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Hanford Site Composite Analysis Technical Approach Description: Vadose Zone

Prepared for the U.S. Department of Energy
Assistant Secretary for Environmental Management

Contractor for the U.S. Department of Energy
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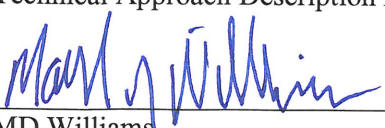
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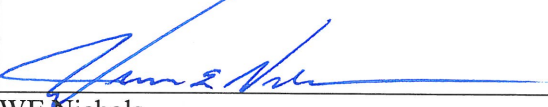
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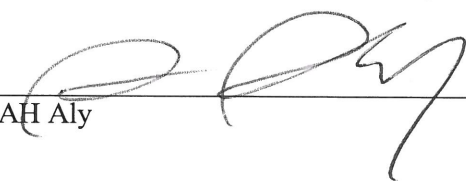
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	Technical Approach Description: Vadose Zone Flow and Transport

MODELING VADOSE ZONE FLOW AND TRANSPORT

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Terms

CA	composite analysis
CHPRC	CH2M HILL Plateau Remediation Company
DAS	disposal authorization statement
DOE	U.S. Department of Energy
ERDF	Environmental Restoration Disposal Facility
FIR	Field Investigation Report
HSDB	Hanford Site Disposition Baseline
IDF	Integrated Disposal Facility
ORP	Office of River Protections
PA	performance assessment
QA/QC	Quality assurance and quality control
RL	Richland Operations Office
SALDS	State-Approved Liquid Disposal Site
TEDF	Treated Effluent Disposal Facility
TTD	Technical transfer document
WMA	Waste Management Area

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1 Introduction

The U.S. Department of Energy (DOE) in DOE O 435.1 Chg. 1, *Radioactive Waste Management*, and DOE M 435.1 Chg 1, *Radioactive Waste Management Manual*, requires the preparation and maintenance of a composite analysis (CA). The primary purpose of the CA is to provide a reasonable expectation that the primary public dose limit is not likely to be exceeded by multiple source terms that may significantly interact with plumes originating at a low-level waste disposal facility. The CA is used to facilitate planning and land use decisions that help assure disposal facility authorization will not result in long-term compliance problems; or, to determine management alternatives, corrective actions, or assessment needs, if potential problems are identified.

A CA is not prepared to demonstrate current compliance; rather, its purpose is to model potential future exposure events. In other words, a CA is a DOE planning tool, used to provide a reasonable expectation that DOE public radiation protection requirements will be met over the long-term after the DOE site achieves its projected end state; and, the CA is a prerequisite to acquire and maintain an operational Disposal Authorization Statement (DAS) and capture concept of tank farm closure support.

CAs are closely linked with performance assessments (PAs) for specific disposal facilities, which DOE uses to demonstrate that there is a reasonable expectation that the performance objectives will be met for a given facility. CAs may be documented in a companion report to the PA, or integrated in the same report with a PA. At the Hanford Site, with numerous separate disposal facilities and tank farms, the CA has been developed and maintained as a separate document that includes all facilities contributing to dose at a specific boundary for supporting PAs for several low-level waste disposal facilities at the Hanford Site.

The initial, and currently maintained, CA for the Hanford Site is documented in PNNL-11800, *Composite Analysis for Low Level Waste Disposal in the 200 Area Plateau of the Hanford Site*, and the subsequent Addendum 1 (PNNL-11800-Addendum-1, *Addendum to Composite Analysis for Low Level Waste Disposal in the 200 Area Plateau of the Hanford Site*). The annual summary report for this initial CA for fiscal year 2015 (DOE/RL-2015-66, *Annual Status Report (FY 2015): Composite Analysis for Low Level Waste Disposal in the Central Plateau of the Hanford Site*) reached the determination that an update to the Hanford Site CA is necessary based on information reviewed for fiscal year 2015 as well as information presented in prior annual status reports. DOE has initiated work to develop a revised CA following a phased approach with planning, scoping, and analysis phases. The scoping phase will culminate in the development of a detailed technical approach for preparing the revised CA. This technical approach description document presents the approach for the vadose zone as one facet of the overall technical approach. This is a companion document to a series of other technical approach description documents for various facets of the revised CA.

Development of the revised CA is being conducted under the provisions of PRC-MP-EP-53107, *Hanford Composite Analysis Project Management Plan*.

2 Background

The objective of the vadose zone task for the Hanford Site CA is to simulate the flow and transport of water and radionuclide releases from the surface to the water table for input into the aquifer model.

Key prior modeling studies of vadose zone flow and transport in the Central Plateau include:

- Initial Hanford Site CA (PNNL-11800; PNNL-11800-Addendum-1)

- PNNL in 2006 developed an approach for the CA using the System Assessment Capability (PNNL-16209, *A Demonstration of the System Assessment Capability (SAC) Rev. 1 for the Hanford Remediation Assessment Project*)
- DOE/EIS-0391, *Tank Closure and Waste Management Environmental Impact Statement*
- CERCLA Operable Units, e.g.:
 - EPA et al., *Record of Decision Hanford 200 Area 200-ZP-1 Superfund Site Benton County Washington, Richland, Washington*
 - EPA et al., *Record of Decision Hanford 200 Area Superfund Site 200-CW-5 and 200-PW-1 200-PW-3 and 200-PW-6 Operable Units September 2011*
 - EPA et al., *Record of Decision for Interim Remedial Action Hanford 200 Area Superfund Site 200-UP-1 Operable Unit*
- Field Investigation Reports (FIRs) of the tank farm waste management areas:
 - RPP-7884, 2002, *Field Investigation Report for Waste Management Area S-SX*
 - RPP-10098, *Field Investigation Report for Waste Management Area B-BX-BY*
 - RPP-23752, *Field Investigation Report for Waste Management Area T and TX-TY*
 - RPP-35484, *Field Investigation Report for Waste Management Area C and A-AX*
 - RPP-354485, *Field Investigation Report for Waste Management Area U*
- Hanford Site PAs:
 - WHC-EP-0645, *Performance Assessment for the Disposal of Low Level Waste in the 200 West Area Burial Grounds* (1995)
 - WHC-SD-WM-TI-730, *Performance Assessment for the Disposal of Low Level Waste in the 200 East Area Burial Grounds* (1996)
 - WCH-520, *Performance Assessment for the Environmental Restoration Disposal Facility, Hanford Site* (2013)
 - RPP-ENV-58782, *Performance Assessment of Waste Management Area (WMA) C, Hanford Site, Washington* (2016)
 - Integrated Disposal Facility Performance Assessment (just completed; in review by the Low Level Waste Disposal Facility Federal Review Group at time of this report); this replaces the older Immobilized Low Activity Waste (ILAW) PA (DOE/ORP-2000-24, *Hanford Immobilized Low-Activity Waste Performance Assessment: 2001 Version*)

This document describes the proposed technical approach for building and simulating the transport of water and radionuclide inventory discharged or disposed at or near the ground, made available for transport through waste form release models (that will be defined in a separate technical approach description document), through the vadose zone and discharging to the top of the aquifer model used in the CA (also to be defined in a separate technical approach description document). Figure 1 illustrates the top-level structure of the CA for all the system components. Figure 2 shows a more detailed view of the vadose zone task with the linkages to the other task.

3 Overview of Key Features, Events, and Processes

Vadose zone flow and radionuclide transport for the CA involves accounting for the flow of water in the partially saturated zone and transport of radionuclide contaminants. The sources of water include natural recharge and water discharged to ground resulting from industrial processes associated with Hanford Site operations that commenced in 1944. Contaminant sources include radionuclides discharged with the water discharged to ground during operations, and radionuclides disposed “dry” in burial grounds or other means than as liquid discharges.

3.1 Key Features

An important feature of the vadose zone in the Central Plateau is its substantial thickness, which ranges up to approximately 80 m thick. This makes the vadose zone a substantial component in the groundwater pathway that can result in very long transit times from surface to the saturated zone for water and contaminant mass under relatively dry conditions. Under historic conditions for large liquid discharge sites, the transit time was dramatically less.

Other key features are the material properties of the vadose zone sediments (e.g., bulk density, porosity, intrinsic permeability, pressure-saturation-relative permeability relations, dispersion) including the spatial variability of these properties, and physical properties of the radionuclides (decay, sorption, diffusion). Finally, another key feature is the construction of the many disposal sites (liquid and dry), including locations, dimensions, and engineered features (e.g., underground tanks, grouting of waste where used, waste packaging, surface covers over time including engineered covers where used or planned, backfill, surface covers, etc.).

3.2 Key Events

The principal key events that must be addressed in simulation of the vadose zone are liquid disposal events (sometimes termed artificial recharge). This was very significant during the operational period of the Hanford Site (1944 to 1989) as shown in Figure 3. Large volumes of liquids with radionuclides were discharged to the surface in this period; some were planned discharges while others were accidental. In response to these immense liquid discharges, the water table elevation rose in the operational period. Figure 4 shows the water table response from selected wells with up to a 15-m increase in the 200W area and a 5-m increase in the 200E Area. The unconfined aquifer has a much higher permeability in the 200E Area. The water table has been slowly receding since cessation of most operational discharges in the 1990s. Since cessation of operational discharges, limited liquid disposal continues at the State Approved Liquid Disposal Site (SALDS) and the Treated Effluent Disposal Facility (TEDF); these liquid discharges are expected to continue while Hanford Site environmental restoration activities are pursued, likely for a few more decades. WRPS is still developing estimates for the radionuclides and activities to be discharged at SALDS which would include H-3, I-129, and Tc-99. We will coordinate with WRPS to include the latest estimates for disposal at SALDS in the CA inventor., The liquid effluent disposed to ground at TEDF does not include significant radionuclide content, but liquid disposals constitutes an important artificial recharge event from a water balance perspective that is important to the groundwater flow component of the CA.

Another event to account for in vadose zone modeling is the changes at discrete times of surface conditions, with the direct impact on natural recharge rates at waste site locations. For example, when a surface condition was changed at the beginning of operations from natural soil and shrub steppe to a gravel cover maintained vegetation free (commonly the case), natural recharge increased dramatically (from about 4 mm/yr to about 63 mm/yr). When a future engineered barrier cover might be applied, the

rate will decrease dramatically (from about 63 mm/yr to 1 mm/yr). Such changes are discrete events in time over the life of a specific waste site, can differ for each waste site, and may vary spatially at a waste site.

3.3 Key Processes

A key process for water flow and associated radionuclide transport through the vadose zone is natural recharge. This process is continuous, but as noted in the preceding subsection, is subject to abrupt rate changes in response in discrete events that change the surface conditions (e.g., changes in surface soil type and/or vegetation condition).

Initial conditions of the vadose zone, namely moisture content, are also needed and are obtained by simulation of steady state conditions for natural recharge conditions prevalent before any disturbance events associated with the onset of Hanford Site operations.

Boundary conditions for the vadose zone models include the recharge at the surface (spatial and temporally variable) and the elevation of the water table at the bottom, which is variable in response to the changes in water table elevation noted above.

4 Applicability of the Tank Closure and Waste Management Environmental Impact Statement Vadose Zone Models to the Composite Analysis Scope

Figure 5, Figure 6, and Figure 7 illustrate the main vadose zone features of the three previous site-wide assessments at the Hanford Site.

The TC&WM EIS (DOE/EIS-0391) modeling set was transferred from DOE's Office of River Protection (DOE-ORP) and its EIS contractor, SAIC, to DOE's Richland Operations Office (DOE-RL) and its integration contractor, CHPRC, in May 2013. The transfer was accomplished through the *Tank Closure and Waste Management EIS Technical Transfer Document (TTD)*, which was not publicly released. This document included an electronic appendix to transfer modeling files. A second transfer was accomplished through a formal data call in May 2013 to release additional modeling files identified as needed based on review of the TTD. The transfer formally provided all vadose zone (STOMP¹) model input files used to develop the TC&WM EIS. The TTD did not provide the tools or geologic framework used to develop the STOMP grids. The TTD also did not provide the full means to modify inventory and revise STOMP input files to reflect those changes. The release-to-vadose-zone codes used in the analysis were provided, but only for reference purposes in response to the data call, and are not part of the formal modeling capability transfer.

The TC&WM EIS vadose zone models reflect key advances deemed important to the CA scope (see Figure 7):

1. All vadose zone models were explicitly three-dimensional, accounting for lateral flow at liquid discharge sites.
2. All vadose zone models were implemented in the STOMP code, consistent with DOE direction for the Hanford Site (Klein 2006; Williams 2012).

¹ Battelle Memorial Institute (Battelle) retains copyright on all versions, revisions, and operational modes of the Subsurface Transport Over Multiple Phases (STOMP) software simulator, as permitted by the U.S. Department of Energy. STOMP is used here under a limited government license.

