Groundwater/Vadose Zone Integration Project

Preliminary System Assessment Capability Concepts for Architecture, Platform, and Data Management

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September 30, 1999

PREFACE

The Groundwater/Vadose Zone Integration Project will initiate the design of a site-wide cumulative impact assessment for the Hanford Site during the first quarter of fiscal year (FY) 2000. This assessment and the system of tools that are required to perform it is called the System Assessment Capability (SAC). The design process will begin with the definition of requirements for the system, followed by development of a specification of system performance to meet those requirements. It will also include a test plan for the initial capability and will identify analyses to be performed in an initial assessment. This letter report lays the groundwork for developing the system design.

A conceptual model is outlined for movement of contaminants from waste sites through the vadose zone, groundwater, and Columbia River to receptors. The measures to be used to assess risk and impact to human health, other living systems, the local economy, and cultures are also outlined. The required data for each element and the linkages between the elements of the system have been outlined. This information will provide the basis for understanding memory, storage, and computational resource requirements of the assessment capability. Preliminary thoughts about how components of the system will be linked and pass information (system architecture and data management) are presented. Options for the system architecture, data management, and computational platform employed in the initial SAC (Rev. 0) are discussed. Questions are posed that must be resolved prior to completion of the design. The information presented and the unresolved questions will serve as the starting point for the design process and the basis for continuing stakeholder, Tribal Nation, and regulator engagement in the development of the assessment.

Conceptual models for elements of the system to be used in the initial assessment are presented in Appendices A through F of this letter report. Each of these appendices discuss how uncertainty in the understanding of the physical environment represented by that element will be treated in the assessment. Appendix G presents options for approaches to treating uncertainty in the overall system. Appendix H is a summary of plans for FY 2000, including a schedule of activities.

As mentioned above, this document lays the groundwork for developing the SAC (Rev. 0) design. That design will be developed during the first half of FY 2000. Design options for subsequent revisions of the SAC will be identified during the first quarter of FY 2000. Requirements for these later revisions will be identified following completion of a requirement definition process that is being performed for the overall Groundwater/Vadose Zone Integration Project. The requirements for later assessments will be identified by the end of FY 2000. The design options, requirements, lessons learned from SAC (Rev. 0) development and testing, as well as input from science and technology development and characterization efforts carried out by the Groundwater Vadose Zone Integration Project (and other projects onsite) will be used to develop the design for future revisions of the SAC.

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ACRONYMS

CERCLA	*Comprehensive Environmental Response, Compensation, and Liability Act of 1980*
CEKSF	C. E. Kelly Support Facility
COBRA	Common Object Request Broker Architecture
CRCIA	*Columbia River Comprehensive Impact Assessment*
DCOM	Distributed Component Object Model
DNFSB	Defense Nuclear Facility Safety Board
DOE	U.S. Department of Energy
EIS	Environmental Impact Statement
EM	Environmental Management
EPA	U.S. Environmental Protection Agency
ER	Environmental Restoration
ERDF	Environmental Restoration Disposal Facility
ERS	Environmental Release Summary
FEPs	Features, Events, and Processes
FRAMES	Framework for Risk Analysis in Multimedia
GB	Gigabytes
GUI	Graphical User Interface
GW/VZ	Groundwater and Vadose Zone
HEDR	Hanford Exposure Dose Reconstruction
HRA	Hanford Remedial Action
HSTD	Hanford Site Technical Database Baseline
HWIR	Hazardous Waste Identification Rule
ILAW	Immobilized Low Activity Waste
ORP	Office of River Protection
RCRA	*Resource Conservation and Recovery Act of 1976*
RL	Richland Operations Office
RVP	Risk Visualization Processor
SAC	System Assessment Capability
TWRS	Tank Waste Remediation System
WIDS	Waste Information Data System
WIPP	Waste Isolation Pilot Plant

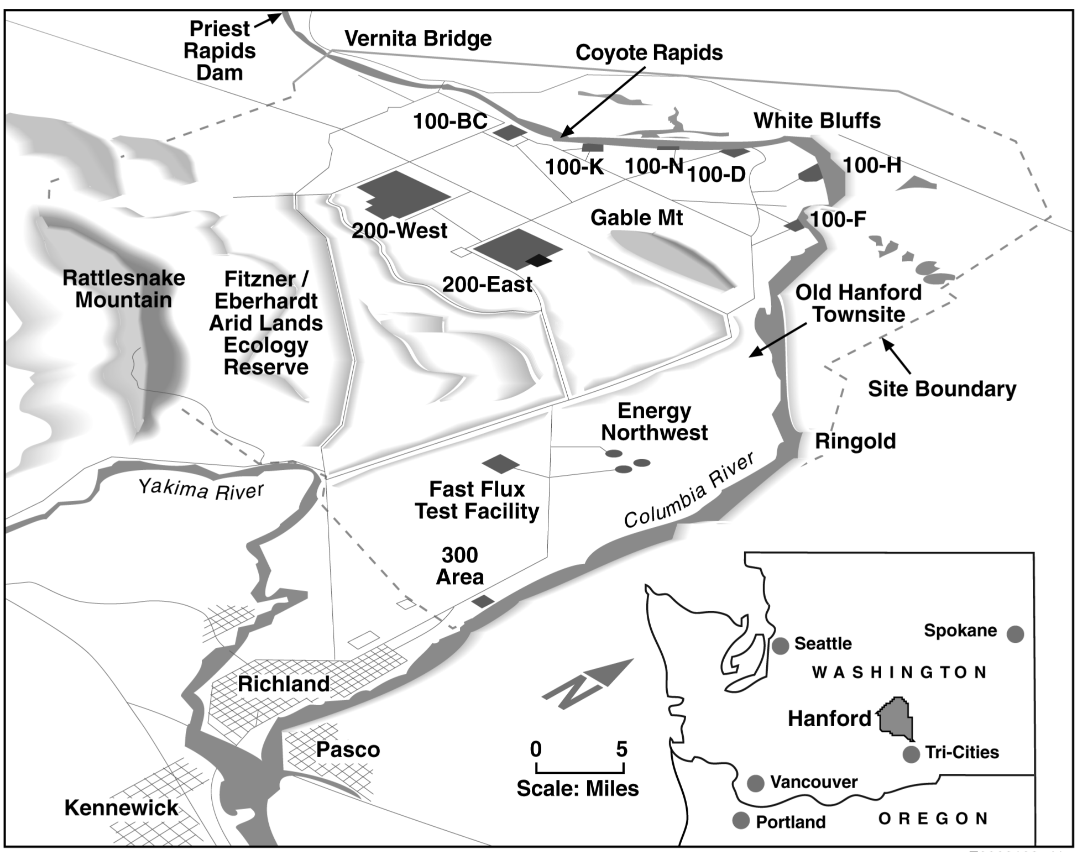
1.0 INTRODUCTION

The Hanford Site lies within the semi-arid Pasco Basin of the Columbia Plateau, in southeastern Washington State (see Figure 1-1 [Gephart et al. 1995]). The site occupies an area of approximately 1,450 km^2 (560 square miles), and is located north of the city of Richland, Washington. About 6% of the land area has been disturbed and is actively used. The site is located upstream of the confluence of the Yakima and Snake Rivers with the Columbia River, approximately 25 miles north and upstream of the Oregon border. A dry area known for its sandy soils, basalt ridges, and shrub-steppe vegetation, the Hanford Site is bordered by the Columbia River on the north and east. The Yakima River flows near a portion of the southern boundary of the site before it joins the Columbia River, south of the city of Richland.

A complete description of the Hanford Site can be found in an annual report on the environment (Dirkes et al. 1999). Details on the Hanford Site groundwater setting can also be found in an annual monitoring report (Hartman et al. 1999). The environmental setting is summarized in the background information presented in DOE-RL 1999b.

Note: Internet addresses for these documents, and the documents in Section 1.1, are included in Section 6.0.

Figure 1-1. Hanford Site Location.



1.1 THE HANFORD SITE

From its creation in 1943 until recently, Hanford Site facilities were dedicated primarily to the production of weapons-grade plutonium for national defense (Gephart and Lundgren 1995, DOE 1997). The current missions of the Hanford Site are to safely clean up and manage the site's legacy wastes, and to develop and deploy Science and Technology (S&T) (DOE-RL 1996). During its nearly 40-year mission to produce special nuclear materials, the Hanford Site has:

- Fabricated reactor fuel (300 Area)
- Performed research and development (300 Area)
- Operated nine production reactors (100 Areas)
- Operated five chemical separation facilities (200 Areas)
- Fabricated plutonium components for nuclear weapons (200 West Area).

As a result of this work, the Waste Information Data System (WIDS) database currently shows approximately 2,600 waste sites at the Hanford Site. These waste sites range in severity from contaminated tumbleweed to radioactive and chemical wastes in tanks at high pH containing high concentrations of organic complexant and salts. The bulk of these wastes were discharged or disposed within the 100, 200, and 300 Areas. However, some wastes were discharged or disposed outside of these operational areas (e.g., the Gable Mountain Pond, the waste disposal caissons located adjacent to the Energy Northwest property, the 300 North burial grounds, and the Environmental Restoration Disposal Facility [ERDF], located between 200 West and 200 East Areas). The site also includes the commercial low-level waste disposal site operated by US Ecology, which is located southwest of the 200 East Area.

For additional information about past operations at the Hanford Site, readers should refer to the state of knowledge document produced by the Groundwater/Vadose Zone (GW/VZ) Integration Project (DOE-RL 1999b). Further details can be found on the Internet at *http://www.hanford.gov/doe/culres/historic/index.htm*. Two links from that address to areas of special interest are 1) *Historic District Book*; and 2) *More Historic Information*. Other resources are provided in a report on Hanford Site tank cleanup, by Gephart and Lundgren (1995), and the U.S. Department of Energy's (DOE's) publication on legacy wastes (DOE 1997).

1.2 THE GROUNDWATER/VADOSE ZONE PROJECT

The DOE, Richland Operations Office (RL) has established and directed several projects (and multiple contractors) to execute the Hanford Site cleanup mission. While many important milestones have been accomplished that support the Hanford Site strategic goals, the cleanup mission is complex and the potential exists for fundamental gaps, overlaps, and inefficiencies to occur among the multiple projects. A key area of concern involves the characterization and remediation of contaminants in specific regions of the Hanford Site's subsurface sediments (i.e., the vadose zone and groundwater). Federal and state regulators, stakeholders, and Tribal Nations have voiced concerns over real and perceived threats that Hanford Site contaminants pose to the aquifer underlying the Hanford Site and to the Columbia River. Those concerns are clearly expressed in three key documents: 1) the *Columbia River Comprehensive Impact Assessment* (CRCIA), *Part II* (DOE-RL 1998); 2) *Defense Nuclear Facility Safety Board Recommendation 94-2* (DNFSB 94-2); and the expert panel status report on contamination in the vadose zone beneath the tank farms (DOE-RL 1997).

In response to these concerns, the DOE established the GW/VZ Integration Project (Integration Project) in late 1997. The Integration Project is to be a catalyst for fundamental change at the site. One dimension of that change involves the creation and application of an assessment of cumulative impacts for Hanford Site wastes on the subsurface environment and the Columbia River. Through the application of a system assessment capability (SAC), decisions for each cleanup and disposal action will be able to take into account the composite effect of other cleanup and disposal actions. The Integration Project is to use the CRCIA Part II document as a starting point for designing the assessment, and has been directed to ensure that DNFSB 94-2 requirements are met through this resulting assessment.

The challenge of predicting the migration and fate of contaminants, and the risks and impacts associated with their release to the accessible environment, is monumental. All aspects of the problem introduce uncertainty - from the inventory and release, through the environmental pathways, to the quantification of risk and impact. The natural environment of the vadose zone, groundwater, and Columbia River is highly variable and complex. Clearly, in the case of some wastes, portions of the associated vadose zone have been altered, thereby making it more difficult to understand and forecast the future migration of contaminants.

Past Hanford Site operations have created a variety of complex wastes, a large number of waste sites, and a number of radioactive and hazardous chemical contaminants of potential interest. The regulator, stakeholder, and Tribal Nation communities have identified a number of risk and impact metrics. The size, scope, and scale of a site-wide or system assessment of cumulative impact must be understood before any assessment capability can be designed, developed, and applied.

The GW/VZ Integration Project and the role of the SAC within the Project are described in the project summary (DOE-RL 1999a). This document and two others (DOE-RL 1999b, 1999c) describe the integration project, provide background information on the Hanford Site and past operations, and summarize the S&T portion of the project. These documents are accessible at http://www.bhi-erc.com/vadose/docsl.htm#published on the internet.

