is a test of how well the tool is able to perform a stochastic analysis of the massive and complex problem of Hanford Site contaminant disposal, migration, and fate. The overall capability will be evaluated based on intermediate as well as final results. An assessment will be made of the inventory used to drive the model on a site-by-site basis. The overall ability of the model to deliver contaminant to the water table and create groundwater

plumes will be evaluated by simulating the inventory, release and vadose zone modules, and evaluating the mass of contaminant delivered to the aquifer as a function of time and position. This will be compared to the estimated mass of contaminant in groundwater plumes.

The ability of the SAC Rev 0 tool to simulate the delivery of contaminants to the Columbia River will be evaluated by simulating tritium releases through groundwater to the river and its subsequent migration and fate in the river environment. Tritium is the most distinctive of the contaminants because it is released in the river at detectable levels. The mass of tritium below the Hanford Site is roughly double the background value in the river at Priest Rapids Dam. The inventory, release, and subsequent migration and fate of technetium-99 will also be simulated using the overall capability.

History match of the overall SAC will be probabilistic, but limited to fewer than 100 realizations because of computing resource and time limitations. Hence, the overall SAC history match will reveal the resource requirement of the model by simulating the complex period of past Hanford Site operation.

### The Initial Assessment

Upon completion of the overall history match, the initial assessment will be simulated and the full suite of environmental, human and ecological health, economic and socio-cultural impacts will be calculated and displayed. While an incomplete suite of radionuclides and chemicals are simulated, the cumulative risk, dose, and impact from them will be simulated to illustrate application of the capability.

Using the various risk/impact metrics, results of the initial assessment will be used to examine the relative significance of:

- wastes disposed in the river corridor versus wastes disposed on the central plateau,
- tank wastes versus all other wastes,
- past tank leaks versus future tank losses,
- past practice liquid waste discharges, facilities, and solid waste disposals, and
- radioactive wastes versus hazardous chemical wastes.

The relative uncertainty in the various metrics will also be evaluated.

# CONCLUSIONS

Clearly, a probabilistic analysis using mechanistic, even if simplified, computational tools is a challenging endeavor. However, regulatory agencies, the public, and Tribal Nations all want to see more comprehensive and realistic simulations conducted, and they want the analyses that represent the uncertainty in past actions and future migration and fate estimates. It is being demonstrated that it can be done. While work is still in progress, indications are that a site-wide probabilistic assessment of the scope and scale of the Hanford Site, when conducted in a time frame of interest to decision makers, is possible but will fully utilize computational resources in the current software/hardware architecture.

### REFERENCES

- Defense Nuclear Facilities Safety Board (DNFSB). "Recommendation 94-2 to the Secretary of Energy – Conformance with Safety Standards at DOE Low-Level Nuclear Waste and Disposal Sites". Letter from JT Conway to H.R. O'Leary dated September 8, 1994 (1994).
- 2. U.S. Department of Energy (DOE). DOE Order 435.1, "Radioactive Waste Management." as amended, U.S. Department of Energy, Washington, D.C. (1999).
- C. T. Kincaid, M. P. Bergeron, C. R. Cole, M. D. Freshley, V. G. Johnson, D. I. Kaplan, R. J. Serne, G. P. Streile, D. L. Strenge, P. D. Thorne, L. W. Vail, G.A. Whyatt, and S.K. Wurstner. "Composite Analysis for Low-Level Waste Disposal in the 200 Area Plateau of the Hanford Site." PNNL-11800. Pacific Northwest National Laboratory, Richland, Washington (1998).
- CRCIA Management Team Representatives (CRCIA). "Screening Assessment and Requirements for a Comprehensive Assessment; Part II Requirements for a Columbia River Comprehensive Impact Assessment." DOE/RL-96-16, Revision 1. U.S. Department of Energy, Richland, Washington (1998).
- C. T. Kincaid, P. W. Eslinger, W..E. Nichols, A. L. Bunn, R. W. Bryce, T.B. Miley, M. C. Richmond, S. F. Snyder, R. L. Aaberg. "System Assessment Capability (Revision 0); Assessment Description, Requirements, Software Design, and Test Plan." BHI-01365, Draft A. Bechtel Hanford, Inc., Richland, Washington (2000).
- T. M. Poston, R. W. Hanf, and R. L. Dirkes. "Hanford Site Environmental Report for Calendar Year 1999." PNNL 13230. Pacific Northwest National Laboratory, Richland, Washington (2000).
- M. J. Hartman, L. F. Morasch, and W. D. Webber. "Hanford Site Groundwater Monitoring Report for Fiscal Year 1999. PNNL-13116. Pacific Northwest National Laboratory, Richland, Washington (2000).
- S. F. Agnew, "Hanford Tank Chemical and Radionuclide Inventories: HDW Model Rev. 4." LA-UR-96-3860. Los Alamos National Laboratory, Los Alamos, New Mexico (1997).
- U.S. Department of Energy (DOE). "Linking Legacies; Connecting the Cold War Nuclear Weapons Production Processes to Their Environmental Consequences." DOE/EM-0319. U.S. Department of Energy, Washington, D.C. (1997).
- 10. R. E. Gephart and R. E. Lundgren. "Hanford Tank Cleanup: A Guide to Understanding the Technical Issues." Battelle Press, Columbus, Ohio (1995).
- 11. WIDS (Waste Information Database System). http://www.erc./~dm/wids.htm
- 12. IAEA-TECDOC-477 Radioactive Waste Management Glossary, 2<sup>nd</sup> edition (1988).
- Pacific Northwest National Laboratory. "Screening Assessment and Requirements for a Comprehensive Assessment; Part I Screening Assessment." DOE/RL-96-16, Revision 1. U.S. Department of Energy, Richland, Washington (1998).
- M. J. Kupfer, A. L. Boldt, K. M. Hodgson, L.W. Shelton, B. C. Simpson, R. A. Watrous, B. A. Higley, R. M. Orme, M. D. LeClair, G. L. Borsheim, R. T. Winward, N. G. Colton, S. L. Lambert, D. E. Place, and W. W. Schulz. "Standard Inventories of Chemicals and Radionuclides in Hanford Site Tank Wastes." HNF-SD-WM-TI-740, Rev 0C. Lockheed Martin Hanford Corporation, Richland, Washington (1999).

- 15. C. R. Cole, S. K. Wurstner, M. P. Bergeron, M. D. Williams, and P. D. Thorne. "Three-Dimensional Analysis of Future Groundwater Flow Conditions and Contaminant Plume Transport in the Hanford Site Unconfined Aquifer System: FY1996 and 1997 Status Report." PNNL-11801. Pacific Northwest National Laboratory, Richland, Washington (1997).
- 16. M. C. Richmond, W. A. Perkins, and T. D. Scheibe. "Two-Dimensional Hydrodynamic, Water Quality, and Fish Exposure Modeling of the Columbia and Snake Rivers. Part 1: Summary and Model Formulation." Final Report submitted to U.S. Army Corps of Engineers, Walla Walla District. Battelle Pacific Northwest Division, Richland, Washington (1999).