3. All vadose zone models have temporally variable recharge rates, based on based on surface soil and vegetation type.

With respect to the CA scope, certain limitations to the TC&WM EIS STOMP models are identified:

1. The means to effectively modify/update the inventory within the EIS framework was not provided;
2. The means to modify/update the geologic basis of the vadose zone model grids was not provided;
3. Analysis reveals that the vadose zone model domains exhibit significant overlap;
4. Model implementation, as documented in the TTD, is very labor-intensive (no automation); and
5. The so-called “cumulative impacts” waste sites were modeled under no-further action.

The first limitation (cannot effectively modify/update the inventory) clearly hinders direct application of the TC&WM EIS vadose zone models for the CA. The CA, as a planning tool for DOE, must be able to accommodate inventory basis changes efficiently. This includes updated inventory information generated since the issue of the TC&WM EIS. It is evident that a new methodology is required to maintain the Hanford Site inventory basis for the CA and efficiently pass this through a waste-form release model tool and into the STOMP models is needed.

The second limitation noted (lack of geoframework supporting the STOMP model grids, and therefore means to maintain and update this basis) also hinders the CA scope. A new *Central Plateau Vadose Zone Geoframework* is in development under the CA scope to provide such as maintainable basis for vadose zone fate and transport models.

The third limitation identified (significant spatial overlap in the models) is illustrated for the BC Cribs models (as an example) in Figure 8. The objective of simulating these sites in three dimensions was to account for lateral water flow in the vadose zone explicitly. However, because of the very significant overlap apparent in many instances shown in Figure 8, many liquid discharge sites are effectively simulated in isolation, with no accounting for the lateral flow of liquid from other nearby liquid discharge sites. Where liquid discharges occur nearby, both spatially and temporally, the effect of neglecting interactions may be important. Absent a modeling approach that accounts for these features, events, and processes, it is not possible to determine whether the impact of this modeling construct is significant.

The fourth noted limitation (a labor-intensive model application approach) is important because of the role of the CA to serve as a DOE planning tool, with a required annual maintenance cycle. Accordingly, the CA must be efficient enough to rerun with updated inputs to support annual status reporting as the most efficient way to provide for CA maintenance. The current implementation of the TC&WM EIS vadose zone models required running 580 separate STOMP models, times the number of contaminants of interest, individually. This was done with some scripting to speed work during scoping studies for the CA, the maintenance of this many individual models would be challenging.

The final limitation deals with how to manage alternative future dispositions for waste sites effectively. The so-called “cumulative impacts” waste sites were modeled under no-further action in the TC&WM EIS. This means that, for several hundred STOMP models, the recharge rates used as boundary conditions, and the contaminant mass remaining in the vadose zone, do not reflect DOE plans for waste site disposition. While this resulted in bounding estimates of impacts suitable for EIS analysis purposes, it is not appropriate to the scope of the CA as a DOE planning tool. A means to revise STOMP models efficiently to impose planned and alternative waste site dispositions for all waste sites is required.

Consideration of the above limitations leads to the following recommendations considered in the development of this technical approach description document for the vadose zone.

The three-dimensional treatment of the vadose zone implemented in the STOMP code as used in the TC&WM EIS is to be retained, with these recommendations for adaptation to meet the CA scope and needs:

1. Three-dimensional models should be developed that consider overlapping influences areas for liquid discharge sites;
2. These three-dimensional models should have a geologic basis in three-dimensional geoframeworks that account for available recent geologic interpretative information and are subject to periodic maintenance;
3. New tools are needed to provide for modeling waste form release from inventory database(s) that are subject to periodic maintenance to account for updated inventory information; and
4. The vadose zone models need to be incorporated into an efficient, integrated computational framework suitable to CA maintenance needs.

5 Methodology

Figure 9 illustrates the proposed approach for the CA vadose zone facet for comparison with the previous approaches shown in Figure 5, Figure 6, and Figure 7.

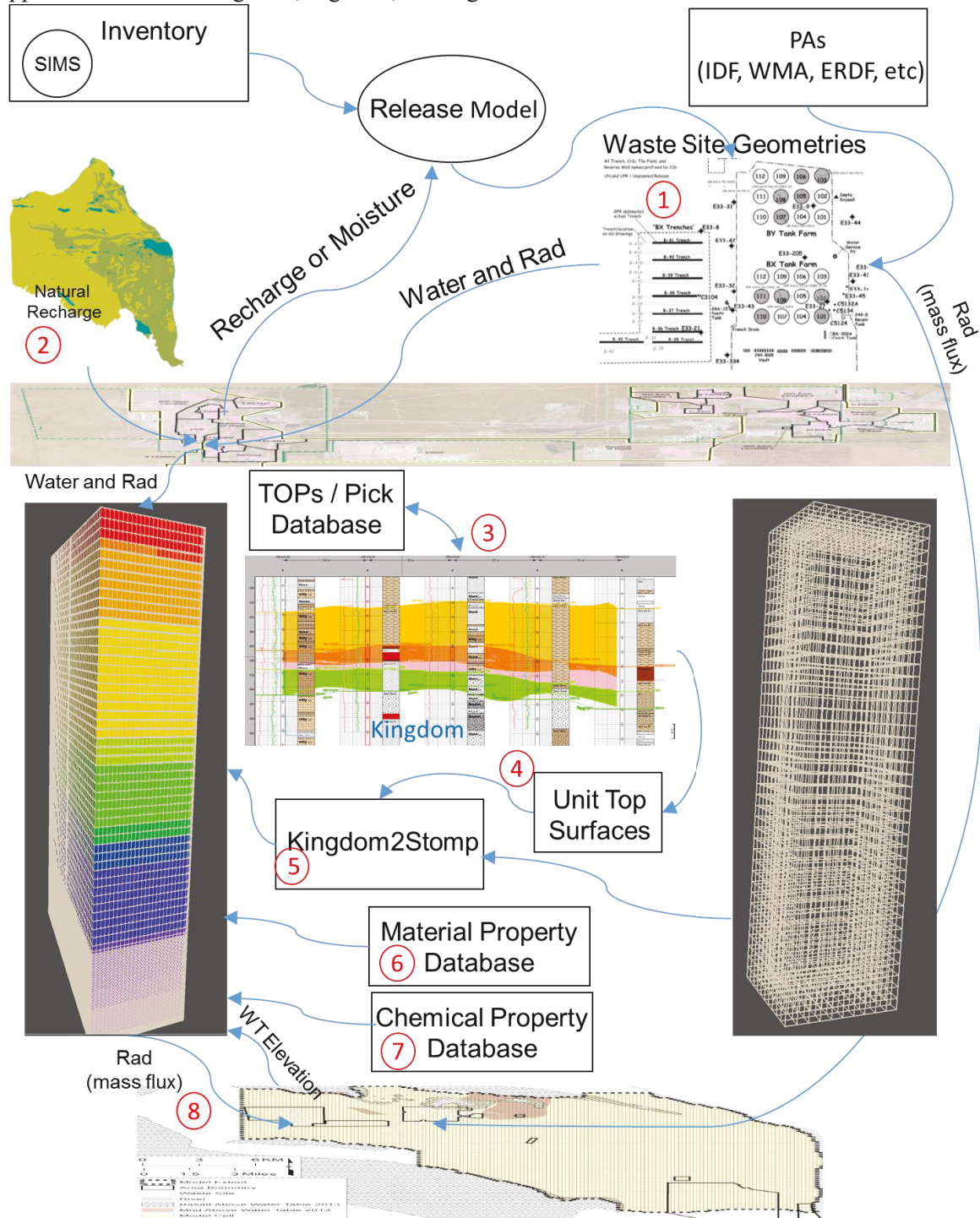


Figure 10 shows the overview of the workflow and dataflow for the CA vadose zone model. The vadose zone model for the CA will use the *Subsurface Transport Over Multiple Phases* (STOMP)² software for simulating unsaturated flow and radionuclide transport (PNNL-12030, *Subsurface Transport Over Multiple Phases Version 2.0 Theory Guide*; PNNL-15782, *Subsurface Transport Over Multiple Phases Version 4.0 Users Guide*). The technical approach for the inventory /source term inputs to the vadose zone models are described in CP-60195, *Hanford Site Composite Analysis Technical Approach Description: Radionuclide Inventory and Waste Site Selection Process*. The outputs of the vadose zone models will be transmitted to the groundwater model, with the technical approach described in CP-60406, *Hanford Site Composite Analysis Technical Approach Description: Groundwater Flow and Transport*. The updated hydrostratigraphic framework used for the structural basis of vadose zone modeling of the Central Plateau (see Figure 11 for location) in this effort are documented in a separate modeling data package (CP-60925).

The overall approach to simulate the flow and transport through the vadose zone of the surface discharges of the Central Plateau is to subdivide the 200W and 200E Areas into numerous three-dimensional models that permit the interaction of nearby releases. The number of three-dimensional vadose zone models required for this approach is estimated to range from as few as 20 to as many as 30 models, with each model having between 0.75 million and 2 million computational nodes. The computational requirements for this modeling effort necessitates the use of the parallel version of the STOMP code (eSTOMP, online user guide at http://stomp.pnnl.gov/estomp_guide/eSTOMP_guide.stm) for executing the simulations in a timely manner. Preliminary models will be tested early in the development process to determine the specific cluster requirements and estimated simulation run times.

A standardized approach is being developed for constructing each of the models with scripting being used to automate as many of the steps as possible. Scripting will also be used for post-processing the model results and for reporting / visualizations. In addition to streamlining the construction process, the reliance on scripting provides documentation of the data linkages, algorithms, and sources. Scripting also will enable easy rerunning of the models when changes occur in the upstream data sources and during the initial model development.

In addition to the three-dimensional, multi-waste site vadose zone models developed for the CA as described in this approach, the vadose zone models developed for DOE/EIS-0391 will also be run with the mass flux routed to the CA aquifer model. This will provide for comparison of results with the different approaches and provide a contingency to accommodate late changes in the models and/or upstream data due to the computational requirements of the new vadose zone models.

5.1 Assumptions

The major assumptions in this vadose zone modeling effort are:

- Isothermal, with constant fluid density and viscosity
- Availability of NQA-1 version of eSTOMP that includes the qualified features used in the model
- Same water table elevation in each vadose zone model domain (but temporally variable)
- Size of footprint for unplanned releases (to be decided on a case by case basis)

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- Size of footprint for tank farm releases / residuals
- Use of same aqueous-solid partition coefficient (K_d) for each radionuclide in different sediments (but may vary based on waste stream chemistry and distance to release)

5.2 Vadose Zone Geoframework

A major effort is underway by CH2M HILL Plateau Remediation Company (CHPRC) to create a vadose zone geoframework for the Central Plateau expressly to support the development of vadose zone numerical models described in this technical approach description document. Previously developed geoframeworks covering this area focused on the saturated zone and did not provide detail for the vadose zone. All well and geophysical borehole logs are being evaluated for sufficiency in developing the vadose zone geoframework. Wells that have reasonable data available are being interpreted for the elevations of different units and are being documented in a database following standardized forms and terminology.

The IHS Kingdom®³ seismic and geological interpretation software is being utilized in this effort to help evaluate unit picks for each well in relation to neighboring wells. The software is also being used for visualization and generation of cross sections for comparison with previously interpreted geologic maps. Lastly, three-dimensional surfaces for each of the units identified are being generated in Kingdom and exported for use in a separate program being developed for this project, Kingdom2Stomp, for assigning

³ IHS™ Kingdom® software and all of its components, 2dPAK®, 3dPAK®, 2d/3dPAK®,... IHS and the IHS globe design are registered trademarks of IHS.