2.0 PURPOSE

The SAC is the capability needed to assess the cumulative impacts of radioactive and chemical waste at the Hanford Site on water resources, living systems, cultures, and regional economics. The SAC consists of a suite of tools and databases that are evolving and maturing as new data knowledge are gained. Results from SAC assessments will allow site-specific cleanup decisions and disposal authorizations to be made in the context of the overall impact of the Hanford Site on the region, including the Columbia River. The SAC will also provide useful information for making operational Hanford Site decisions, such as cleanup prioritization, funding allocation, and the need for additional data. In the long term, the SAC will provide important information to site closure decisions.

2.1 STRATEGIC OBJECTIVES

The SAC is developing the tools and information required to perform these assessments, based on the needs and interests of a broad range of customers. Customers for SAC information and products include the organizations responsible for decisions at the Hanford Site (i.e., DOE, U.S. Environmental Protection Agency [EPA], State of Washington) and the organizations and people who desire to understand the risks and impacts (e.g., the contractor public, stakeholders, and Tribal Nations). Based on these customer needs, three strategic objectives have been identified for the assessment:

1. **Promote a common understanding** of environmental concerns and cumulative effects of contaminants from the Hanford Site among all interested parties including DOE, regulators, Hanford Site contractors, Tribal Nations, stakeholders, and the public.

2. **Provide consistent information for decisions** at the Hanford Site. In the near term, these include operational and remedial decisions. In the long term, these include closure decisions.

3. **Identify specific needs** for better protection of resources and improved information for decisions, including science and technology needs and information input from core projects.

The Integration Project has adopted an iterative approach for development of the SAC. This approach will maximize learning, improve customer acceptance, and maintain flexibility.

2.2 PURPOSE OF THE INITIAL SYSTEM ASSESSMENT CAPABILITY

The initial SAC, also described as SAC (Rev. 0), will demonstrate that an assessment of the scale and scope of the Hanford Site and the Columbia River can be conducted and yield information needed to design a decision support tool later revisions. While the initial assessment will be limited in some respects, the assessment capability is being designed to:

- Examine radioactive and hazardous chemical contaminants that are expected to be dominant and representative contributors to risk and impacts.

- Determine the long-term (i.e., 1000-year post closure period), migration and fate of dominant and representative contaminants in the Hanford Site operational areas (i.e., 100, 200, and 300 Areas).

- Include a quantification of uncertainty (e.g., both conceptual model, and parametric).

- Include a suite of quantitative and qualitative risk and impact metrics.

A subset of dominant and representative contaminants will be investigated in the SAC (Rev. 0) effort. Current plans call for the study of four mobility groups for radionuclides; mobile (e.g., tritium and techetium-99); somewhat mobile (e.g., iodine-129, uranium); immobile (e.g., strontium-90, cesium-137); and highly immobile (e.g., plutonium-239, 240). Two chemicals will be studied: carbon tetrachloride (i.e., an organic) and chromium (i.e., an inorganic metal). A greater number and variety of radionuclides and chemicals will be studied in future revisions of the SAC to better represent the potential impacts to humans, other living systems, cultures, and the regional economy.

In addition to these general objectives, the initial SAC will be designed to distinguish the risk and impacts of the various waste types within each operational area, as well as sources located in the different operational areas (e.g., plateau sources versus near-river sources). A demonstration of the significance of waste types and source areas may be achieved without requiring individual site-specific analyses. Waste inventories will be aggregated within each operational area, according to waste type (e.g., pre-1970 solid waste burial grounds, past-practice liquid discharge sites, canyon buildings, past tank leaks).

2.3 THE INITIAL ASSESSMENT

The initial SAC will be a proof-of-principle, and not a prototype of the decision assisting capability. It will demonstrate that an overall assessment of the scope and scale for a Hanford Site post closure setting can be accomplished. It will also provide performance information for design of the decision assisting capability to be created and deployed as future iterations of the SAC. Because of the dependence of virtually all aspects of the assessment on the assumed physical and geochemical setting at the time of site closure, it is necessary to choose a final waste disposal and contaminated site remedial action configuration. The GW/VZ Integration Project has looked to the regulatory, stakeholder, and Tribal Nation community for input on the configuration to analyze with the initial SAC (i.e., Rev. 0). Clearly, the initial assessment will be followed by future iterations (e.g., SAC Rev. 1, 2, etc.), that consider and analyze other configurations as environmental restoration (ER) (remedial action) and environmental management (EM) (disposal) options are evaluated and closure actions are implemented. The basis for project planning of the SAC (Rev. 0) effort has been an assessment of the *Hanford Site Disposition Baseline*.

The following guidance contained in the CRCIA, Part II (DOE/RL 1998), details the requirements for a comprehensive assessment of the river, and provides a basis for the definition of the post-cleanup end state (i.e., the Hanford Site Disposition Baseline):

> (the Columbia River comprehensive impact assessment) … "is to be performed maintaining as much consistency as possible with each set of Hanford Site-wide cleanup/disposal decisions and with each subsequent revision. In other words, for the collection of DOE documents which, at any given time, constitutes the approved Hanford Site post-cleanup end state, there will be a corresponding CRCIA assessment of resultant impact." (DOE/RL 1998, page II-1.10)
>
> "If no officially recognized end-state plan exists for the overall Site, the (…) analysts will develop with DOE's recommendations, the most credible surrogate end-state information available." (DOE/RL 1998, page II-1.10)
>
> "The requirements in this section call for the Columbia River impact assessment to be consistent with the current definition of the Hanford Site after all cleanup and waste disposal actions are complete." (DOE/RL 1998, page II-A.36)

Clearly, with many decisions yet to be made, (e.g., long term groundwater cleanup, tank waste recovery, carbon tetrachloride contamination in the 200 West Area vadose zone), there is no single collection of DOE documents that constitute (or identify fully) the approved post-closure end state. However, the collection of multi-year work plans for projects at the Hanford Site represent DOE's current assumed surrogate end state. This set of assumptions is the basis for the life cycle cost estimate for closure of the site. Use of the post-closure end state assumptions from the multi-year workplans as the *Hanford Site Disposition Baseline* for the initial SAC will provide an assessment of post-closure risk and impacts that is consistent with the current life-cycle closure budget. Other post-closure settings will undoubtedly be the subject of subsequent iterations of the SAC.

2.4 LIMITATIONS OF THE INITIAL SYSTEM ASSESSMENT CAPABILITY

In the initial SAC, assessment scenarios that pose perturbations from the *Hanford Site Disposition Baseline* (i.e., the baseline) will not be examined. Such perturbations will be examined in later iterations. Thus, the baseline assessment will assume a static situation for many features and events. Examples are assumptions that the Columbia River will remain as it is today for the duration of the assessment, and that the climate of the region will remain unchanged. Correspondingly, assumptions of river flow and erosion/deposition patterns from wind and runoff will also remain unchanged from the current setting.

The assumption that existing conditions prevail is extended to the background contamination upon which Hanford Site contaminants are superimposed. Background is defined here to include naturally occurring contamination and anthropogenic contamination from other non-Hanford sources. Background contaminant levels resulting from fallout, mining, agriculture (etc.) are assumed to continue, and the initial SAC will provide an estimate of Hanford Site contribution above these background conditions. Where total contamination levels are observed and simulated, results will be presented as the total contamination level and the Hanford Site contribution to the total.

The initial SAC is posed as a limited analysis of human and ecological health, as well as cultural and economic impacts. It will not address occupational health risks or estimates of the cost associated with the decommissioning, remedial actions, disposal alternatives, or closure actions implied by the end state(s) analyzed. In the initial SAC, past and future disposals, remedial actions, and tank waste recovery operations are considered as occurring when they did occur or when they are planned to occur. Because the assessments capture the long-term risk and impact associated with present day operational decisions dealing with disposals and remedial actions, future SAC assessments will inform the decision making process.

2.5 PURPOSE OF THIS PRELIMINARY SYSTEM ASSESSMENT CAPABILITY CONCEPTS DOCUMENT

This report is a preliminary description of the architecture, platform, and data management options available for the design of a SAC for the assessment of the Hanford Site's present and post-closure cumulative and composite effects of radioactive and chemical materials that have accumulated throughout Hanford's history. Section 3 describes the conceptual model of the overall SAC (Rev. 0), and its incorporation of conceptual models for each of the technical elements (i.e., inventory through risk-impact). Section 4 describes the interface and output data requirements of the SAC (Rev. 0). An appreciation of the information to be passed between technical elements is essential to understand constraints on the system architecture, platform, and data management options. Section 5 provides a description of the alternative architecture for performing the assessment and managing data. It also outlines the experience gained through participation in several large-scale assessments that included uncertainty simulations. Recommendations are made regarding the architecture and data management structure for SAC (Rev. 0), and for the computational platforms to be utilized.

This report includes appendices describing the conceptual models for each of the components of the Hanford Site SAC (i.e., inventory, release, vadose zone, groundwater, river, and risk/impact). This document describes the data linkages between system components, and the form and general requirements of the output requirements for each technical element. These interface linkages and output requirements contribute to an understanding of the constraints on and functionality of alternate architecture. Assessment or simulation results of the first five (inventory through river) provides an indication of what the future contaminant distribution might be at selected moments in time and at selected locations. Assessment or simulation of risk/impact can be viewed as people, other living systems (the ecology), or cultures being exposed to the future environment through prescribed scenarios of exposure. An appendix is included as a report on aspects of uncertainty, its representation, and its simulation in assessments of similar scale, especially the large-scale and long-term assessments of the Waste Isolation Pilot Plant (WIPP) and Yucca Mountain Projects, and how those approaches might be applied to an assessment performed with the SAC.

3.0 SYSTEM ASSESSMENT CAPABILITY CONCEPTUAL MODEL AND ARCHITECTURE

A conceptual model is an evolving hypothesis identifying the important features, events, and processes controlling our understanding of consequences in the context of a recognized problem. A conceptual model evolves as more is learned about the environment or problem in question. It involves the identification of controlling or dominant features, events, and processes because one wishes to develop an efficient means of understanding and perhaps predicting observed behavior.

Problems requiring conceptual models vary. For example, one can use a simple conceptual model of an aquifer to develop water table elevation estimates to support drilling cost estimates. One can also use a conceptual model of an aquifer to forecast the direction of flow in support of a monitoring plan. Drilling cost estimates and monitoring plans may rely on a simple conceptualization that is never formalized as an analytical or numerical model. The development of a long-term quantitative assessment requires considerably more detail in the conceptual model, and will be formalized in a predictive or forecasting model. One purpose for identifying conceptual models for the SAC development effort is to provide the basis for quantitative and qualitative assessment. Another purpose is to define the data linkages between SAC technical elements and their output requirements, and to understand the magnitude of the analysis proposed and any constraints on its design.

The propagation of uncertainty through the SAC will ultimately include uncertainties in the environmental setting (e.g., climate change, onset of an ice age), uncertainties in remediation and closure actions, uncertainties in conceptual models of the geologic structure and the processes governing the movement and fate of contaminants, and parameter uncertainty. Uncertainty in the environmental setting and the remediation and closure actions will be considered in future revisions to SAC (Rev. 0). The capability to quantify uncertainty in the system assessment arising from uncertainty in conceptual models will be incorporated into the SAC (Rev. 0) design; however, applications will be limited. The majority of SAC (Rev. 0) uncertainty evaluations will focus on parameter uncertainty.

3.1 CONCEPTUAL MODELS AND THEIR RELATIONSHIP TO NUMERICAL MODELS

Conceptual models form the basis for interrogation or investigation of field and laboratory observations. They form the basis for the construction of a simulator. The concept of a conceptual model applies to all aspects of the system assessment. Conceptual models form the basis of models implemented to provide inventory projections, forecasts of contaminant release, migration, and fate in the environment, and risk and impact. While not commonly used to describe the modeling approaches to inventory or risk and impact, the approach of defining conceptual models as a precursor to the modeling process is applied (here) to all aspects of the SAC.

The modeling process is a sequence of events that most often involves feedback loops. In general, the sequence involves the following:

- Identification of the specific problem.
- Conceptualizing the important features, events, and processes in a conceptual model.
- Assembly of a quantitative description or model (e.g., a spreadsheet, an analytical model, or a numerical model).
- Verification of its ability to simulate.
- Gathering and analyzing field and laboratory data to support model calibration and history matching.
- Conducting assessments and providing predictions used to resolve the identified problem.

Feedback within the modeling process can occur at various points in the cycle. If history matching is not successful, one could return to the "conceptualization" step to alter the important features or processes included. If the predictions are too uncertain, one could return to the "gather and analyze data" step and assemble and assimilate more data, to become more certain about the conceptual model and its parameter sets, before proceeding with the assessment. Certainly, when field observations or laboratory data are gathered that conflict with the accepted conceptualization, the "conceptualization" step would be revisited and the conceptual model revised to use or explain the new data.

The development of conceptual models can be subjective and biased. These models are dependent on a limited suite of field observations and laboratory data, and on the experience and insights of the investigative team. Conceptual models can also be influenced by biases created by the disciplinary background of individuals on the investigative team. However, the GW/VZ Integration Project has established a structured logic for the identification of important or dominant features, events and processes (i.e., the features, events, and processes [FEPs] process). By establishing an interdisciplinary investigative team and the FEPs process, the conceptual models adopted for future editions of the SAC will suffer less from subjective decisions and disciplinary bias.

The initial SAC is based on existing data and conceptualizations that may be prone to these issues; however, as a proof-of-principle, the assessment achieved will still be relevant and its findings of value to the design of the SAC (Rev. 1) capability. Existing data, its interpretation, and conceptualization provide the basis for existing capabilities. These capabilities are representative of the analysis capabilities applied elsewhere to address similar problems. As such, the combination of the capabilities in a site-wide scale system assessment will be tested in principle, and relevant performance information will be gathered for the design of future SAC iterations.

3.2 CONCEPTUAL MODEL OF THE SYSTEM ASSESSMENT, INCLUDING UNCERTAINTY SIMULATION

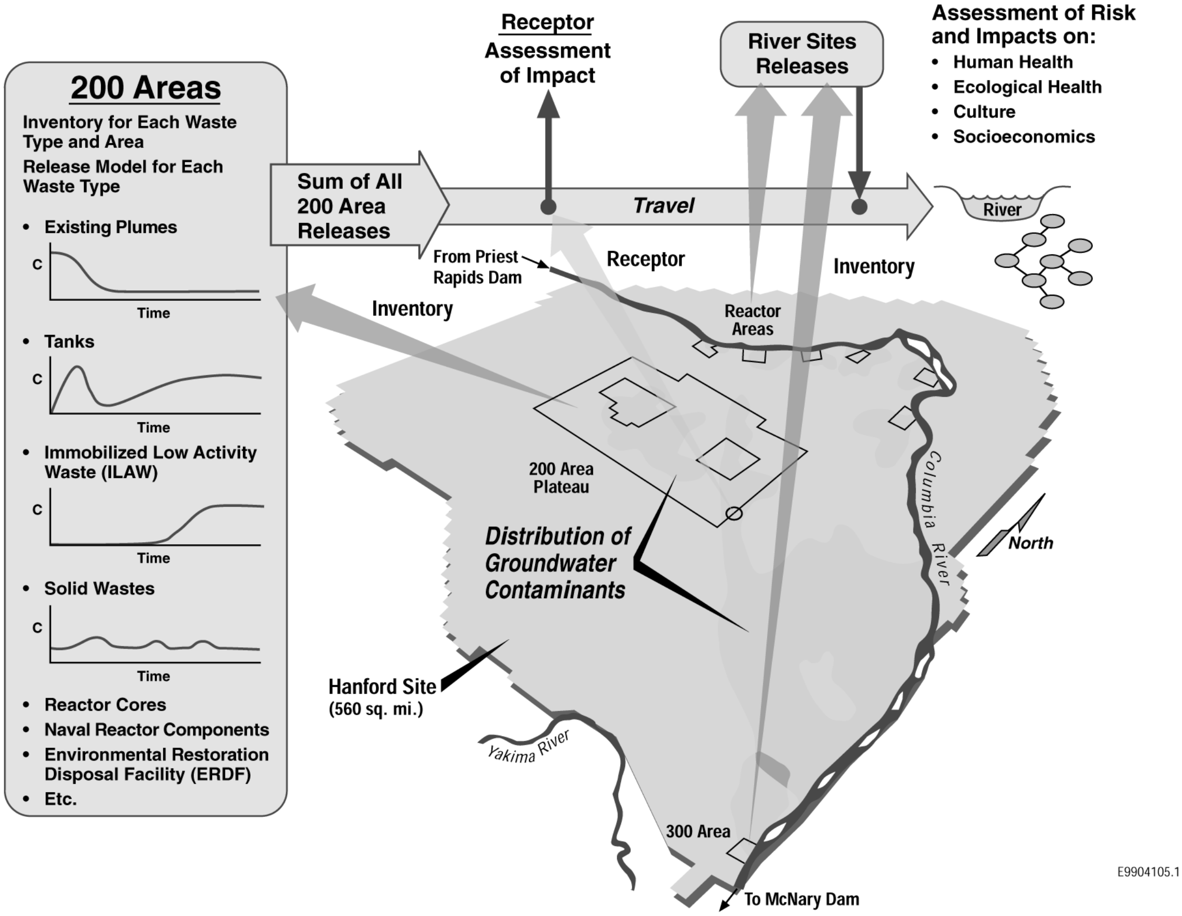
At a high level, the conceptual model of the Hanford Site must represent inventories and releases from operational areas, transport of released contaminants through the environment to the Columbia River, subsequent transport downstream to the Pacific Ocean, and exposure and risk to people, the ecology, and cultures to contaminant levels. Figure 3-1 illustrates the scope of this problem at the scale of the Hanford Site. The figure omits the downstream Columbia River aspect of the assessment capability; however, the initial SAC will address contaminant migration downstream on the Columbia River to the pool behind McNary Dam.

Operations in the reactor areas (i.e., 100 Areas), the fuel fabrication and research & development laboratories area (i.e., 300 Area), and the chemical separations areas (200 East and 200 West) generated waste. Releases have occurred to the Columbia River, to the atmosphere, to the vadose zone, and to the groundwater. The initial SAC will consider the dominant long-term threat pathways of the vadose zone and groundwater that have been identified and analyzed in several prior analyses (Mann et al. 1998, Kincaid et al. 1998, Wood et al. 1996). That is (a) release to the vadose zone; (b) subsequent migration through the vadose zone and groundwater aquifer to the Columbia River; and (c) the downstream migration and fate of contamination to McNary pool, which lies below the confluence of the Snake and Columbia Rivers. Finally, the assessment of risk and impact will examine a suite of metrics including human health, ecological health, socio-cultural and economic impacts. Conceptual models for each of the technical elements contributing to the SAC (Rev. 0), (i.e., inventory, release, vadose zone, groundwater, Columbia River, and risk and impact), are presented in Appendices A through F.

As mentioned in Section 2.2, the SAC is being designed to distinguish between the risks and impacts of the various waste types (e.g., solid wastes, liquid discharges, immobilized low-activity waste [ILAW]). This will be achieved by applying distinct release models to different wastes. The number of waste types used in the analysis will be determined by the characteristics of the waste release and its mobility in the environment. Waste types (such as solid waste, graphite cores, and glass) have different release characteristics. Liquid releases to ground via cribs, french drains (etc.) all use the same release model, but are distinguished by their geochemical mobility because of their pH, organic content, and salt content.

The SAC is also being designed to distinguish between the risks and impacts of the wastes disposed in the Central Plateau, and wastes disposed adjacent to the Columbia River within the 100 and 300 Areas. To maintain an economic and efficient initial assessment, the analysis will aggregate sources within these operational areas while maintaining realistic waste concentrations in the environment. This is being done to ensure the groundwater analysis can be conducted in a format that allows unit releases to be used and overall releases to be scaled. Single release locations will be used in the 100 and 300 Areas; however, on the 200 Area plateau, several locations may be used (up to 3 in each 200 Area) to best represent contaminant migration in the vadose zone, and contaminant plumes in groundwater.

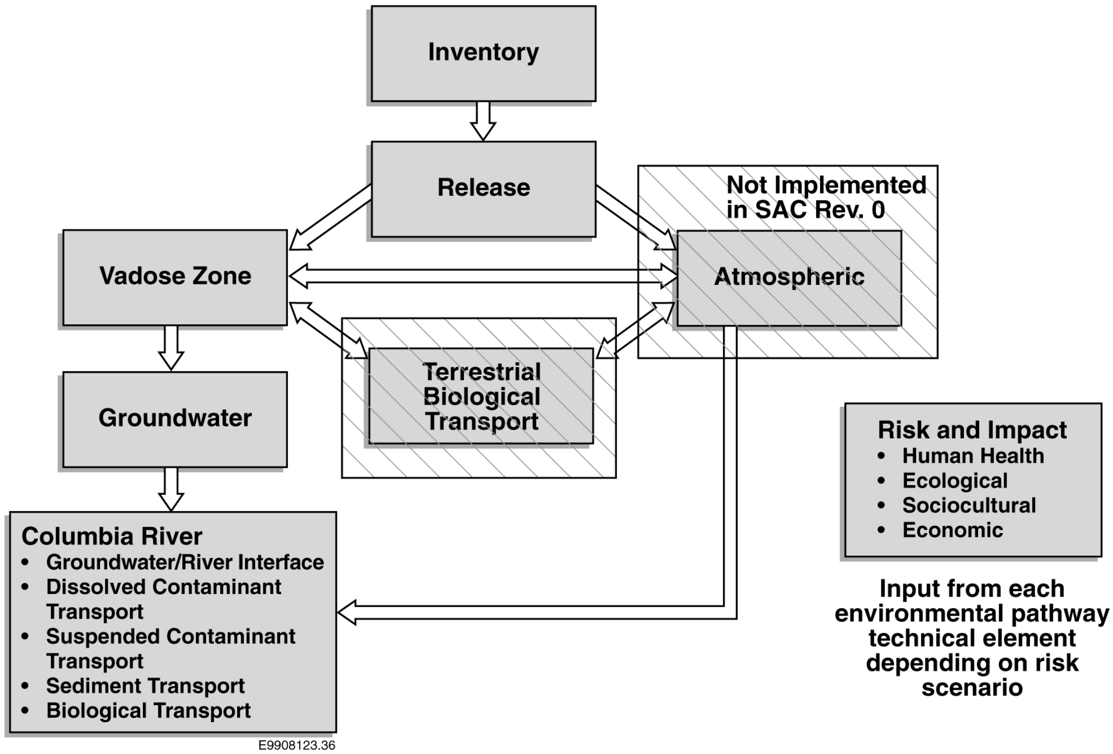
Figure 3-1. System Assessment Capability (Rev. 0) Conceptual Model.



3.2.1 System Assessment Capability Conceptual Model

The initial SAC is being designed as a relatively simple demonstration capability. Figure 3-2 illustrates the technical elements and the flow of information. The assessment of the environmental conceptual model of the SAC, by showing the linkage of pathways, exhibits a linear flow of information. No feedback loops to predecessor technical elements are allowed in this initial assessment. Inventory feeds to release, feeds to vadose zone, feeds to groundwater, and feeds to the Columbia River. The Columbia River includes groundwater/river interface, river flow and transport, and biological transport. The groundwater and Columbia River technical elements feed the risk and impact assessment capabilities. Figure 3-2 notes the omission of the atmospheric and terrestrial biological transport pathways in the initial SAC. The atmospheric pathway is omitted from the SAC (Rev. 0) because of its relatively small contribution to contaminant migration in a post-closure setting (when waste forms and disposal are stable). Terrestrial biological transport would quantify the biological migration and fate of contamination at the soil-atmospheric interface. The inclusion of feedback and atmospheric and terrestrial biological transport pathways will be considered during the design of the SAC (Rev. 1).

Figure 3-2. System Assessment Capability System Conceptual Model.