units to each of the numerical model nodes. The center portion of

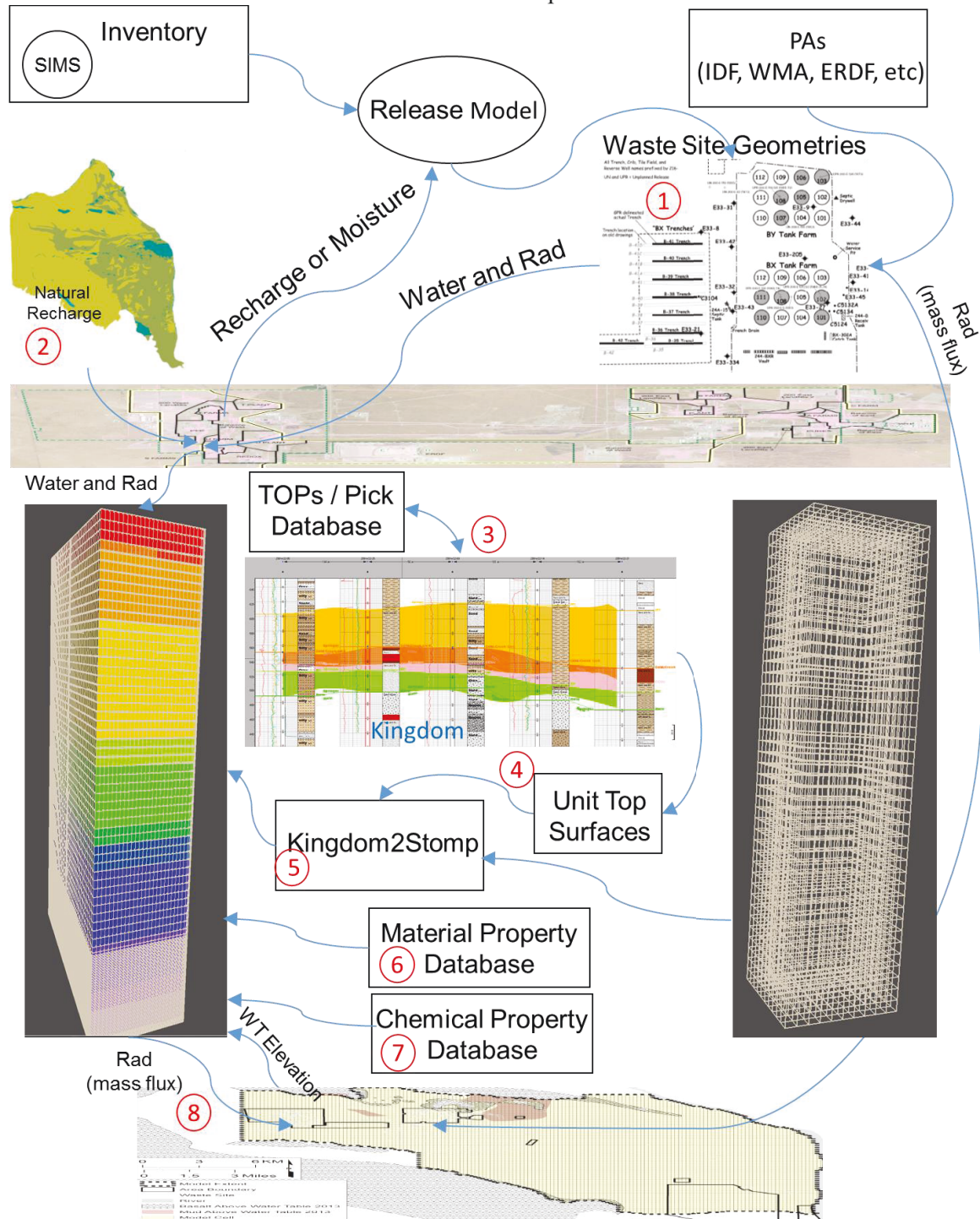


Figure 10 illustrates the workflow of these software packages and data.

The three-dimensional surfaces that are generated in Kingdom are being checked by comparison with the elevations documented in the database for each well location, within a specified tolerance for validation. This is to make sure there are no spurious artifacts created by the surface generation algorithms due to the

irregularly spaced, sparse well data. Since the surfaces are being interpreted and generated in the Kingdom software, no additional well interpretation is required downstream (e.g. Leapfrog®⁴).

The results of the hydrogeologic framework interpretation of the Central Plateau are documented in a model package report (CP-60295).

5.3 Domain Selection and Grid Spacing

The 200W and 200E Areas of the Central Plateau (see Figure 11) will be subdivided into several three-dimensional vadose zone models, with each model containing multiple source terms. This will provide for the potential interaction of nearby source terms. For example, large water sources could increase the vadose zone moisture content in an area causing adjacent sources to have faster travel times to the aquifer.

To develop these models, plan-view rectangular polygons for the model domains are created in ArcGIS®⁵ around each of the source term areas (see Figure 12). These areas are guided by plotting preliminary estimates of the total water discharged along with the total technetium-99 (Tc-99) and iodine-129 (I-129) activity (Curies) for each of the waste sites. These are shown in Figure 13, Figure 14, and Figure 15, respectively. A close-up view of these domains is shown with the water discharges in Figure 15. The objective is to include adjacent waste sites into a single model, but to minimize boundary effects (i.e., no large water sources near the model boundaries). For each of the model areas, an additional, smaller, plan-view polygon will be developed inside for the selection of source terms that will provide a buffer zone out to the model boundary to minimize boundary effects. An example of an inner, source term polygon for the S-SX Tank Farm is shown in Figure 16.

Proposed initial grid resolution for these models is 10 m in the X and Y directions, and 0.5 m in the vertical (Z) direction. In comparison for prior site-wide studies, the System Assessment Capability (PNNL-16209) used a 0.5-ft vertical grid spacing (for all units except the Cold Creek units that used 0.2-ft vertical grid spacing) for the vadose zone while the *Tank Closure and Waste Management Environmental Impact Statement* (DOE/EIS-0391) vadose zone models used a uniform 2-m vertical grid resolution for all vadose zone models. Grid spacing tests will be conducted to determine the adequacy of the selected grid spacing. In these tests, grid spacing in each direction will be reduced, and the results will be compared to the nominal case to see if any major differences in the predicted moisture contents, arrival times, and mass fluxes. It is estimated from the preliminary models built that the number of nodes for the nominal grid spacing selected will range from 0.75 million to 1.5 million. The total number of models needed to cover the waste sites in the 200W and 200E areas is estimated to be between 20 and 30 models.

The top of each of the model domains are set to the highest topographic elevation within the domain. Nodes in the domain with surface elevations less than the maximum will be set to inactive. The topography used in this effort is taken from the geologic framework. The bottom of each model domain will be set to the elevation of the pre-Hanford Site operational period water table as shown in Figure 9, which is the lowest potential water table elevation.

To reduce the computational requirements for some of the models, the rectangular plan-view domain can be altered to using inactive node zones if the spacing of the source terms permits it. An example of this can be seen in the preliminary S-SX Tank Farm as shown in Figure 16.

⁴ Leapfrog® is a registered trademark of ARANZ Geo Limited.

⁵ ArcGIS is a registered trademark of Esri.

5.4 Material Properties

Material properties required for simulated processes for sediments in the vadose zone include grain density, porosity, compressibility, tortuosity, intrinsic permeability, and dispersion, along with saturation and relative permeability relationships. Some of these properties are anisotropic, most notably intrinsic permeability.

Several sources will be used to develop a database of material properties for units in this modeling effort. These include:

- PNNL-14702, *Vadose Zone Hydrogeology Data Package for Hanford Assessments*
- DOE/RL-2011-50, *Regulatory Basis and Implementation of a Graded Approach to Evaluation of Groundwater Protection*
- Tank Farm FIRs (RPP-7884; RPP-10098; RPP-23752; RPP-35484; RPP-35485)
- PAs (WCH-520 for the Environmental Restoration Disposal Facility; RPP-ENV-58782, for Waste Management Area (WMA) C; and documentation developed for the forthcoming Integrated Disposal Facility [IDF] PA)
- PNNL-19277, *Conceptual Models for Migration of Key Groundwater Contaminants Through the Vadose Zone and into the Unconfined Aquifer Below the B-Complex*
- PNNL-23711, *Physical, Hydraulic, and Transport Properties of Sediments and Engineered Materials Associated with Hanford Immobilized Low-Activity Waste*

A limitation of most of the measurements for material properties within sediments of the vadose zone is that they are mostly measured on core samples. These may not be representative of the field scale values. Large discrepancies exist in some previous modeling studies where permeabilities used for a sediment type in the vadose zone can be an order of magnitude less than the values for the same sediment in the aquifer. Aquifer permeability has the advantage of being capable of field scale measurements (e.g., aquifer tests or inverse model calibration). Upscaling of certain parameters measured in the vadose zone from core samples will be investigated or correlation to aquifer measurements with the same sediment / texture.

Material properties will also be assessed through initial simulations for cases where sufficient vadose zone characterization exists (e.g., 200-WA-1 and 200-EA-1 Operable Unit) to compare simulated concentration and moisture content profiles with measurements. Additionally, runs will be developed for comparison with resistivity measurements (primarily responding to nitrate) as documented in SGW-50056.

The material properties in the above references, including scaling issues, will be assessed for applicability for use in the CA vadose zone models. The final property values selected, along with the rationale, will be documented in the final CA report.

5.5 Chemical Properties

Standard values of the radioactive decay rates for the simulated radionuclides have been compiled for use on new Hanford Site Assessments and will be used in this modeling effort⁶.

Sorption of radionuclides will be simulated using a reversible linear sorption isotherm (K_d , or distribution coefficient). Nominal values for the K_d s of radionuclides in this study are published in Section 4.6 of DOE/RL-2011-50. K_d values are influenced both by aqueous geochemistry and sediment mineralogy. While single values for each radionuclide will be used for most of domain for vadose zone modeling, K_d values may be changed in certain areas near a source where the discharge chemistry could significantly impact these values and therefore transport behavior. Aqueous diffusion for these radionuclides will also be simulated.

5.6 Boundary Conditions

Boundary conditions for the vadose zone models include no-flow boundaries on the sides and transient boundaries on the top for natural recharge and on the bottom for the water table elevation. These boundaries are discussed in more detail below.

5.6.1 Lateral Boundaries

Given that multiple waste sites are being simulated in a single model domain, the impacts of the no-flow side boundaries need to be assessed for each model. The initial model domains are being selected to provide a distance from the large water discharge sites. However, the distances may need to be adjusted based on the amount of plume spreading as they migrate from the surface to the water table. Dipping layers within a model domain may also cause water and radionuclides to migrate toward boundaries. These factors necessitate examining the water and plume development from the simulation results to assess if there is any interference from the side boundaries. In cases where boundary interference is detected, a larger domain of the other boundary type will be used.

5.6.2 Natural Recharge Boundary

Natural recharge specified at the top boundary (Neumann) is both spatially and temporally variable based on soil type, vegetation, and changes in land use through time. Natural recharge rates across the Hanford Site are discussed in DOE/RL-2011-50. ECF-HANFORD-15-0019, *Hanford Site-wide Natural Recharge Boundary Condition for Groundwater Models*, compiled data from several sources, interpreted imagery, and developed natural recharge values for the different soil and land use types. This study developed recharged maps for different time periods based on land disposition and documented the process used in developing these maps. A second study, (CP-60254, *Hanford Site Composite Analysis Technical Approach Description: Hanford Site Disposition Baseline*), compiled an extensive database of the condition and disposition of all the waste sites available. This will be used to augment ECF-HANFORD-15-0019 to develop the final natural recharge maps used in this vadose zone modeling effort.

An automated approach, using scripting, will be developed to sample each model surface node from ArcGIS or exported grid files for the recharge layers at the different periods to generate the spatially and temporally variable recharge rates for the models.

⁶ Electronic Model Data Transmittal EMDT-DE-0006, *Half-lives for Typical Hanford Site Radioactive Contaminants*, Rev. 0, INTERA.

5.6.3 Water Table Boundary

The bottom boundary of the vadose zone models is a transient specified head boundary (Dirichlet-type boundary condition) that is set to the water table elevation. Since the water table elevation varies significantly in the 200 Areas due to the large volumes of water discharged to the surface during Hanford Site operations, the specified head will be varied. For each period, only a single water table value is specified for the bottom of each vadose zone model (i.e., no hydraulic gradient across the bottom). Water table elevations will be based on the CA groundwater model predictions (see CP-60406). The water table is currently declining due to cessation of most surface discharges as shown in Figure 4.

5.7 Initial Conditions

Initial conditions for each of the vadose zone models are set to be pre-Hanford Site operational period conditions for moisture content and water table elevation. Additionally, no existing contamination is specified. This initial condition is achieved by running a pseudo-steady state simulation with undisturbed site values for natural recharge at the top and the pre-Hanford Site operational period water table elevation at the bottom (see Figure 9). The pressure results of these simulations for each model domain is used for the starting values for the transient simulations and the time-constant dirichlet boundary conditions for the sides of the three-dimensional models.