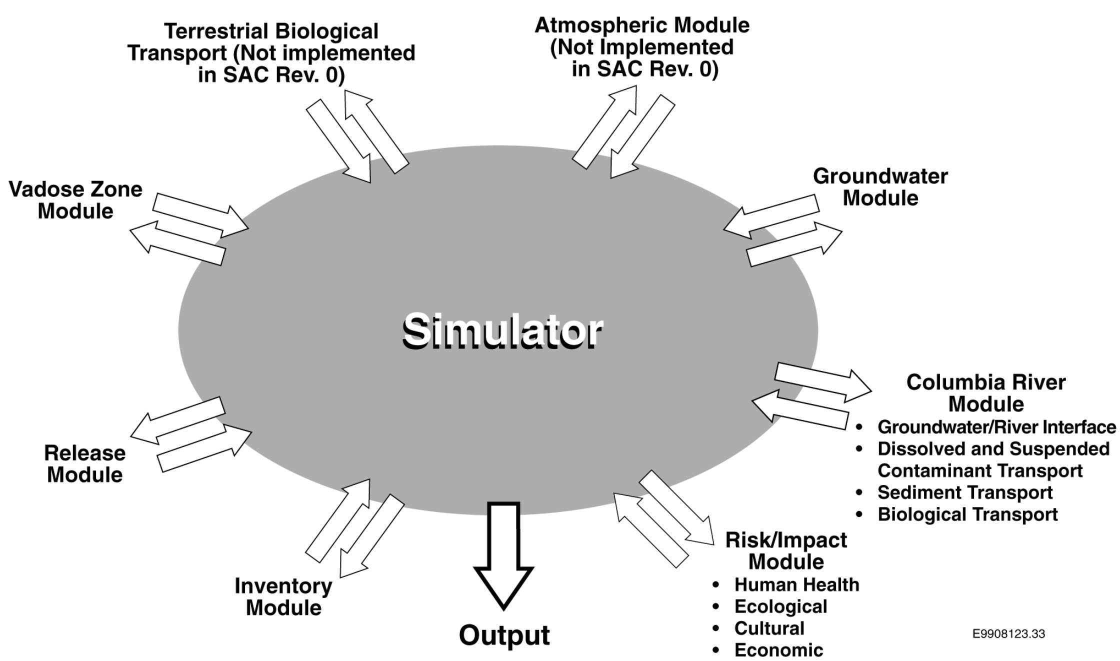
3.2.2 System Assessment Capability Simulator

The SAC simulator itself can be described (in concept) as a sequence of simulations proceeding from inventory through risk and impact. Each technical element component of the overall simulator would be based initially on a deterministic understanding and an existing simulation capability. Following the assembly and verification of the initial capability, multiple realizations will be simulated of technical element conceptual models and model parameter variations. While viewed as a sequence of simulations, the overall simulation can be viewed as two largely independent events. First, there is the combination of technical elements that yields a representation of the physical world. This is captured as the contaminant distribution in space and time, resulting from a suite of environmental (e.g., climate), remediation (e.g., *Hanford Site Disposition Baseline*), conceptual model, and model parameter scenarios. Second, there are the individual risk and impact assessments that essentially use the contaminant distributions in space and time as plausible future environments to which we expose humans, other living systems (the ecology), and cultures according to accepted scenarios for exposure and impact.

Two approaches exist for the development of the SAC simulator. First, assuming that experience and knowledge of the simulation options (computing resource requirements) is complete, or at least adequate, one can proceed immediately using a requirements, design, and assembly sequence to create the desired capability. Second, if the design would benefit from additional experience and knowledge regarding the computing resource requirements associated with different options, then a rapid and less structured initial development should be followed by an evolutionary prototyping improvement period. In the latter case one could replace the initial technical element components to the overall SAC with alternate components, ranging from reduced-form capabilities or analytical solutions to the most complex and sophisticated simulation tools. One could also replace a computational component with a pre-run simulation stored for use in the SAC simulator. Thus, one would be determining the resources and speed of direct computing as opposed to input/output speed of data file transfers. Using either approach, the intent is to learn the physical constraints (resource, memory) and performance requirements of alternatives, and use this information to design the decision assisting capability of the SAC (Rev. 1). The evolutionary prototyping approach acknowledges the dynamics of changing requirements, and reduces risk in achieving a satisfactory design of SAC (Rev. 1).

In general, the simulator facilitates a sequence of simulations of technical element modules. Output of one transfers through the simulator and becomes the input to the next. Under either approach described in the preceding paragraph, the basic design of the SAC is represented by a simulator hub (in Figure 3-3) with stubs that interface to technical element components. Each stub has well defined interface protocols for the transfer of data to the technical element, and for the transfer of data back to the simulator hub. The simulator sequentially calls technical element simulators, beginning with the inventory, and ending with the risk and impact components. Information is passed through the simulator to successor simulations. Sensitivity could be examined by running the simulator on a series of cases that alter one or more scenarios of environment, remediation, conceptual model, or model parameters. Uncertainty is examined by cycling the simulator and saving output from numerous cases selected (or designed) to represent the full spectrum of uncertainty of interest to the users of the decision assisting capability (e.g., alternate remedial actions, alternate conceptual models, alternate model parameters).

Figure 3-3. System Assessment Simulator.



This is a Monte-Carlo method of analyzing uncertainty. Scenario and data selection methods could be optimized (e.g., through use of Latin Hypercube methods), to minimize the number of cases requiring simulation to achieve an uncertainty assessment. Because of the resource requirements of propagating uncertainty through the overall simulation, it may be desirable to use fewer simulations and achieve a general indication of the variability in the performance of the entire system.

3.3 CONCEPTUAL MODELS FOR TECHNICAL ELEMENTS

A conceptual model of inventory estimation for the Hanford Site is based on hypotheses about the processes and waste streams arising from a series of events. These events include the fabrication of fuel rods, the irradiation of fuel in reactors, the chemical separation of special nuclear materials from irradiated fuel, the disposal of some wastes, and the storage and subsequent reprocessing of other waste streams. In addition to waste transfer records, a conceptual model of inventory must be based on the imported and exported quantities of radionuclides and chemicals, and on the estimated efficiencies of chemical extraction processes. The final disposition of waste at site closure, and the Hanford Site end state, must be captured in the inventory conceptual model. The conceptual model provides a framework in which to estimate the location and quantity of radioactive and chemical wastes in Hanford Site facilities and the environment. Appendix A provides a more complete description of the inventory conceptual model.

Conceptual models for the waste form release and environmental pathways of the vadose zone, groundwater aquifer, and Columbia River have in common the context of the long-term release, migration, and fate of contaminants. Appendices B, C, D, and E provide a more complete description of the release and environmental pathway technical elements. Their conceptual models are the evolving hypotheses that identify the important features, events, and processes controlling the flow of fluid and transport of contamination of consequence for the Hanford Site and downstream Columbia River in the context of accepted risk and impact metrics. With respect to release calculations and environmental pathways, the definition of conceptual models is an accepted approach to the definition of the necessary models, their supporting data, and the necessary output.

Conceptual models for risk to human health and ecological health rely on hypotheses regarding the dominant processes and events governing human and ecological exposure and resulting risk. They are described in Appendix F. Scenarios are the series of events resulting in human and ecological exposure. Dose or risk conversion factors are commonly used to quantify the human or ecological response to observed or predicted levels of contamination in the environment. These dose or risk conversion factors are based on hypotheses regarding the pathway taken by contaminants in the human body, and in ecological species of interest, and the resultant impacts of the contaminants on the health of the living system.

Details of the interface linkages between technical elements provide another avenue for understanding the conceptual models of each technical element of the SAC. These data interface and output requirements are outlined in Section 4.0.

4.0 INTERFACE AND OUTPUT DATA REQUIREMENTS

Data requirements are a significant consideration in the design and application of the SAC. A clear understanding of the data and information to be passed from one technical element to the next is essential to the design of interfaces. Certainly, a clear understanding of the desired results is essential to design of the risk and impact component. Those requirements trace back through the entire assessment design. In the following sections the predecessors and successors relationships are outlined, and the interface and output data requirements are described.

4.1 TECHNICAL ELEMENT PREDECESSORS AND SUCCESSORS

Linkages between and among the technical elements of the SAC are described below, in terms of the predecessors and successors (Table 4-1). While it is acknowledged that feedback exists, the SAC (Rev. 0) will exclude feedback and assume that a forward flow of information dominates the overall assessment.

Table 4-1. Technical Element Predecessors and Successors. (2 Pages)

Technical Element	Predecessor Technical Element(s) or Information	Successor Technical Element(s) or Output
Inventory	• Inventory models, e.g., Hanford Defined Waste Model • Inventory spreadsheets and databases (e.g., SWITS, WIDS, Radionuclide Inventories of Liquid Waste Disposal Sites on the Hanford Site) • Synthesis of model and databases (e.g., Best Basis Inventory for Tank Wastes) • Hanford Site Disposition Baseline	• Release
Release	• Inventory	• Vadose Zone
Vadose Zone	• Release	• Groundwater • Groundwater-Columbia River Interface
Groundwater	• Vadose Zone	• Groundwater-Columbia River Interface • Columbia River & Biological Transport • Risk – Ecological • Risk – Human • Risk – Cultural • Risk – Economic
Groundwater-Columbia River Interface (part of the Columbia River technical element)	• Vadose Zone • Groundwater	• Columbia River & Biological Transport • Risk – Ecological • Risk – Human • Risk – Cultural • Risk – Economic
Columbia River & Biological Transport	• Groundwater • Groundwater-Columbia River Interface	• Risk – Ecological • Risk – Human • Risk – Cultural • Risk – Economic

Table 4-1. Technical Element Predecessors and Successors. (2 Pages)

Technical Element	Predecessor Technical Element(s) or Information	Successor Technical Element(s) or Output
Risk – Ecological	• Groundwater • Groundwater-Columbia River Interface • Columbia River & Biological Transport	SAC Output for Ecological Risk
Risk – Human Health	• Groundwater • Groundwater-Columbia River Interface • Columbia River & Biological Transport	SAC Output for Risk to Human Health
Risk – Cultural Impact	• Groundwater • Groundwater-Columbia River Interface • Columbia River & Biological Transport	SAC Output for Cultural Impact
Risk – Economic Impact	• Groundwater • Groundwater-Columbia River Interface • Columbia River & Biological Transport	SAC Output for Economic Impact

Predecessors to the inventory technical element are unique in that they include models of inventory, (e.g., the Hanford Defined Waste model), inventory databases, and databases that represent a synthesis of inventory records, measurements, and model results (e.g., the best-basis Office of River Protection [ORP] inventory for tank wastes). Inventory databases differ from a synthesis of data and models in the sense that an inventory database can be a record of actual waste transfer. The synthesis database includes expert judgment as to the relative worth of a waste transfer record, a measurement, and a model result. Depending on the application to be made, measurements may be more highly valued than waste transfer records. The end state of the Hanford Site for the SAC (Rev. 0) is the Hanford Site Disposition Baseline, which is also an example of predecessor knowledge needed for implementation of the inventory model.

The initial SAC will consider the main flow of information in the environmental models from inventory to release, from release to vadose zone, from vadose zone to groundwater, and from groundwater to the river. Information flow to and from the groundwater-Columbia River interface is called out because this component of the Columbia River technical element is important to ecological risk considerations.

The vadose zone and groundwater-river interface is significant because of the potential for river stage change and bank storage to affect a release of contamination adsorbed or precipitated in the vadose zone of the near-shore environment. Past releases to the vadose zone in the 100, 200, and 300 Areas raised the water table in these regions, and created the deposits which now lie above the normal water table. Water-table rise in response to river stage rise periodically floods these deposits in the 100 and 300 Areas, and causes a release of contamination.

Groundwater releases occur to the Columbia River. At an intermediate to large spatial scale, release from the groundwater aquifer to the river is a long-term event governed by the annual flux of contamination from the aquifer to river. At the fine scale of the ecology of the riparian zone, the fine sand river sediments, and the coarse gravel river sediments; seasonal-to-daily changes in river stage, temperature, etc., impact the concentrations of contaminants and the life cycles of living systems. Thus, the groundwater-river interface is an important aspect of the Columbia River technical element receiving input from the groundwater technical element.

The groundwater, groundwater-river interface, containment transport in the Columbia River, and biological transport all interface with each of the risk technical elements (i.e., ecology, human health, socio-cultural, and economic). Each of the risk technical elements will produce tabular and graphical displays of their associated metrics of risk resulting from the Hanford Site's present and post-closure cumulative effects of radioactive and chemical materials.

4.2 INTERFACES BETWEEN TECHNICAL ELEMENTS AND REQUIRED OUTPUT

Unambiguous interface definition is critical to the success of the SAC. The required interface or output data are summarized below, and in Table 4-2 for each technical element. This information will contribute to an understanding of the information to be simulated and passed between simulation components. It will also contribute to an appreciation of the potential mass storage requirements for a simulation cycle. The interface and output data are presented in reverse order, (i.e., from final SAC output back to inventory), to achieve an appreciation for the interface information required to enable the risk quantification.

Table 4-2. Technical Element Interface and Output Data. (3 Pages)

Technical Element	Interface or Output Data
Risk – Economic Impact	SAC Output from Economic Impact • Economic impacts associated with (among others): - avoidance of products - avoidance of recreational activities - alternate water supplies - loss of business recruiting options
Risk – Cultural Impact	SAC Output from Cultural Impact • Plots illustrating the diminished natural resource quality of cultural importance (e.g., groundwater) • Plots illustrating the proximity of known cultural resources to impacted zones
Risk – Human Health	SAC Output from Risk to Human Health • Risk contours for groundwater impact • Plots of human health risk versus river mile at selected times for exposures to the riparian zone, the Columbia River water (dissolved and suspended contaminants), the Columbia River sediment, and the living biological systems in the Columbia River • Plots of human health risk versus time at selected locations of concern for above
Risk - Ecological	SAC Output on Ecological Risk • Plots of ecological risk versus river mile at selected times for specific living systems, according to exposure scenarios • Plots of ecological risk versus time at selected locations of concern for above

Table 4-2. Technical Element Interface and Output Data. (3 Pages)

Technical Element	Interface or Output Data
Columbia River & Biological Transport	River interface data forwarded to all risk technical elements – ecology, human health, cultural, economic • Water mass flux • Dissolved and suspended contaminant concentrations in water • Contaminant concentration on suspended material • Contaminant concentration on sediment • Contaminant concentrations associated with living biological systems
Groundwater-Columbia River Interface (part of the Columbia River technical element)	GW/CR interface data forwarded to risk – ecology, human health, cultural, economic, and to the Columbia River & Biological Transport technical elements • Contaminant concentrations in water, on suspended sediment, and on sediment at identified locations of concern and as a function of time (e.g., seasonal cycles) and events (e.g., river stage) in the riparian zone, in the fine (i.e., sand) river sediments, and in the coarse (i.e., gravel) river sediments.
Groundwater	Groundwater data forwarded to the Columbia River & Biological Transport technical element • Mass flux of water and contaminants, and concentrations of contaminants introduced to the Columbia River along the Hanford Reach for a period of analysis - Distinct flux for 4 radionuclide groups, and 2 chemicals (CCl_4, Cr^{+6}) Groundwater interface data forwarded to all risk technical elements – ecology, human health, cultural, and economic • Concentrations in groundwater over the Hanford Site for the period of analysis • Maximum predicted concentration of contaminants as a stand alone result and as the basis for predictions of maximum risk and dose for the period of analysis - Distinct plumes for 4 radionuclide groups and 2 chemicals (CCl_4, Cr^{+6})
Vadose Zone	VZ interface data forwarded to the GW technical element • Mass flux in aqueous phase to unconfined aquifer per unit area beginning in 1944 and continuing throughout the period of analysis • Distinct releases for the following locations - 100 Area (one) - 300 Area - 200 West – up to 3 zones - 200 East – up to 3 zones • Distinct flux for 4 radionuclide groups, and 2 chemicals (CCl_4, Cr^{+6}) • Distinct releases for several waste site groups • VZ interface data forwarded to the GW/CR Interface technical element • Same as above but for 100 and 300 Areas only • Transient effect of vadose zone leaching caused by river stage and bank storage effect
Release	Release interface data forwarded to the VZ technical element • Mass flux to vadose zone per unit area, beginning in 1944 and continuing throughout the period of analysis • Distinct releases as a function of time in the 100, 200, and 300 Areas for the following: - Liquid discharges - Solid waste - Tank salt cake & sludge - Glass waste - Cement waste - Graphite Core - Reactor Compartments

Table 4-2. Technical Element Interface and Output Data. (3 Pages)

Technical Element	Interface or Output Data
Inventory	Inventory interface data forwarded to the Release technical element, for the period 1944 until Hanford Site closure • Location • Physical Description (end states) • Operational History - Dates - Volumes - Time to Closure • Future inventories

4.2.1 Risk Technical Element Output

The risk technical elements produce displays or tabular summaries of risk as a consequence of contamination in the environment. Areal plots of risk, diminished resource quality, or impacted zones will present contours of risk/impact based on contaminant concentrations in space at a moment in time. These same metrics and those for economics will also be portrayed as risk or economic impact as a function of time at a point in space, or as the maximum risk or impact as a function of time at any point within the domain of interest. Assuming the use of a classical Monte Carlo simulation with Latin Hypercube methods to optimize data selection, risk could be portrayed in several ways. Risk could be portrayed in the form of cumulative distribution function plots of risks, from which exceedance probabilities could be read. Risk could also be shown using box and whisker plots (e.g., graphical displays showing the 75%, 50%, and 25% probability).

4.2.2 Groundwater and Columbia River Interface

Interface data to be transferred to the risk/impact technical elements derives from the technical elements for groundwater and the Columbia River. The interface between these elements and the risk/impact elements is composed of water and contaminant flux over the simulation period at internal and external boundaries of interest (e.g., the shoreline of the Columbia River, the sediments dredged from McNary pool, the spillway and power plant releases at McNary Dam). The interface also includes contaminant concentrations at these boundaries, and within the interior of the domain of interest (e.g., in the unconfined aquifer underlying the Hanford Site, and in dissolved, suspended, and sediment phases of the Columbia River). The Columbia River technical element includes a component on the biological transport within the river. Its interface with the risk elements includes contaminant concentrations associated with the life cycle of living biological systems. To support the risk/impact assessment, these contaminant distribution will be reported over all space at selected times, and over all time at selected points.

4.2.3 Vadose Zone Interface

The vadose zone is an interface to groundwater and to the Columbia River. An important component of the Columbia River is the groundwater-river interface. As noted in the previous section it is unique with regard to the transient release behavior associated with changes in river stage.

Otherwise, the vadose zone interface to the Columbia River is very similar to the interface with groundwater, and contains the mass flux in the aqueous phase to the unconfined aquifer. To avoid the necessity of knowing the initial conditions, (i.e., where contaminants are in the vadose zone at the beginning of the simulation), releases to the groundwater are forecast beginning with the first releases at the Hanford Site in 1944. Releases from the vadose zone will reflect the aggregation of sources obtained by the release models and inventory. Thus, vadose zone release to the groundwater will be aggregated by operational area, by radionuclide mobility, and by waste types.

To enable the examination of issues related to near-shore releases and plumes (as compared to those from the Central Plateau), the analysis will include releases from one of the 100 Areas, the 300 Area, and both the 200 West and 200 East Areas. Releases on the Central Plateau will be further subdivided to better reflect the observed migration of contaminants through the vadose zone and in the aquifer. Thus, both the 200 Areas may be subdivided into 2 or 3 zones exhibiting distinct transport and mobility behavior.

The initial SAC will examine a limited number of the more significant radionuclides and chemicals. Including the range of contaminant mobility was a primary consideration in the selection of radionuclides for study. The highest mobility group represents contaminants that move with water, e.g., tritium and technetium (technetium-99). A somewhat less mobile group represents contaminants that are somewhat but not greatly sorbed by Hanford formation and Ringold Formation sediments (e.g., uranium and iodine [iodine-129]). The next group represents contaminants that are moderately sorbed on Hanford Site sediments, e.g., cesium and strontium (cesium-137, strontium-90). Finally, the last group represents highly sorbed contaminants, e.g., plutonium (plutonium-239, 240). Chemicals to be studied include an organic compound, carbon tetrachloride, and an inorganic metal (chromium).

The aggregation of vadose zone releases to groundwater will follow that of the release models for distinct waste site groupings (or waste types). Distinct models for release to the vadose zone will be created for solid waste, tank residuals, glass waste forms, wastes in cement products or concrete, graphite cores of production reactors, naval reactor compartments, and liquid releases of unique fluids, (e.g., pH, organic content, salt content). To support the groundwater and Columbia River assessment, vadose zone releases will be reported at the aggregation locations for the assessment time period.

4.2.4 Release Interface

The release technical element of the initial SAC will provide contaminant release rates only to the vadose zone. Information on releases to other environments (e.g., Columbia River, atmosphere) will be captured in the inventory technical element. However, those releases will not be addressed in this version of SAC. The interface to the vadose zone will provide the mass flux of contaminants leaving waste sites beginning in 1944. The releases will be aggregated as noted in the preceding section according to operational area, radionuclide and chemical, and waste type. Release projections will be reported at the aggregation locations for the assessment time period.

4.2.5 Inventory Interface

The inventory technical element will provide the release module with the aggregated inventories described above. Interface data will go beyond simple reports of curies of radionuclides and kilograms of chemicals. Information on operational history (including dates of facility operation), facility dimensions (including depth), the volumes of disposal, and the assumed time of closure will be included. In addition, a physical description of the facility end-state will include mention of anticipated stabilization efforts and cover design or performance. Finally, the inventory will include estimates of future disposals and the routing and final disposition of *Resource Conservation and Recovery Act of 1976* (RCRA) and *Comprehensive Environmental Response, Compensation, and Liability Act of 1980* (CERCLA) cleanup wastes. Because of the need to avoid the specification of initial conditions, the inventory will be reported beginning in 1944, and continuing to Hanford Site closure.

5.0 PRELIMINARY CONCEPTS FOR ARCHITECTURE, PLATFORM, AND DATA MANAGEMENT

5.1 ABSTRACT LOGICAL LAYER FOR SYSTEM ASSESSMENT CAPABILITY ARCHITECTURE

Conceptually, the SAC is comprised of three layers of components: (1) the environmental simulator layer; (2) the risk and impact layer; and (3) the client interface allowing the user to interact with the system. Figure 5-1 illustrates these three layers.

Figure 5-1. Abstract Logical Architecture for the System Assessment Capability.

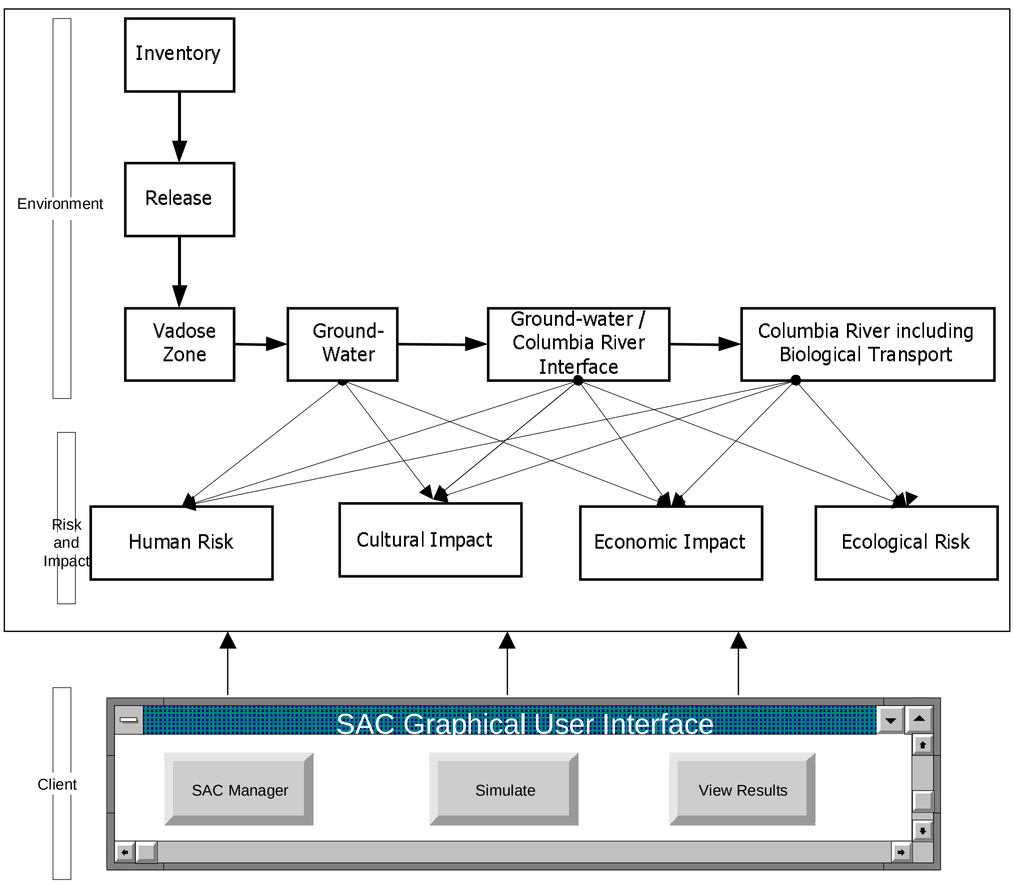


Figure 5-1 presents an *abstract logical architecture* of the SAC. It is "abstract" because each component is presented as a black box where all implementation details are hidden. It is "logical" because it is concerned with the interaction of the various components, and does not show how these components are mapped onto a set of machines running the codes (the physical layer). This architecture follows from the information in Sections 3.0 and 4.0 (see Table 4-1).

The set of components from "Inventory" to "Columbia River" is used for modeling and simulation. This set of components is given the label "Environment." Each element is necessary for the overall simulation. The second set, called "Risk and Impact," is required to inform decisions. However, one can remove any of the components of the risk section and the SAC application should continue to function. Finally, the "Client "application consists of the interface between the end-user and the system.