5.8 Sources

The top of

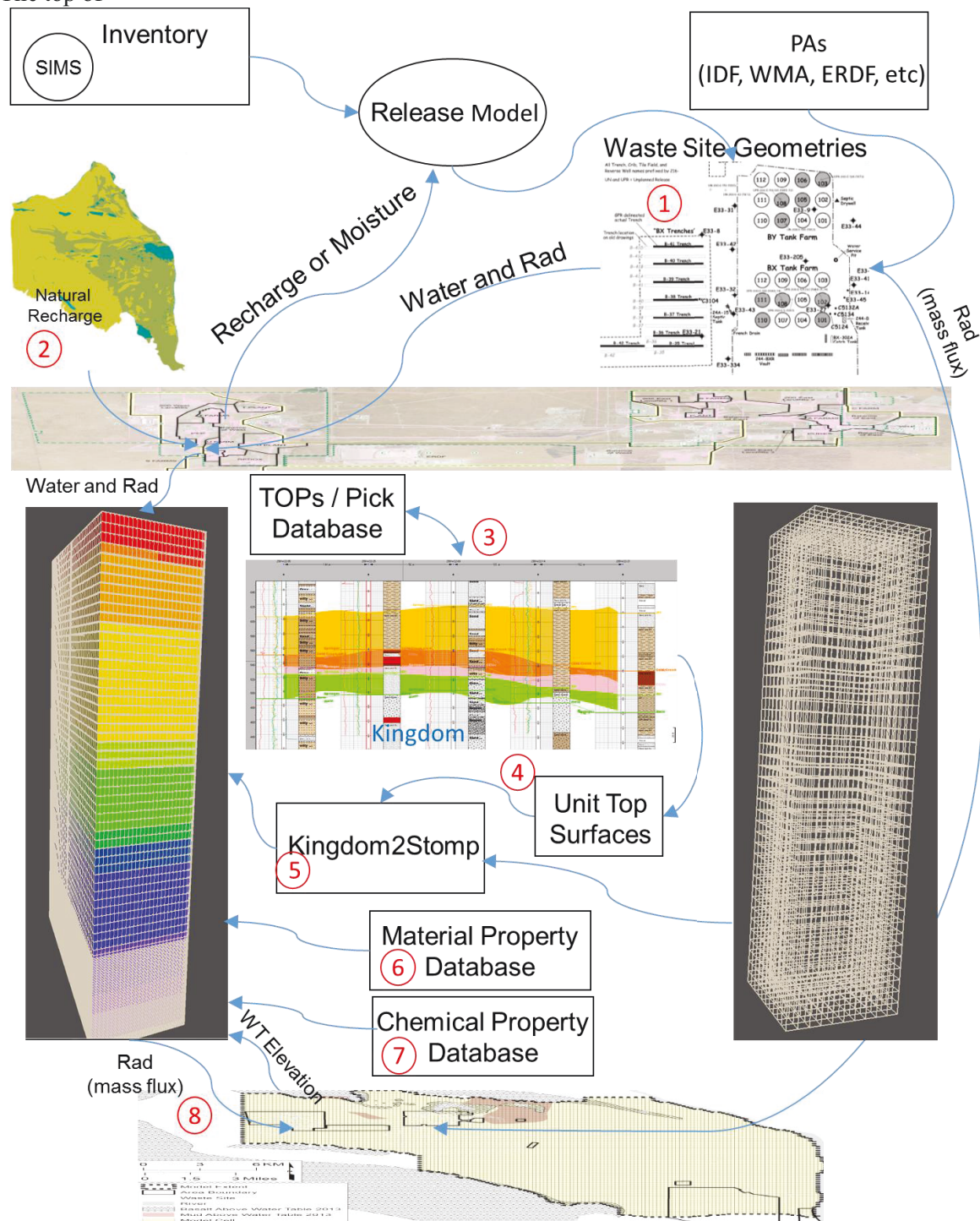


Figure 10 illustrates the data flow of the water and radionuclide releases to the top of the vadose zone model. The waste inventory, water discharges, and release models are being developed for the CA under other tasks as shown in Figure 1. A more detailed process showing the minimum data requirements and the mapping of the releases is shown in Figure 17. The mapping of the releases to the top nodes of the

vadose zone models will be automated using scripting. Water and contaminant releases will be spread out over all the grid blocks within the waste site footprint (see Figure 18).

The general geometry of most of the waste sites are described in PNNL-14725, *Geographic and Operational Site Parameters List (GOSPL) for Hanford Assessments*. Additional information on waste site geometries will be extracted from the ArcGIS shapefiles as shown in Figure 17. Unplanned releases and tank farm releases (including residuals) may not have a defined footprint so assumptions must be made for minimum sizes. These assumptions will be documented in the final report.

Releases to the aquifer that have already been simulated from existing PAs and site closure (e.g. IDF; Environmental Restoration Disposal Facility [ERDF]) will be mapped directly to the CA aquifer model. Reverse wells will also bypass the vadose zone model and be routed directly to the aquifer model. The mapping of these sources will be conducted in a similar process as described in Section 4.10.

For sites where there is adequate vadose zone contaminant characterization (e.g. 200-WA-1 and 200-EA-1 Operable Units), initial conditions for concentrations in the vadose zone may be set based on these data at the collection date rather than simulated through source discharge. Source discharge simulations will also be conducted in these cases for comparison and evaluation of results between the two methods. Uncertainties in source terms, recharge, and material properties could account for the differences.

In addition to the CA Inventory and Source Terms, several other documents will be assessed to inform model development and simulation assessment, including:

- DOE/RL-2011-102, *Remedial Investigation/Feasibility Study and RCRA Facility Investigation/Corrective Measures Study Work Plan for the 200-DV-1 Operable Unit*
- SGW-59881, *200-IS-1 Operable Unit Scoping*
- SGW-60540, *200-EA-1 Operable Unit Scoping*
- ECF-200EA1-17-0046, *Assessment and Presentation of Available Waste Site Data for the 200-EA-1 Operable Unit*
- DOE/RL-2010-49, *Remedial Investigation/Feasibility Study Work Plan for the 200-WA-1 and 200-BC-1 Operable Unit*
- DOE/RL-2004-60, *200-SW-2 Radioactive Landfills Group Operable Unit RCRA Facility Investigation/Corrective Measures Study/Remedial Investigation/Feasibility Study Work Plan*

5.9 Simulations

The transient flow and transport simulations will be run for a 10,000-year period starting at the commencement of Hanford Site operations in 1944. Variable time stepping will be utilized since the transient impacts of large water discharges should dissipate in later periods. An automated Courant limiter on the time step size available in STOMP will be used to control numerical dispersion.

Output options specified for the simulations include:

- Pressure, saturation, and radionuclide concentrations at selected reference nodes that will be output every time step.
- Plot files of pressure, saturation, concentrations, and velocity for the entire model domain at selected periods.

- Contaminant mass in system at every time step.
- Water and contaminant fluxes (instantaneous and cumulative) for horizontal planes at different depths.
 - o These will be used at the bottom of the domain for use in calculating radionuclide flux to the aquifer model starting at the time selected as the initial time for aquifer modeling, which under the selected approach will begin from initial measured contaminant plume conditions at a year designated as the present and accept additional vadose zone inputs thereafter.
 - o These fluxes will also be available from 1944 to the present from the vadose zone model, but under the selected approach will not be used in the historic period (1944 to the present) by the groundwater model.

To reduce computational requirements for single models, two runs for each model may be developed with one simulating the short-lived radionuclides (which may not need to run for 10,000 years) and the second simulation for the longer-lived radionuclides.

To condition and constrain model response, site data will be used to guide selection of material properties:

- Material properties will be assessed through simulations for cases where sufficient vadose zone characterization exists (e.g., 200-WA-1 and 200-EA-1 Operable Units) to compare simulated concentration and moisture content profiles with measurements.
- Simulations will be developed for comparison with plume extents derived from resistivity measurements, as documented in SGW-50056.
- Historical site groundwater monitoring data will be used for comparison with early arrival predictions or for situations where simulated radionuclides have not reached the water table but monitoring shows impacts.

5.10 Linkage to Aquifer Model

The primary output of the vadose zone model is the radionuclide fluxes at the water table for input into the aquifer model (See Figure 2). The spatial and temporal differences between these models requires mapping of the nodes and synchronization of the major time stepping. The nominal grid cells for the vadose zone model in the X and Y direction is 10 m, while the proposed aquifer model uses 200 m cells in the horizontal dimensions. Therefore, many vadose zone cells will be mapped to a single aquifer model cell.

The code “stomp_mf2k_mt3d” is a utility that uses surface flux files from STOMP (water and contaminant flux files that STOMP generates) to write water and solute flux files for the MODFLOW and MT3D simulators that will be used for the proposed CA aquifer model. MODFLOW is used for fluid flow and uses the FHB file (Flux and Head Boundary Condition) for specifying fluid boundary conditions / source terms. MT3D is used for radionuclide transport based on the flow field from MODFLOW and using the HSS file (Hydrocarbon Spill-Source Package) for activity flux boundary conditions / source terms. This current version of this code needs to be updated to be applicable for the CA.

The proposed CA aquifer model will start with initial condition plumes for the radionuclides based on Hanford Site-wide monitoring data starting at a year to be designated as the present. The vadose models will start at the beginning of the operational period of 1944. Therefore, the radionuclide flux simulated to

the water table in the vadose zone model will not be passed to the aquifer model until the present. The cumulative radionuclide flux prior to this period will be tallied for comparison with the starting curies for each radionuclide in the initial condition plumes. Additionally, the proposed CA aquifer model already represents recharge (natural and artificial) directly, so simulated water fluxes from the vadose zone models will not be added to the aquifer model.

5.11 Sensitivity Analysis

A primary sensitivity analysis for the full CA will be based on two cases for end members of land use / releases based on the Hanford Site Disposition Baseline (HSDB). These will represent the range from least to greatest remedial effort for all waste sites currently without final remedial decisions, based on information provided in DOE/RL-2015-10, 2016 Hanford Lifecycle Scope, Schedule and Cost Report. Other primary sensitivity cases for the full CA may be added during the Analysis Phase, but have not been identified in the scoping process.

5.12 Additional Alternatives to Consider

The assumptions and approach described above will be supplemented with alternative models for evaluation of impacts.

The first set of alternatives will focus on the treatment of basalt in other ways besides a default no-flow unit, specifically the fracture flow tops. Models in the northern portion of the 200 East area will include basalt in the domain. The basalt flow tops will not be differentiated in the geologic framework. However, cases can be developed by specifying a certain thickness with greater permeability and higher porosity. Additionally, the top basalt surface can be modified to include smaller scale features, such as potholes based on site-specific observations, or based on more general observed trends in the surrounding areas. The specific scenarios to be evaluated have not been finalized.

Another potential factor is density-driven flow at some waste sites. For selected wastes sites that had large volumes of high total dissolved solid fluids discharged along with the radionuclides, the density effects will be simulated. Results of these runs will be compared to the constant density case.

The potential impact of other features that have been identified in the Central Plateau (e.g., clastic dikes, thin fine stringers, etc.) will be considered in the framework. These have been addressed in prior modeling studies with sensitivity cases (e.g., FIRs).

6 Quality Assurance and Quality Control

PRC-MP-EP-53107, the approved project management plan for the development of the revised Hanford Site CA, includes the project's quality assurance plan (PRC-MP-EP-53107, Appendix B). That plan notes that

“A critical aspect of preparation of the revised Hanford Site CA is quality assurance and quality control (QA/QC). This *Project-Specific Quality Assurance Plan* documents the plan for QA/QC for the project that is consistent with CHPRC plans and procedures that implement DOE requirements, EPA guidance, and adds additional project-specific requirements deemed necessary to facilitate delivery of a successful product. This Project-Specific Quality Assurance Plan will be updated as required to reflect program and planning changes as the project progresses.”

The project's quality assurance plan will be adhered to in the development and application of vadose zone modeling for the revised Hanford Site CA. This includes provisions for quality control of modeling data, modeling applications, and software quality assurance. All modelers supporting vadose zone model

development and application will be trained to the project's quality assurance plan at the commencement of the project Analysis Phase (scheduled for April 2017).

Scoping work was performed with STOMP to develop the proposed approach detailed in this technical approach description document. Scoping work was not performed under rigorous quality assurance / quality control requirements, but served only to help define tenable approaches and guide the design of models to be developed for this facet of the CA revision. However, as the project moves into the Analysis Phase, the full rigor of the project's quality assurance plan will be applied.

7 Conclusions

The technical approach for the CA vadose zone modeling is currently being tested with preliminary data (geologic framework, source terms, and material properties) and preliminary assumptions for current data gaps. Major refinements to the approach based on these tests will be reported in revisions to this document. The testing will also provide the basis for estimates of the computations requirements for this modeling effort.

This technical approach description document will be finalized as the Scoping Phase of the Hanford Site CA revision project is concluded and before the Analysis Phase commences. It will then serve as the design basis for model development and application in the Analysis Phase.