The Graphical User Interface (GUI) is the means by which the user (a) configures and manages the application via the SAC Manager; (b) sets and runs a simulation; and (c) views the results of the simulation. These activities can be implemented with any desired degree of flexibility and sophistication. The buttons used in Figure 5-1 for the SAC graphical user interface are intended for illustration purposes only.

5.2 AVAILABLE OPTIONS FOR ABSTRACT ARCHITECTURE

There are four broad options for turning the abstract logical architecture section into a fully functional program (Table 5-1).

Table 5-1. Fundamental Architecture Options.

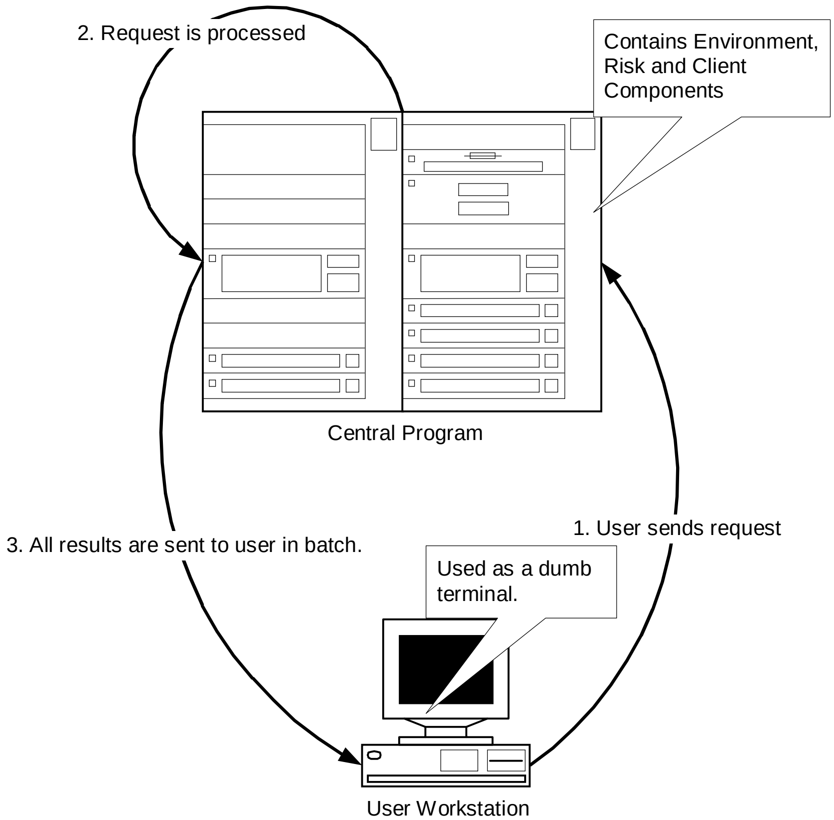
Central Program/ batch interaction	Client/Server	*n*-Tier Architecture	Distributed Collaboration
All three sets are part of one application running on a mainframe or advanced workstation. Output is mainly batch oriented. Interaction is limited.	The environment and risk components are part of the same application running on a server. The client components are written as one or more distinct applications running on client machines.	The environment component is written as one application running on its own server. The risk components are written as a separate application running on a second server. The client applications run on client machines.	Each environment component is its own application. The risk and client components are also their own applications. 'Client' and 'server' become roles played by these components as the need arises.

These four options, which are described in more detail in the following sections, represent a historical progression in software design, ranging from tightly coupled programs running on a central machine to a highly-distributed environment that is largely event driven. However, this should not be construed to mean that the three previous architectures are obsolete and should not be considered. There are problems where a central program/batch interaction approach is optimal.

5.2.1 Central Program/Batch Interaction

The Central Program/Batch Interaction solution may be simpler to develop if starting with all new code (Figure 5-2). It is also a good candidate for use with supercomputers or massively parallel machines. However, new or modified requirements that necessitate structural changes to the program tend to be difficult and costly. Furthermore, this type of application does not readily support modern user interfaces (such as Web browsers).

Figure 5-2. Central Program/Batch Interaction.



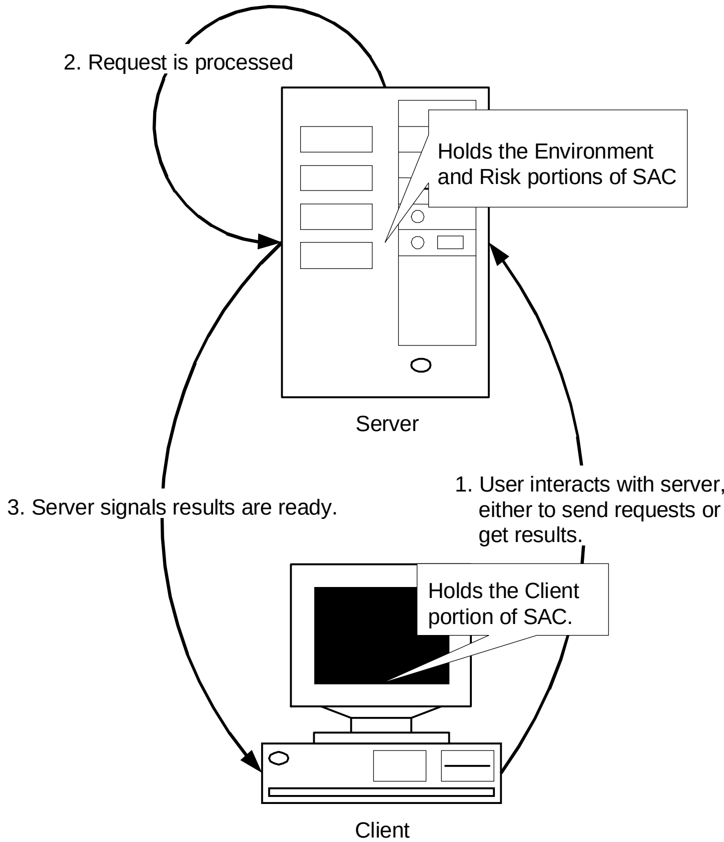
5.2.2 Client/Server

The Client/Server architecture offers better user interaction by de-coupling the client portion (the user portion) from the server (where the work is actually being done). As seen in Figure 5-3, the client portion has now been moved to the client workstation. Further, the interaction between the client and the server is interactive, offering the user an improved environment when compared to the Central Program/Batch Interaction paradigm. Modifications to the user interface become easier to implement (relative to the Central Program/Batch Interaction).

A good rule of thumb for architecture design is that the Client/Server architecture is attractive when:

- The make/type of databases is set for the duration of the project.
- The user interface is set for the duration of the project.
- The application will be implemented on a local area network (LAN), with high bandwidth and fast machines.
- No substantial modifications will be performed on the application.

Figure 5-3. Client/Server Architecture.



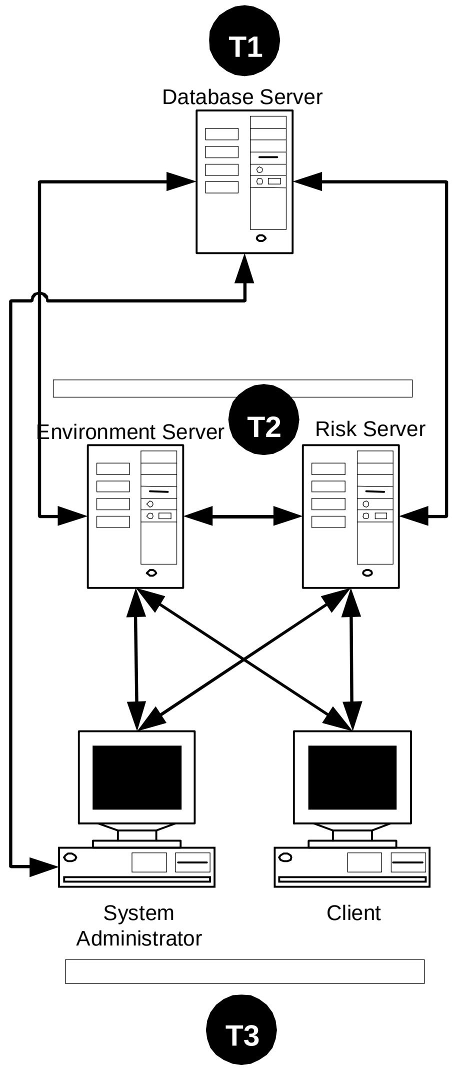
5.2.3 *n*-Tier Architecture

The SAC architecture could also be addressed as a 3-Tier Architecture (Figure 5-4). The first tier houses the database; the second tier houses the Environment and Risk components, with each component in its own server; and the third tier houses the client applications.

This division into tiers is in a *logical* sense. In Figure 5-4, the mapping between logical and physical layers is one-to-one, but it need not be so. It is possible to build an 3-tier application running on one machine.

In this type of architecture, the system administrator workstation has access to the database server via a database console for the purpose of configuring, maintaining, and repairing the database. Also, the environment and risk functions are housed in servers that are functionally independent of the database and GUI. This system is easier to scale if new databases or a new GUI must be added.

Figure 5-4. *3*-Tier Logical Architecture.



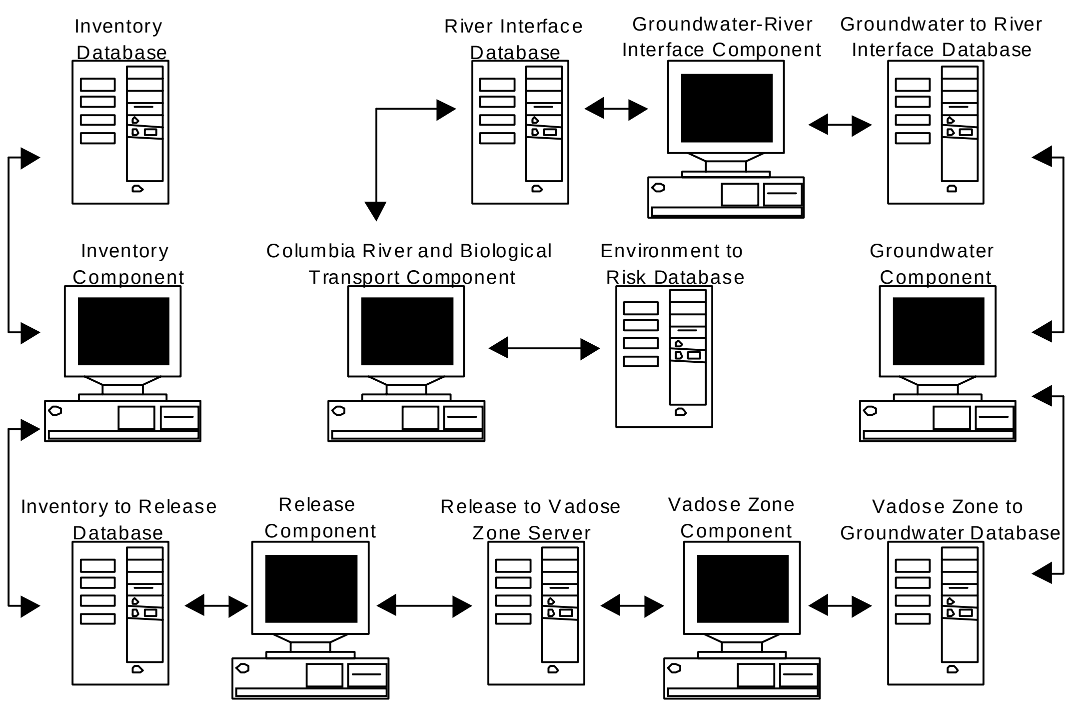
The 3-tier solution presupposes that each tier will not substantially change over the life span of the SAC. In particular, this means that the environment and risk components will remain stable and will not require much change. The 3-tier architecture is built as a set of connected central programs, such that the environment components are tightly coupled, and that the risk components are tightly coupled.

5.2.4 Distributed Collaboration Architecture

In the discussions so far, each layer consisted of one application. For instance, in the 3-tier architecture, the environment components form one application (one executable). The same holds true for the client layer since it is comprised of one application. By its very nature, the environment and risk layer are best realized as a multiplicity of independent components, collaborating together to implement the intended requirements. The Distributed Collaboration architecture is the 3-Tier Architecture taken to its logical conclusion.

Figure 5-5 illustrates a possible distributed architecture for the environmental component. Database servers and simulation components are connected in an order dictated by the needs of the application, rather than following a rigid architectural structure as in the 3-tier approach. This application order starts with the inventory database and continues through to the environment to risk database. In this architecture, the databases can be either formal databases or information exchange through disk files.