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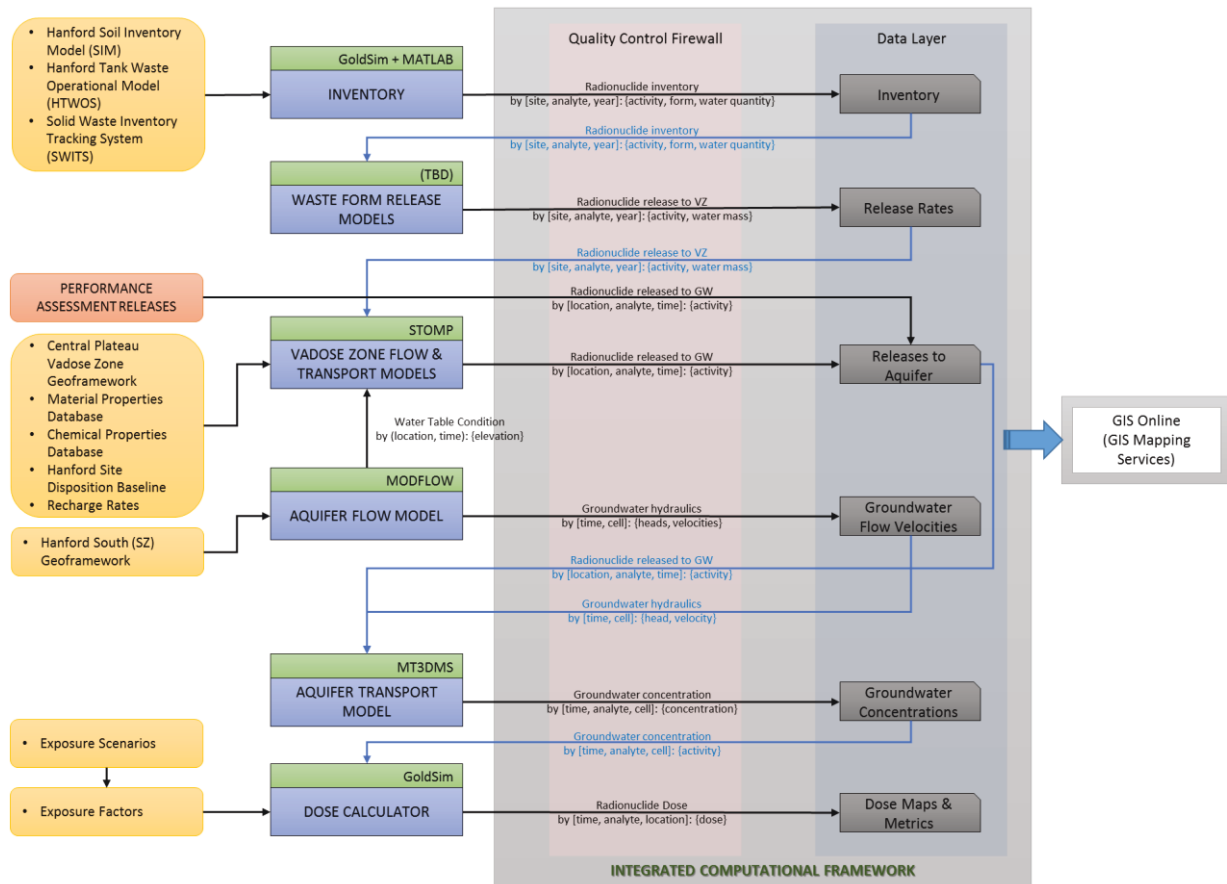


Figure 1. CA Top Level Structure

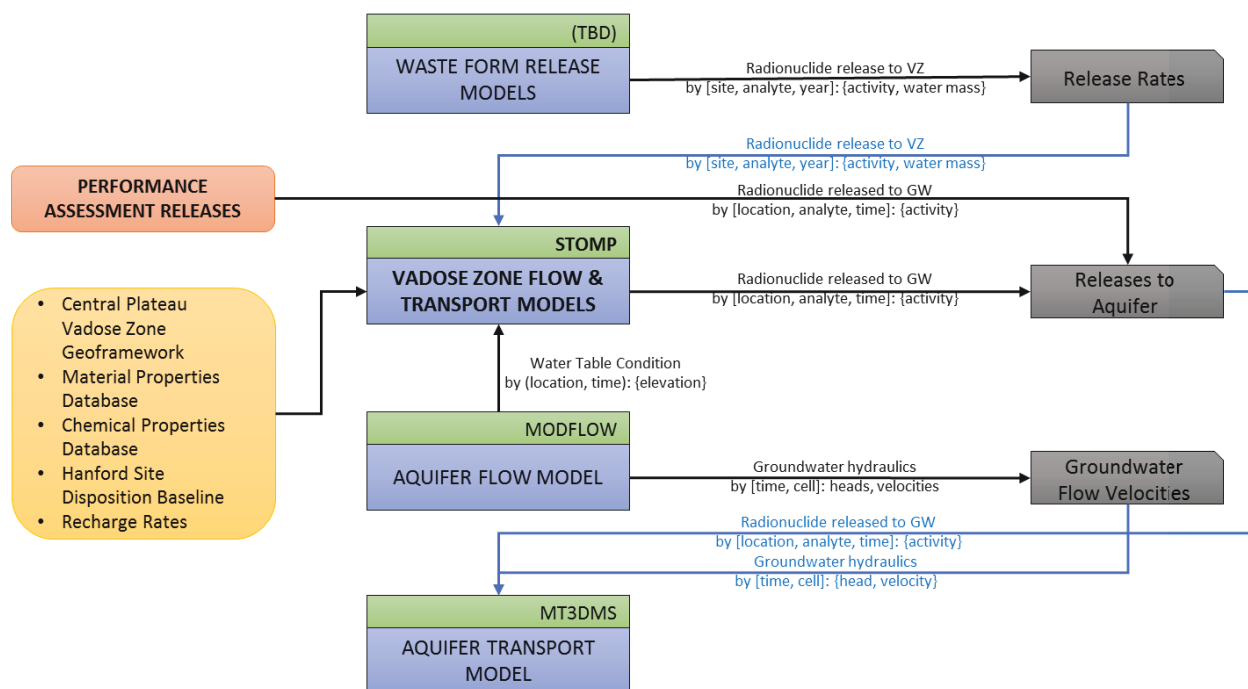


Figure 2. Vadose Zone Flow & Transport Facet of the Composite Analysis

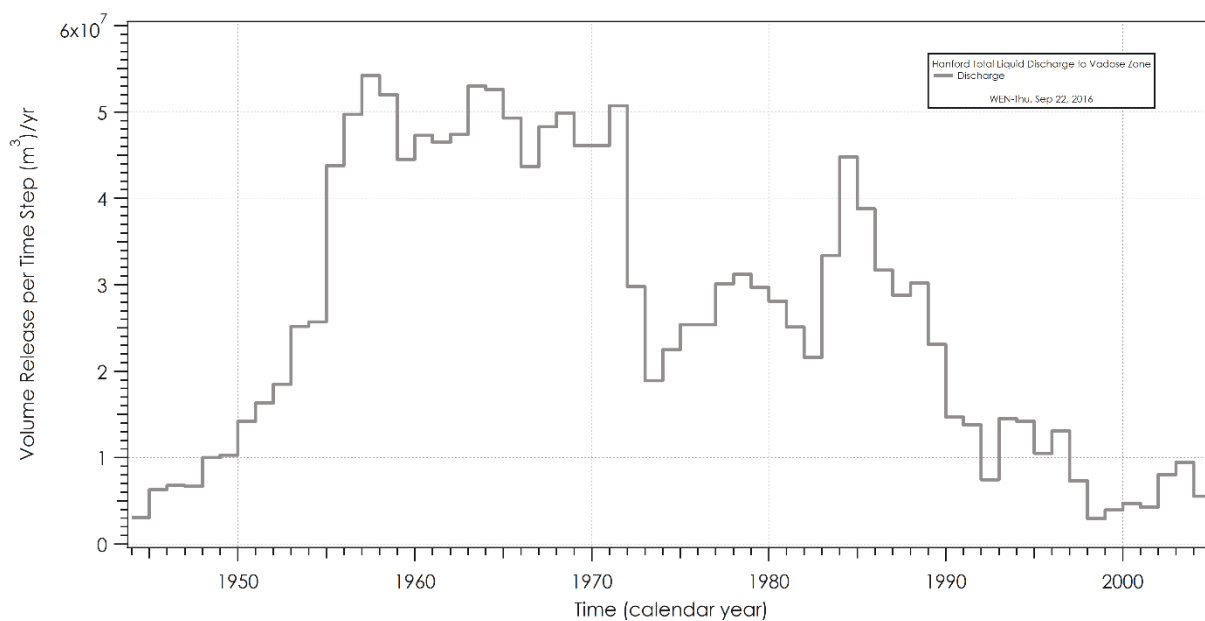


Figure 3. Total Liquid Discharge Record for Hanford Site

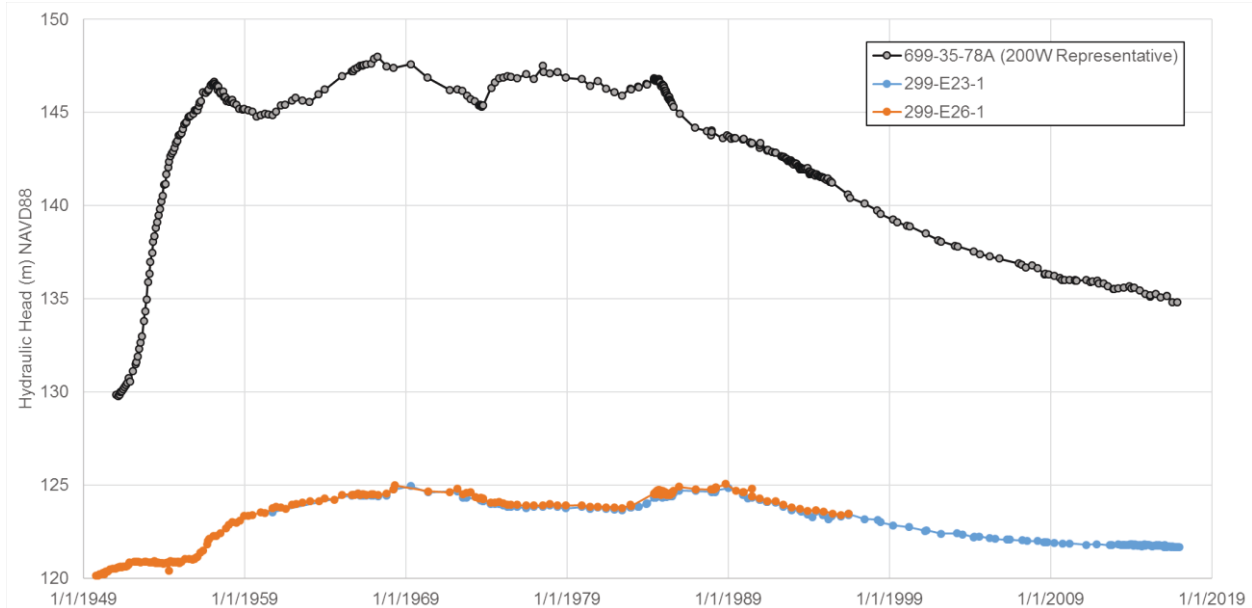


Figure 4. Hydraulic Head Measurements from Representative Wells for the 200W and 200E Area (note elevation datum is NAVD88)

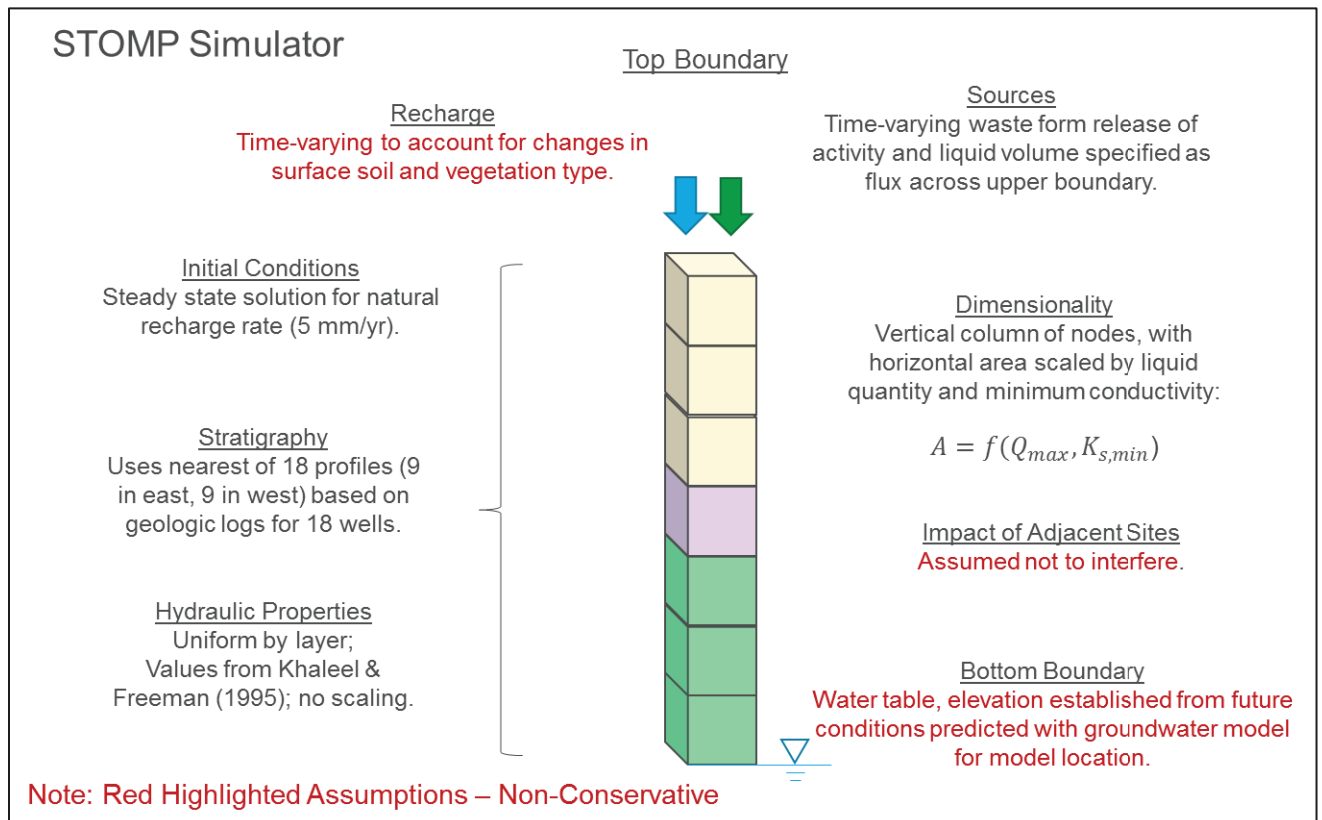


Figure 5. Previous Studies - Initial CA (PNNL-11800)