Figure 5-5. Example of Distributed Collaboration Architecture for the Environment Component.



Under this model, Inventory, Release, Vadose Zone, Groundwater (etc.) are components. Thus, “inventory” may be running in a separate process and/or on a separate machine than “release.” This model allows for the greatest flexibility among the four architectures discussed here.

Distributed Collaboration is attractive when much is unknown about the application, and when requirement creep and change is likely to occur. Under this model, each component can be built separately, and then assembled to meet the current state of the requirements. Component upgrade and replacement has minimal overall impacts. This architecture also scales well because it is very easy to house all core components on one machine, or to distribute them across a set of machines.

5.3 FUNDAMENTAL CONSIDERATIONS IN MAINTAINING A SYSTEM ASSESSMENT CAPABILITY ARCHITECTURE

5.3.1 Maintenance Operations

In order to make an informed decision among available options, it is important to understand the type of maintenance operations that are most likely to be performed in any SAC implementation scenario. There are three fundamental architecture operations: (1) adding a component; (2) modifying an existing component; and (3) removing a component. The main objective from a software-engineering standpoint is to minimize the impact these changes will have on the entire system. A tightly coupled system will be most difficult to modify because the effect of a change can propagate throughout the entire program. On the other end of the spectrum, a Distributed Collaboration architecture will be the easiest to modify *provided that it is operating with a set of well-defined interfaces*.

5.3.2 Separation of Concerns

While a user may readily accept that modifications to the environment component take time, they may be less inclined to be patient if modification of a user interface unrelated to the interface they are using prevents use of the entire system. Here, the argument in favor of a Distributed Collaboration architecture or at the very least a 3-tier distributed architecture becomes compelling.

Use of the *separation of concerns principle* of good software engineering must be employed. This principle can be stated from the perspective of a software developer: what happens in another module should not affect my work, if my work is largely independent from the module being modified.

In the Distributed Collaboration architecture, one can replace any simulator by another simulator or even by a database containing a result set of simulations without affecting the rest of the system. This is an end-result of applying the separation of concern principle, by letting a set of components collaborate through a well defined set of interfaces.

5.3.3 Software Versioning

Versioning is the process through which a component is upgraded to implement new functionality while remaining backward compatible. Backward compatibility allows those components that do not know of the new functionality to be undisturbed by the upgrade, while components that depend on the new functionality have access to it. Decisions on software versioning are required early in the software design process.

5.3.4 Object-Oriented Architecture Considerations

While it is entirely possible to apply distributed collaboration principles using traditional means, it is easier (in some cases) to deal with issues of versioning and scalability using the functionality of Distributed Component Object Model (DCOM) or Common Object Request Broker

Architecture (CORBA). Scalability of a system refers to the system's ability to be re-deployed on a physical layer that is markedly different from the initial one. For instance, the initial physical layer may be a workstation, and the next layer is a set of networked servers. With CORBA and DCOM, this movement becomes a matter of installation. Without these technologies, all the requested connectivity among workstations, the movement of data across the network, and the management of communication between these workstations must be explicitly defined by the programmers. CORBA and DCOM give an industry-standard way of mapping components onto a physical layer.

These considerations must be balanced by constraints of the problem being addressed, such as the ability to break the simulators into a set of well-defined component without rewriting existing software. These key issues need to be addressed when deciding on the type of architecture. Most, if not all, of the candidate simulators for the SAC are written in FORTRAN. There is no readily available interface between FORTRAN and DCOM or CORBA. However, methods now exist to interface FORTRAN libraries with C++.

While this compatibility issue is not limited to the Distributed Collaboration paradigm (Client/Server and 3-Tier architectures suffer from this problem although to a lesser degree), it becomes critical in the Distributed Collaboration architecture. In order to determine the feasibility of using a DCOM or CORBA approach in a Distributed Collaboration architecture for the SAC, the following questions need to be answered.

- Is it reasonable to place C++ wrappers around extant FORTRAN code? This is feasible only if the FORTRAN code has a small set of well-defined entry points (functions), which is a situation that does not exist for any of the legacy codes being considered for SAC (Rev. 0).

- Does the project favor reuse of existing code over scalability of the entire system or can FORTRAN code be rewritten into C++ when wrapping is not feasible?

These questions highlight the tension between the scientific framework where FORTRAN is predominant and the software-engineering framework where Distributed Collaboration via object-oriented design alongside DCOM or CORBA is predominant. Typically, baseline requirements help resolve these issues.

5.4 HISTORICAL SYSTEM DESIGN CONSIDERATIONS

This section examines historical software system designs to extract design concepts and lessons learned for the SAC (Revision 0/1). A brief discussion of criteria for comparing multimedia exposure assessment software systems is needed. Any good modeling exercise starts the software system design with a well-defined set of requirements based on four fundamental questions:

- What is the question the user is asking the software system to answer?
- What data are available at the site to support efforts to answer the question?

- What scientific and model complexity is needed to answer the question?
- What equipment is available to the modeling system?

Because these foundation concepts are so important the comparison of historical modeling systems is broken into these fundamentals.

5.4.1 Historical Project Overviews

Several recent projects that had large systems-like modeling efforts containing an uncertainty component are reviewed in this section.

5.4.1.1 Hanford Exposure Dose Reconstruction 1987-Present. The objective of the Hanford Exposure Dose Reconstruction (HEDR) Project was to provide individualized radiation dose estimates (with uncertainty) to any person who lived within a 75,000 square mile area surrounding the Hanford Site during a period of nearly 50 years (1945 – 1994). Both atmospheric and Columbia River pathways were included. The atmospheric and Columbia River environmental pathways were emphasized over vadose zone and groundwater because releases to the atmosphere and river were dominant during the Hanford Site production mission period. Products included risk maps (with associated uncertainty based on 100 model structures) for a variety of ages and lifestyles at 1,102 locations, and delivery of a code to the client capable of conducting dose assessments for individuals who lived near the site.

The primary computational software dealt with 1 radionuclide in the air and 5 radionuclides in Columbia River water. Spatial resolution is six miles for the air pathways, and several discrete segments of the Columbia River. The major coding effort was aimed at atmospheric pathways, rather than waterborne pathways. The Distributed Collaboration architecture was used.

5.4.1.2 Waste Isolation Pilot Plant 1980-Present. The Waste Isolation Pilot Plant (WIPP) is an operating deep-geologic repository for transuranic wastes in a bedded salt geology near Carlsbad, New Mexico. The most recent performance assessment calculations supported a license application to the EPA to begin waste disposal operations. The system model was implemented as a series of linked complex models in a stochastic framework. Probabilistic analyses were conducted using 100 realizations of the complex models for a moderate number of radionuclides. A single alternative was run through the models. The major products were complementary cumulative distribution functions of cumulative release of radionuclides and individual dose to an individual 5 km from the underground facility. A major feature of the system was implementation of an automated configuration management system that handled computer codes, data sets, and modeling results. This model was developed under stringent quality assurance requirements.

5.4.1.3 Yucca Mountain Project 1986-Present. The DOE is conducting studies at Yucca Mountain, Nevada, on its suitability for constructing and operating a deep geologic disposal system for commercial spent nuclear fuel, DOE spent nuclear fuel, and high-level wastes.
A system model has been developed for the site, with the most recent assessment supporting a report to Congress in 1999 on the suitability of the site for further study. The system model is implemented as a combination of reduced form models and linked complex models on a personal

computer (PC) with a large amount of memory (512 Mb minimum with 1 Gb preferred). The system model is exercised in a stochastic mode, typically with 100 realizations involving 9 radionuclides. The typical model result is a complementary cumulative distribution function of individual dose to an individual 5 km or 20 km from the facility.

5.4.1.4 Columbia River Comprehensive Impact Assessment 1994-1996. The CRCIA, Part 1, was a screening assessment to evaluate the potential impacts resulting from current levels of Hanford-derived materials and contaminants on the Columbia River environment, river-dependent life, and users of river resources. The CRCIA Part 1 scope was limited to the stretch of the Columbia River and its adjacent riparian zone from Priest Rapids Dam to McNary Dam, and to contaminants determined from recent (1990-1996) environmental measurements. No contaminant transport modeling was performed. Both human health risk and ecological risk were evaluated. Twelve radionuclides and sixteen metals or chemical compounds were studied in detail, and uncertainty results were generated using 100 model simulations. The product of the system was a stochastic suite of human and ecological impacts at each of the locations. Because each component was built separately, a central program architecture was used.

5.4.1.5 CE Kelley 1997. This project provided technical support to the U.S. Army Reserve Command's C. E. Kelly Support Facility. The project scope covers a broad range of environmental investigations aimed at evaluating the need for, selecting, and designing remedial alternatives for selected facilities. Technical objectives for this work involved defining the degree and extent of contamination; resolving conflicting previous data; evaluating possible contaminant sources; evaluating contaminant transport pathways and risks, groundwater monitoring needs, various remedial technologies, the effectiveness of Interim Remedial Actions, and the need for further remedial actions. Seven contaminants were analyzed in an uncertainty analysis.

The Framework for Risk Analysis Multimedia Environmental Systems (FRAMES) represented the platform that linked databases and models together in a plug and play environment. The architectural design of FRAMES can best be described as Distributed Collaboration running on a single CPU.

5.4.1.6 Hazardous Waste Identification Rule 1998-Present. The EPA is developing a comprehensive environmental exposure and risk analysis software system for application to the technical assessment of exposures and risks relevant to the *Hazardous Waste Identification Rule* (HWIR). The HWIR is designed to determine quantitative criteria for allowing a specific class of industrial waste streams to no longer require disposal as a hazardous waste (i.e., "exit" Subtitle C) and to (instead) be disposed of in Industrial Subtitle D facilities. The HWIR technology software platform links site-layout, site-specific, regional, national, chemical property, and meteorological databases with 17 different source, transport, and human and ecological exposure/risk/hazard models to evaluate acceptable exit-level criteria for selected organic and heavy-metal contaminants. A separate yet seamless Risk Visualization Processor (RVP), providing graphical and tablular sets of results, was developed so policy analysts could view the results from multiple perspectives to obtain a good understanding of the ramifications of any decision. This RVP captures the uncertainty in the analysis and provides the analyst the option of choosing an acceptable level of protectiveness (e.g., protecting 95% of the population at 95% of the sites). The HWIR software technology system is based on the FRAMES software platform. The architecture design of the FRAMES-HWIR platform can best be described as 3-tier, although FRAMES-HWIR is not prohibited from being modified for Distributed Collaboration.

5.4.2 Historical Project Software Design Comparison

Table 5-2 presents a comparison of many of the features of historical modeling systems that incorporate uncertainty. The first three items in Table 5-2 address user questions and the user who needs answers to these questions. Aspects of the assessment that appear to be important for multimedia exposure assessment software system are as follows:

- The number of sources that can be simulated
- The number of alternatives that can be simulated
- The number of scenarios that can be simulated.

For the purposes of this discussion, an alternative is a difference in the source and transport models. For example, in the Yucca Mountain study two alternatives were 1) a 70,000 and a 105,000 metric ton uranium inventory, and 2) alternate emplacement strategies yielding different thermal profiles. A scenario is defined as a change in the receptor behavior. In CRCIA Part 1 for example, the activity patterns for Native Americans was considered as a different scenario than those associated with recreational use of the area.

The amount of data required for each system is defined as either Low, Medium, or High. This measure was taken on a per site per chemical basis. A “low” value expresses that a software system does not require many data to be able to simulate a site. This is obviously connected to the scientific and model complexity.

The scientific complexity for each system is determined on a medium-by-medium basis. If a modeling system uses all reduced-form models, then it will be labeled as reduced. A reduced model is one that typically can be solved by an analytical or semi-analytical algorithm rather than a purely numerical solutions. A modeling system that is solved by a numerical or adaptive numerical solution is labeled as “complex”. If a modeling system contains a combination of “reduced” and “complex” models, it is labeled as “mixed”. The runtime bottleneck is also listed in scientific and model complexity because it is usually an indication of which media model is the most complicated.

For each software system the operational platform is defined, as well as the memory and storage requirements. Concept and specifications documents are also seen as a requirement of any multimedia software system, and their availability is indicated.

Table 5-2. Comparison of Historical Software Systems that Incorporate Uncertainty.