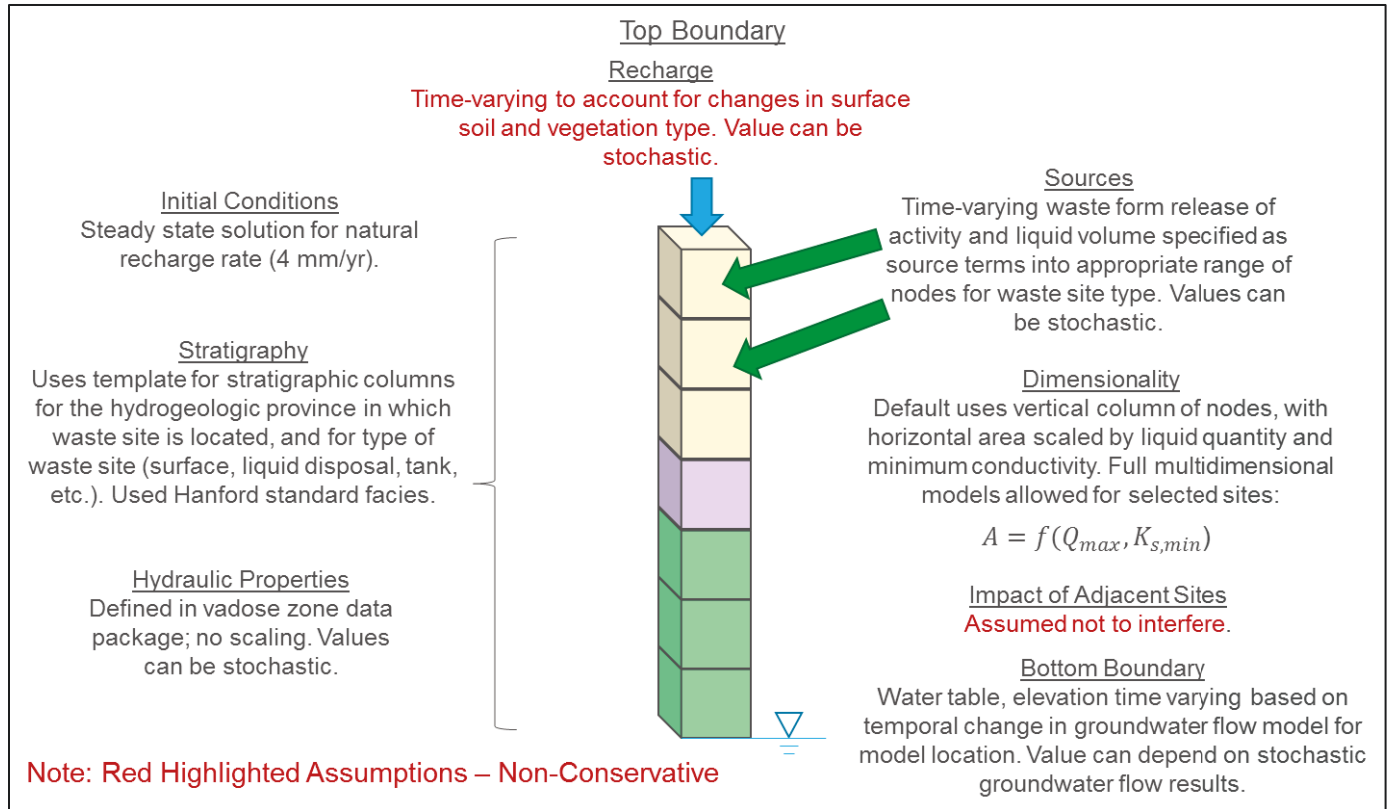


Figure 6. Previous Studies - 2006 CA (Incomplete)

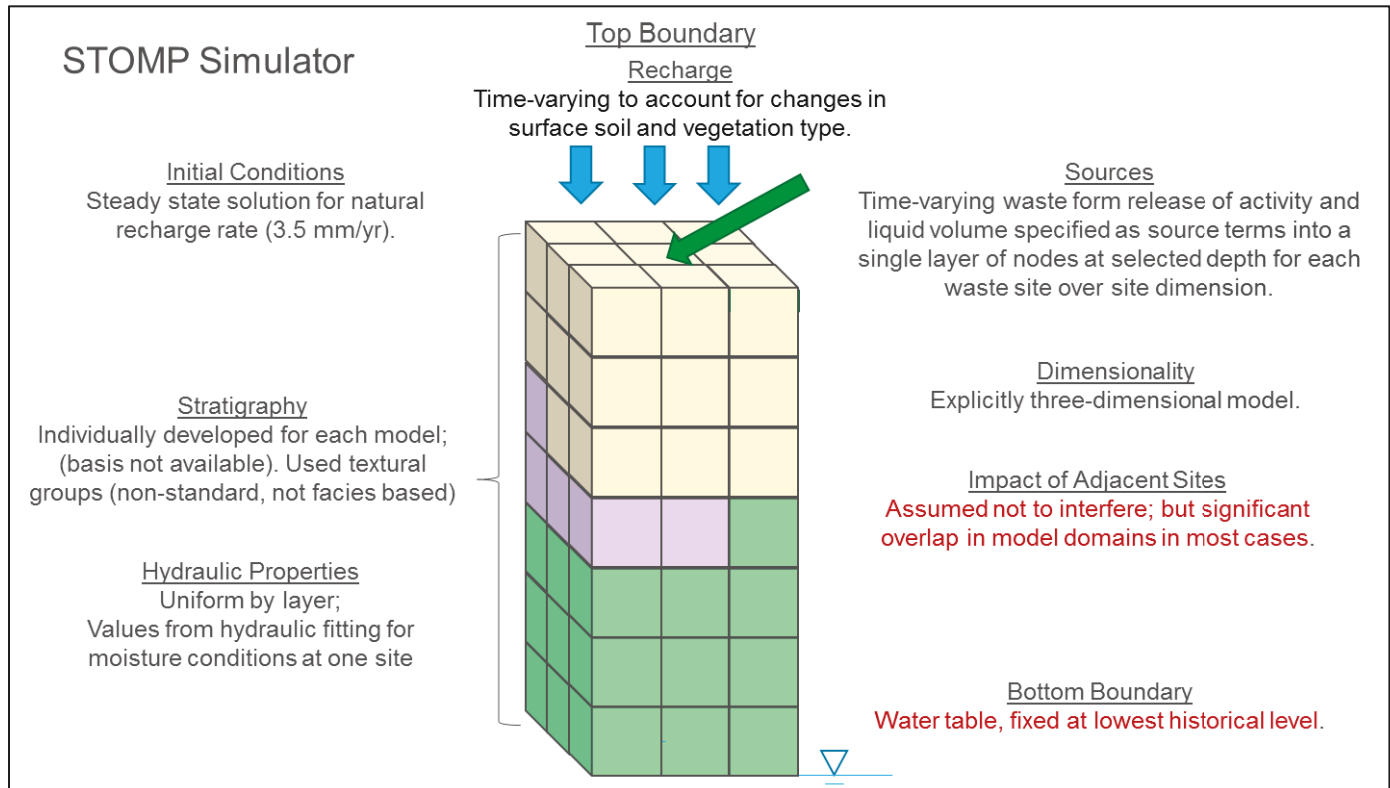


Figure 7. Previous Studies - TC&WM EIS (DOE/EIS-0391)

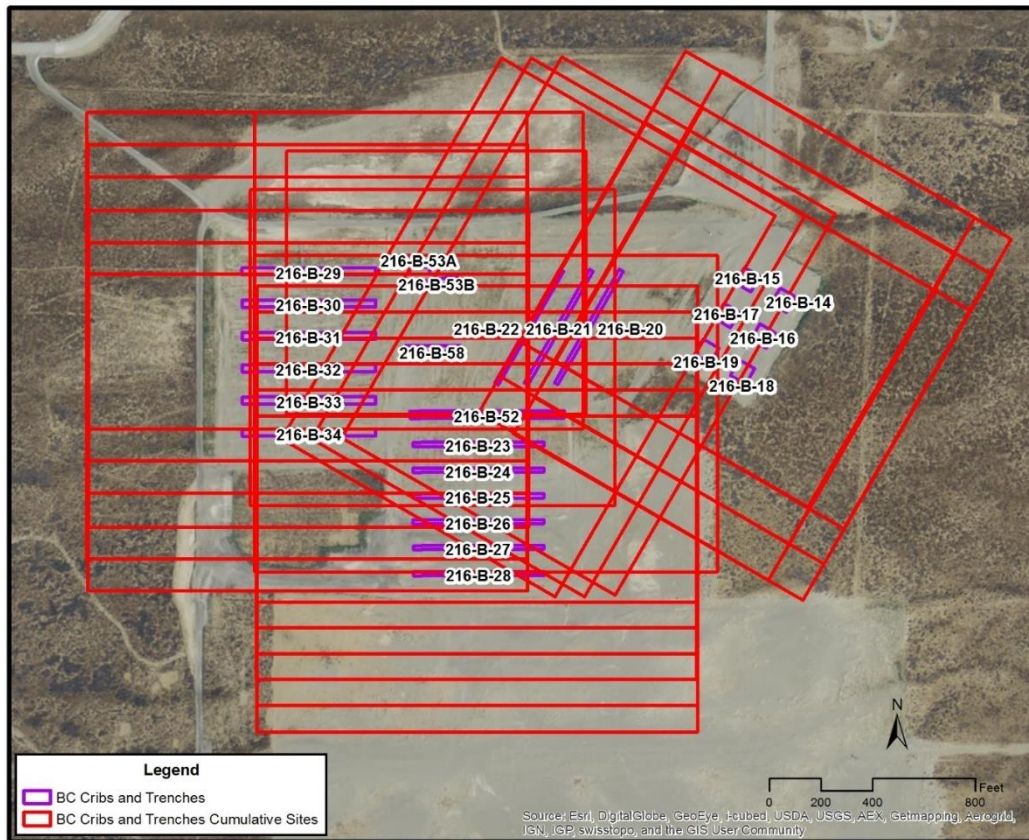


Figure 8. TC&WM EIS 3D Domain Example: BC Cribs and Trenches

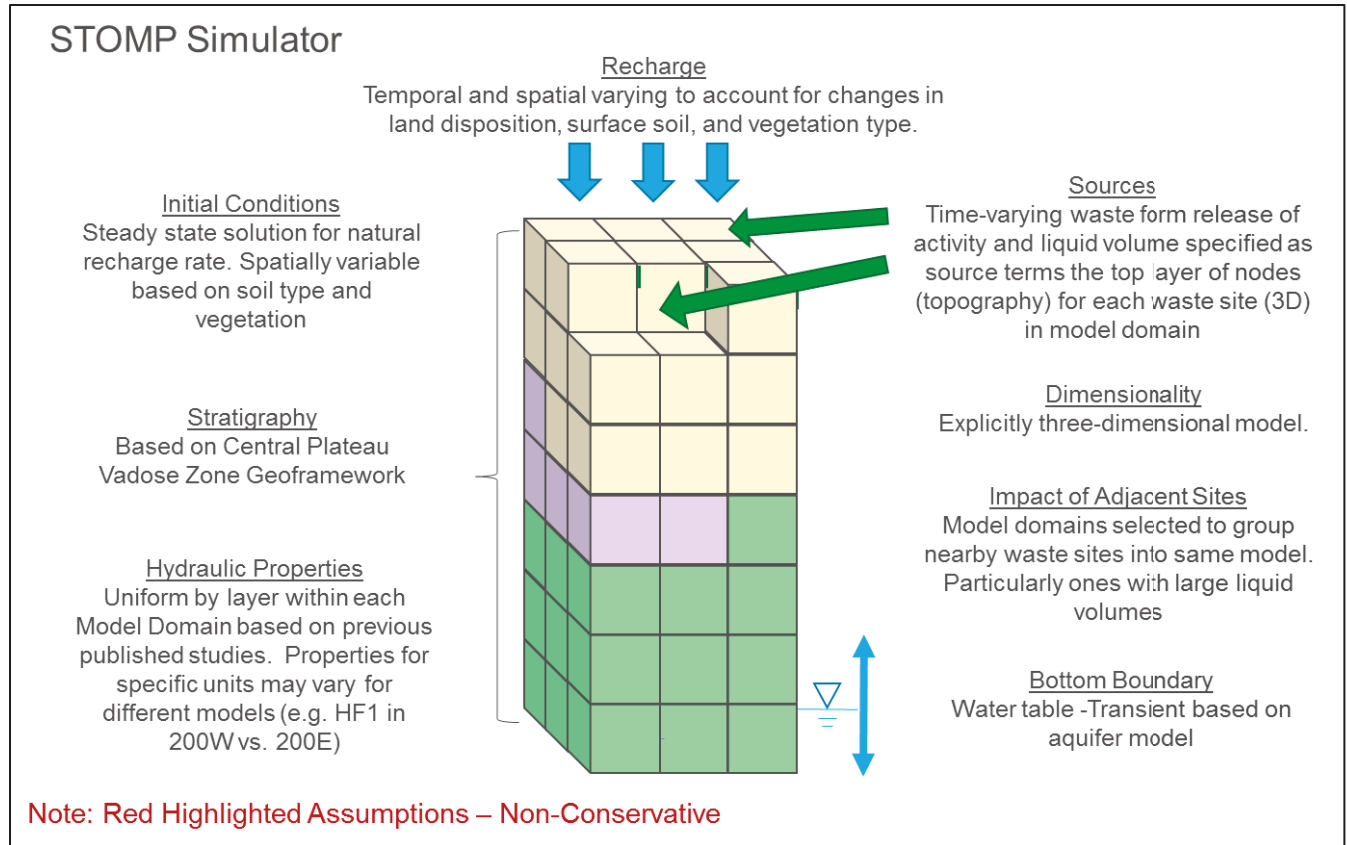


Figure 9. Proposed Approach

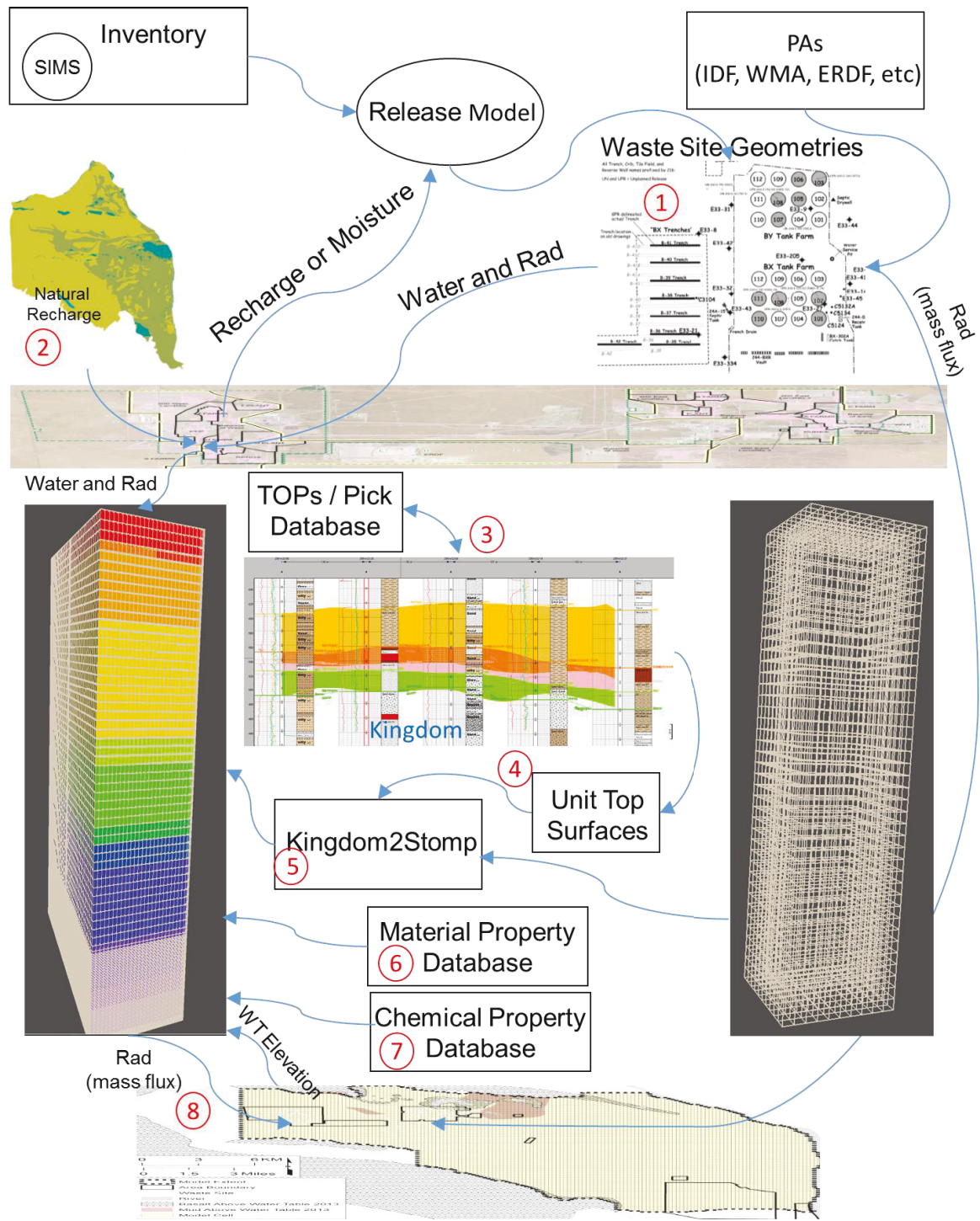


Figure 10. Overview of Vadose Zone Task Showing Workflow / Dataflow and Linkages to Other CA Tasks (Inventory, Release Model, Aquifer Model)

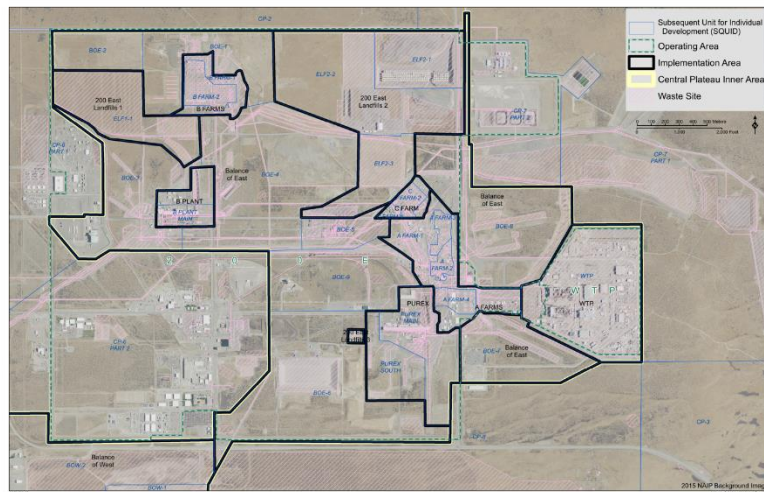
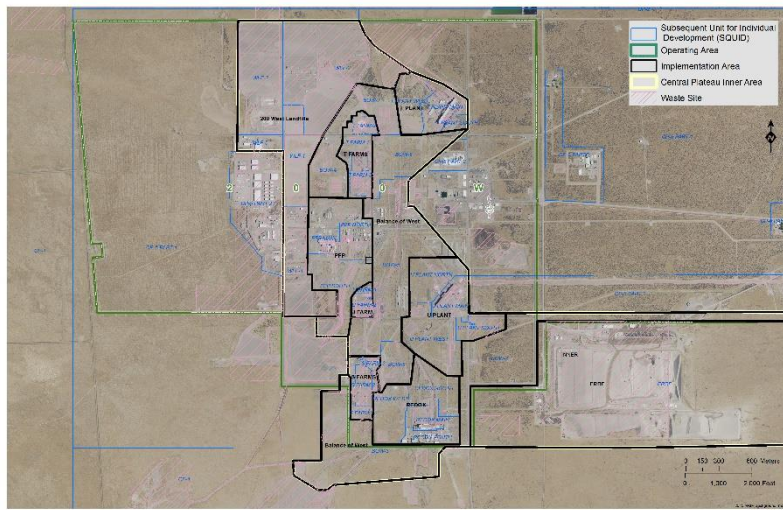
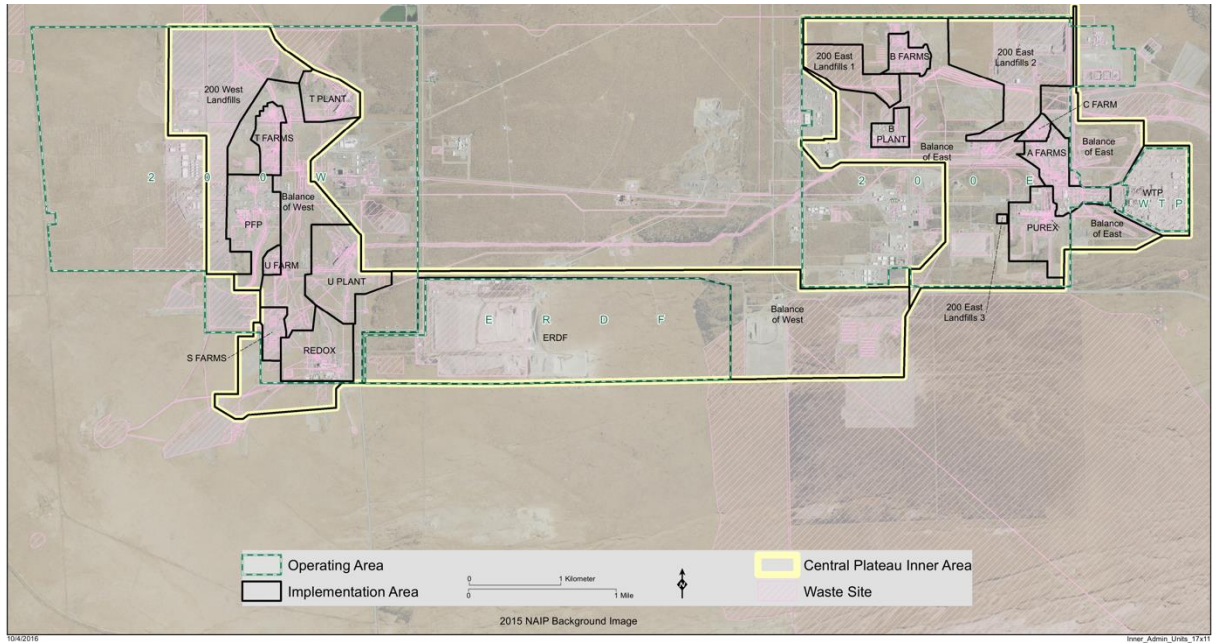


Figure 11. Central Plateau of the Hanford Site with Major Subdivisions of the 200 West and 200 East Areas