	HEDR	CRCIA	WIPP	Yucca Mountain	CE Kelley	HWIR
Question						
Question Dimensions	15 Sources 1 Alternative 2500 Scenarios	1 Source 1 Alternative 16 Scenarios	9 Sources 1 Alternative 3 Scenarios	9 Sources 1 Alternative 4 Scenarios	Multiple sources 1 Alternative Multiple scenarios	Multiple sources 1 Alternative Multiple scenarios
User	Project Personnel	Project Personnel	Project Personnel	Project Personnel	Environmental Engineer	Decision Maker (Regulation)
Deliverable to User	Document with contours of risks and simulation software	Document with stochastic risks	Document with stochastic risks	Document with stochastic risks	Software for conducting simulations and visualization results	Software for visualization of results
Data Availability						
Amount of Data Gathered	High	Medium	High	Medium	Low	Medium
Scientific and Model Complexity						
Complexity of simulations	Complex	Complex	Complex	Mixed	Reduced	Mixed
Access to Source Code **Languages**	Yes FORTRAN, C	Yes FORTRAN	Yes FORTRAN	Yes FORTRAN	Yes FORTRAN, C++, Visual Basic	Yes FORTRAN, C++
Runtime Bottleneck	Air transport, environmental accumulation	None	Deep unsaturated zone flow and transport	Unsaturated zone and saturated zone transport	Aquifer	Human Risk
Platform/Hardware Requirements						
Platform	Sun Workstation, MS-WINNT	MS-WIN95	Dec Workstation	MS-WIN95	MS-WIN95	MS-WIN95
Requirements **Memory** **Storage** **Speed** **Concept Doc.** **Specs Doc.**	 128 MB 7 GB 3 wk, 3 day, 5 min. PNWD-2023 HEDR Rev. 1 PNWD-2251 HEDR	 <26 MB <75 MB 10 minutes Project records Project records	 64 MB 70 GB 45 days Project Records Project Records	 512 MB 10 GB 3 weeks Project Records Project Records	 <32 MB <30 MB 1 day Draft Report PNNL-11748	 < 64MB < 3GB 1 month PNNL-11914 Vols. 6 & 8 PNNL-11914 Vols. 6 & 8

5.5 OBSERVATIONS AND RECOMMENDATIONS

This section summarizes observations from historical projects, along with conclusions and observations about proceeding with design, and includes preliminary recommendations for the system architecture.

5.5.1 Observations

The architecture and design for the SAC (Rev. 0) can benefit from past projects. We provide general observations without developing detailed concepts for the SAC (Rev. 0) software system.

The following observations pertain to the question that is being answered by the software system:

- An uncertainty assessment tends to increase overall run times by as much as two orders of magnitude over that required for deterministic simulations.

- Decision support tools should visually display the results of computation. These tools do not produce new results but, instead, display snapshots of the generated information to assist the decision maker.

- A trained person is needed to produce simulation results. A training course should be developed to train candidates to operate the system.

- The number of potential users and trained operators of the system determines how transferable the software system needs to be. A large number of users and operators drives one to make the system easy to install, test, use and operate.

- Visualization tools for operators are essential for determining simulation and result correctness. Visualization of results is critical for decision makers using the results of the software system.

- Limiting the number of end points will reduce storage and runtime requirements, but are strictly linked to the question being answered. Currently, four endpoints have been defined for the SAC (Rev. 0) (economic impact, ecological risk, human-health risk, and socio-cultural impact).

- A clean system design is key to adding functionality. For example, if all components of a system handle errors using a particular approach, a new component should also follow that approach.

Preliminary Concepts for Architecture, Platform, and Data Management

The following statements pertain to the data availability and management issues for the SAC (Rev. 0) software system:

- Access to data from different databases is important, but a stochastic scientific simulation system probably will not query databases.
- All database and result files produced (or consumed) in the system must have a documented specification and structure.
- Tools to view the "raw" data in databases or result files are required for error checking and quality control. If result files are stored in binary format, a tool must be provided to convert the data to (and from) ASCII format.
- Carrying units in result files and databases decreases the likelihood of unit conversion errors in the software system.
- Range checking of databases and results files will reduce significantly the number of incorrect results from the system. This checking could utilize a component by component approach.
- Management of errors is critical to generating usable results. If a single component of the system generates an error that is not recognized by the system, all other computation after that point could be corrupted.
- Precise definition of data interfaces between components is critical to being able to develop a functioning system.
- Uncertainty analyses elevate data management to a controlling position in the software design.

The following statements pertain to scientific and model complexity issues:

- The science associated with transport and fate issues at a site should determine model complexity.
- In order to enhance run times, the simplest scientifically defensible model should be implemented.
- The specifications of databases or result files require explicit agreement between developers of different modules.

The following statements pertain to the platform requirements of the system:

- Cross-platform software systems are more difficult to maintain and construct.
- A single-platform system reduces overall project time and effort.

- Disk space requirements may be decreased using reproducibility considerations. If system results are repeatable, there is less need to store all the results computed.
- Storage levels less than 50 gigabytes (GB) are convenient for current designs. It is possible to store more information, but file or network management becomes a larger issue if a system stores more than 50 GB.
- Large databases are cumbersome and difficult to analyze within reasonable turnaround times.
- Large files in general make installation of the software systems less tractable.
- Parallel processing can be used when run times are expected to be longer than is acceptable on a single serial system.

5.5.2 Recommendations

Four recommendations are made for the SAC (Rev. 0). These recommendations deal with overall architecture, the platforms, use of historical system code concepts, and system design for SAC (Rev. 0).

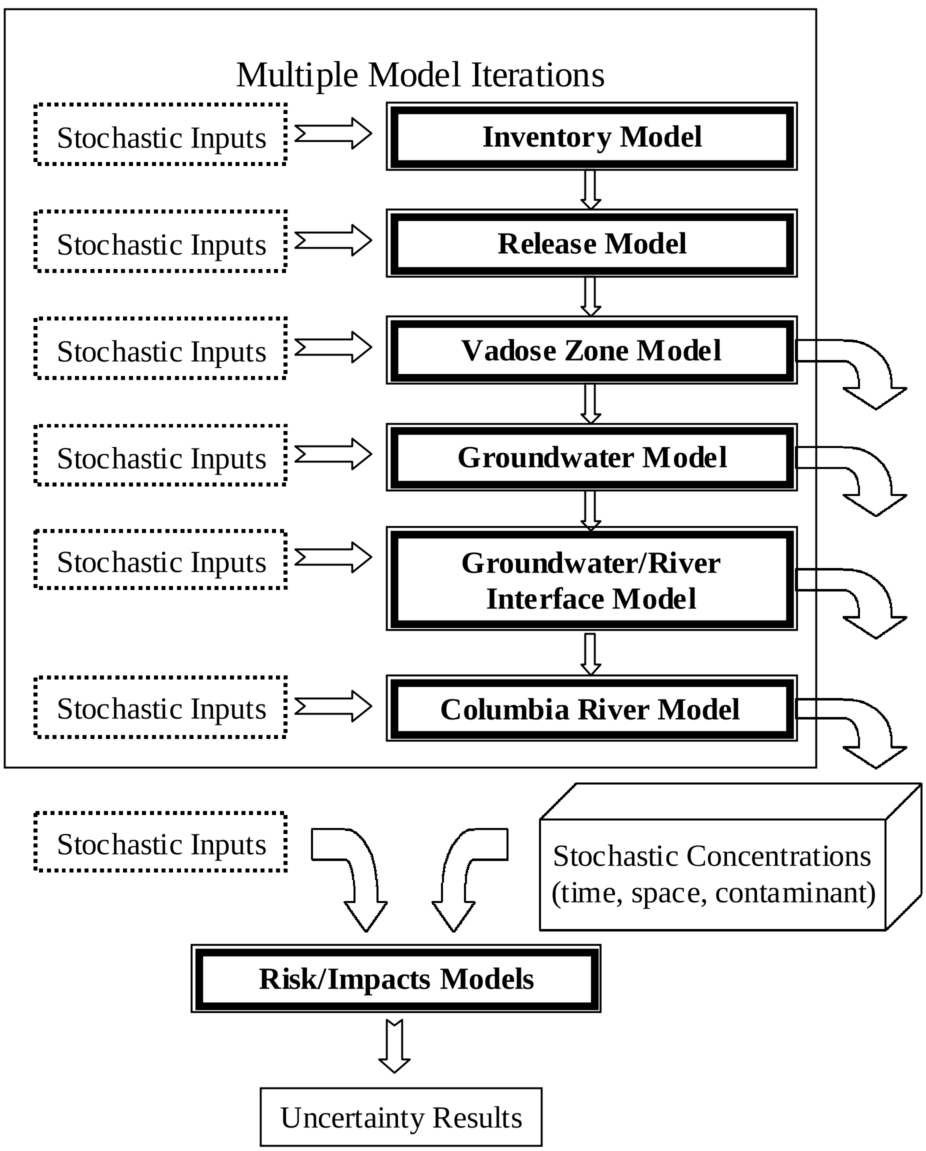
5.5.2.1 Architecture and Data Management Recommendation. A Distributed Collaboration architecture is being recommended for the SAC (Rev. 0). The Distributed Collaboration architecture is attractive when requirement creep and change is likely to occur. Under this model, each component can be built separately and assembled together to meet the current state of the requirements. Component upgrade and replacement has a minimal impact overall, and maintenance is kept to a minimum. This architecture also scales well because it is very easy to house all core components on one machine, or to distribute them across a set of machines, or even to let a cluster of servers implement one component alone. In addition, this architecture allows use of legacy FORTRAN code with minimal modifications.

The architecture and data management concepts are inextricably linked. The two data management options for the Distributed Collaboration architecture are formal database software or individually defined data files. A combination of these options is also possible. The wide variety of data types that must be handled would favor individually defined files over a database manager for most data transfers. The final choice of an approach is deferred until system tradeoffs concerning data file sizes, speed of access, ease of incorporation, and ease of reporting are conducted.

5.5.2.2 Platform Recommendations. Depending on the users and the level of use they are allowed, and the computational requirements of SAC (Rev. 0), the platform could vary. Existing software likely to be incorporated in the SAC may require the computational resources of advanced scientific workstations. Other existing software programs are currently implemented on personal computers running Microsoft Windows NT. Thus, it is envisioned that the Distributed Collaboration architecture will utilize both hardware types.

5.5.2.3 Historical System Code Recommendation. Most of the historical projects discussed in this report used a Distributed Collaboration architecture. We recommend starting with several system concepts from the historical projects. For example, the data handling for HEDR used rigidly controlled interfaces, and was highly optimized for speed and minimal disk storage. In addition, concepts about overall simulation control found in FRAMES may be very useful in a new system. Finally, the stochastic simulation concepts in the human and ecological risk codes for the CRCIA (Part 1) are readily transferable to a new system. Experience in software design for multi-media systems indicates that an incremental approach, building on established codes and concepts, has a higher probability of success than choosing a radically new approach. All of these concepts would support a flow of stochastic data, as illustrated in Figure 5-6.

Figure 5-6. Proposed Flow of Stochastic Data to Support Uncertainty Analyses.



5.5.2.4 System Design Process Recommendation. It is imperative to specify system requirements prior to completing architectural, platform, and data management for any version of the SAC, and before developing software. An illustrative list of questions pertaining to the overall design is as follows:

- **Users**: What type of users will operate the software? Options include one or more of the following: a casual user working on the project; a dedicated user working on the project; a regulator; a stakeholder; a member of a special interest group; or a member of the general public.

- **Level of Use**: Will each user be allowed to run all of the models or will there be different levels of use privileges? Types or levels of information that could possibly be accessed include the following: general project information; summary results from previous simulations; detailed results from previous simulations; summary calculations for a new simulation; and detailed calculations from a new simulation.

- **Access Methods**: How will users gain access to the SAC software suite? Possible avenues include the following: access through a web page; remote access through a stand-alone system; remote use via distributed products; or access on central systems at the Hanford Site.

- **Computation Time**: What length of computation time can be tolerated? The answer may be different for different questions. Some items to consider are the computation times for the following: a deterministic simulation; a stochastic suite of simulations; a new exposure scenario (such as a recreational fisherman or local resident); a revised estimate of inventory at a waste site already modeled; or a new waste site or treatment technology. The solution to reasonable simulation times may require a distributed set of models running on everything from personal computers to scientific workstations to higher end computers.

- **Data Storage**: What types of calculated results are to be saved as intermediate calculations? How many different problems or study sets will be run requiring concurrent data storage? The required amount of data storage depends, among other things, on the number of contaminants, the number of times of interest, the number of exposure locations, and the number of stochastic replications.

Requirements for the SAC (Rev. 0) will be developed during the fall quarter of FY 2000. Requirements for the decision-assisting capability that will be prototyped as the SAC (Rev. 1), and made operational as the SAC (Rev. 2), will be identified by the end of FY 2000. Answers to the above questions, and decisions on the architecture, platform, and data management structure, will be generated as these requirements are developed.

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