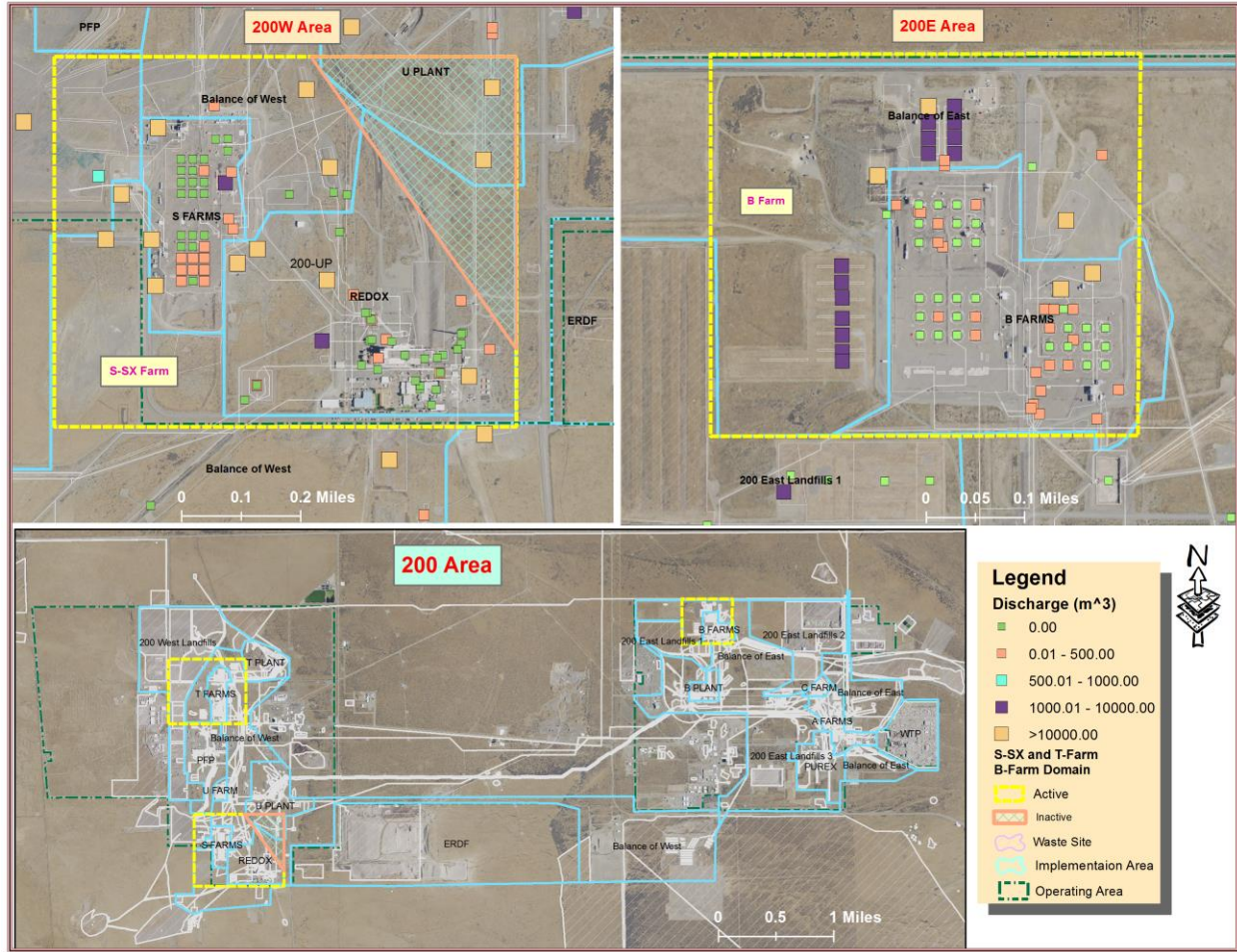


Figure 12. Example of Two Preliminary Model Domains (X-Y) in 200W and 200E Area

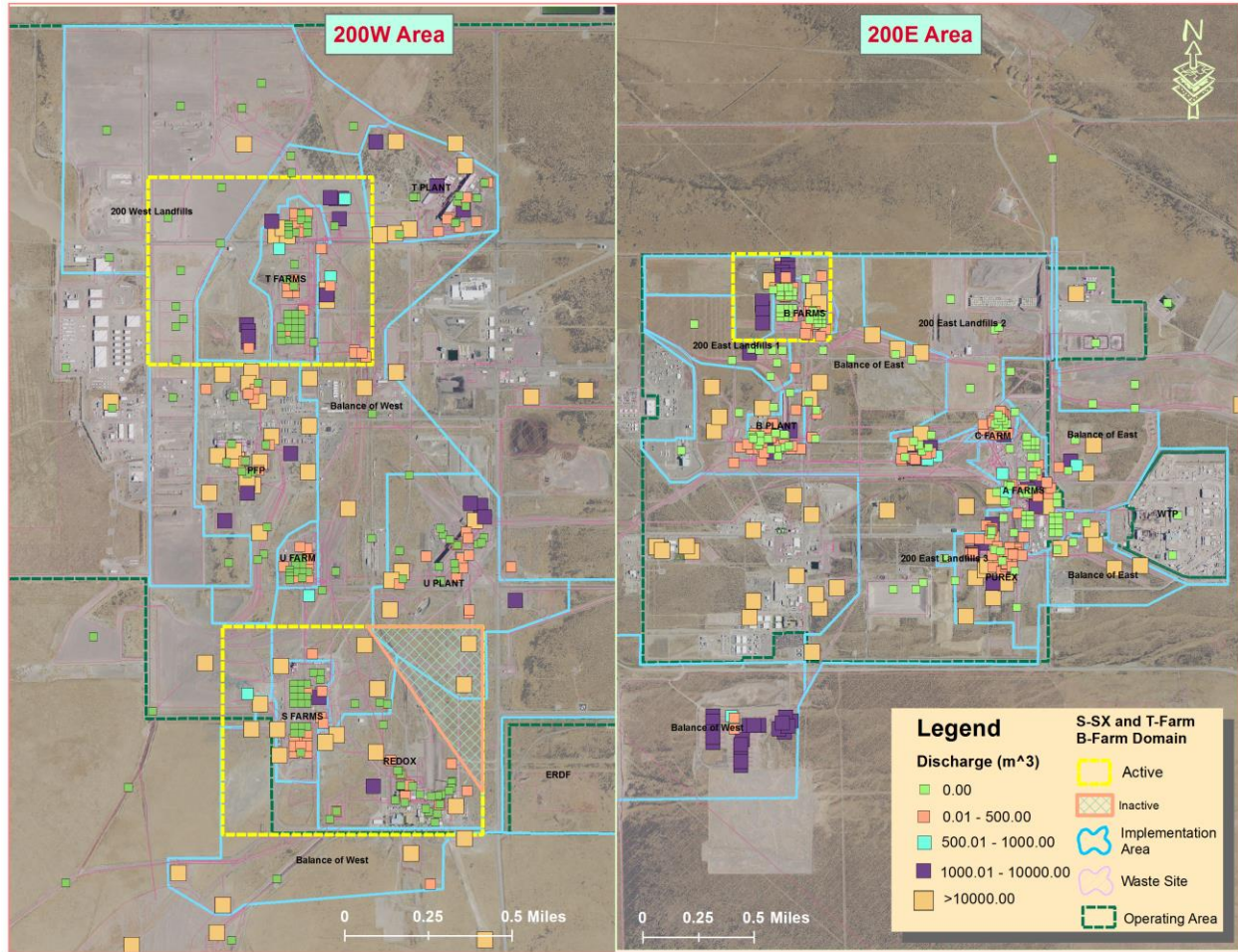


Figure 13. Cumulative Liquid Discharges (m^3) (preliminary data) in the 200 W and 200 E Areas Used to Help Determine Vadose Zone Model Boundaries

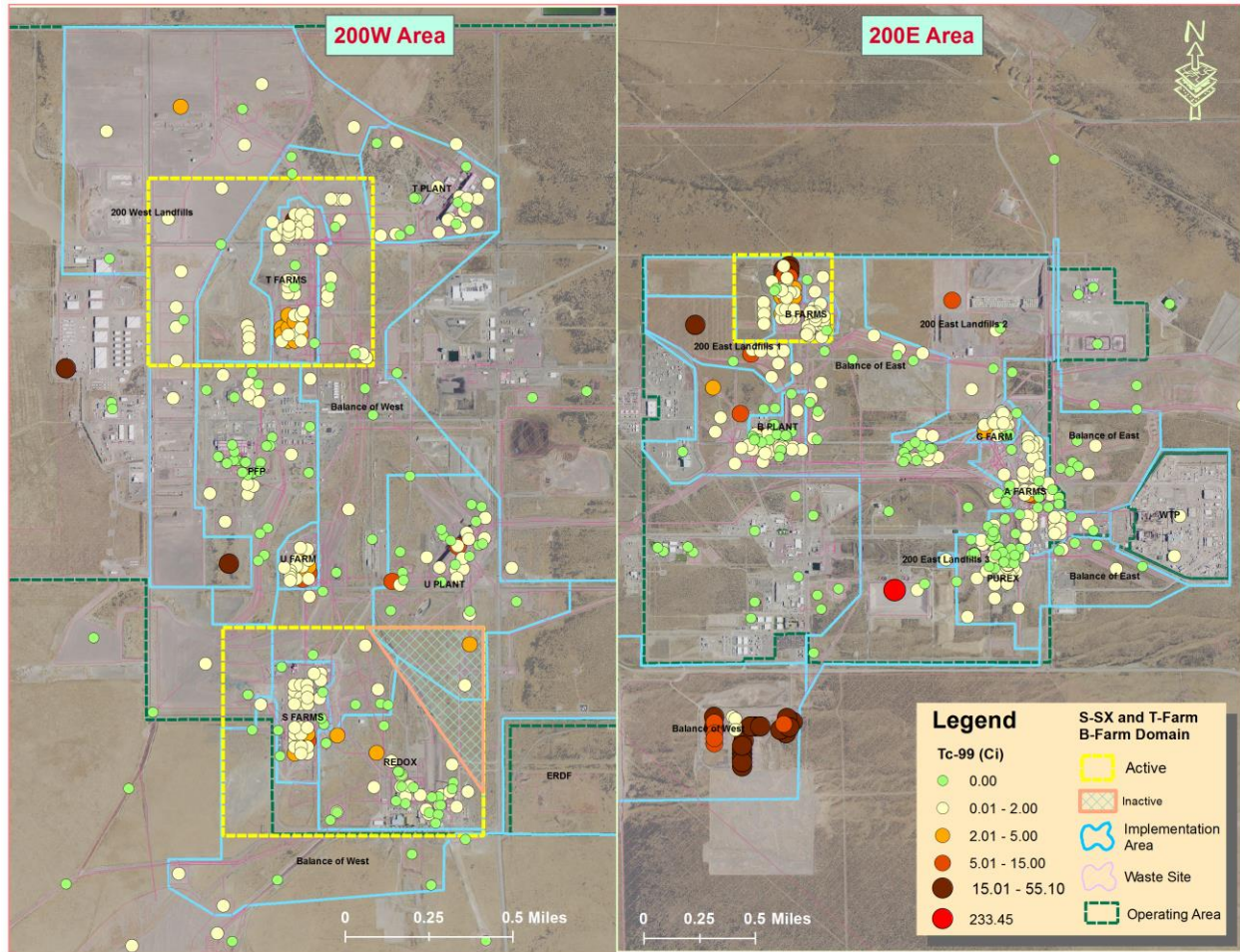


Figure 14. Cumulative Tc-99 Discharges (preliminary data) in the 200 W and 200 E Areas Used to Help Determine Vadose Zone Model Boundaries

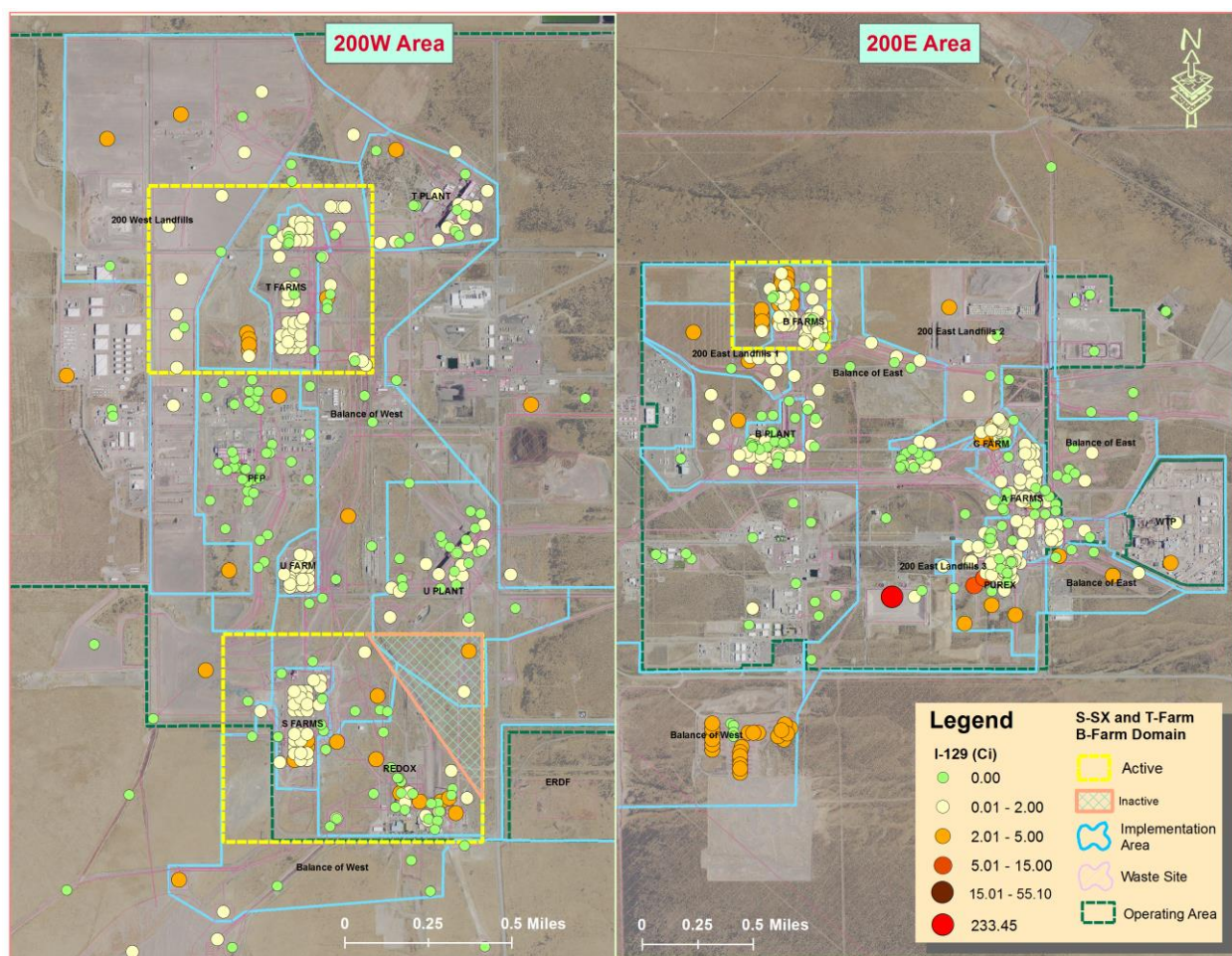


Figure 15. Cumulative I-129 Discharges (preliminary data) in the 200 W and 200 E Areas Used to Help Determine Vadose Zone Model Boundaries

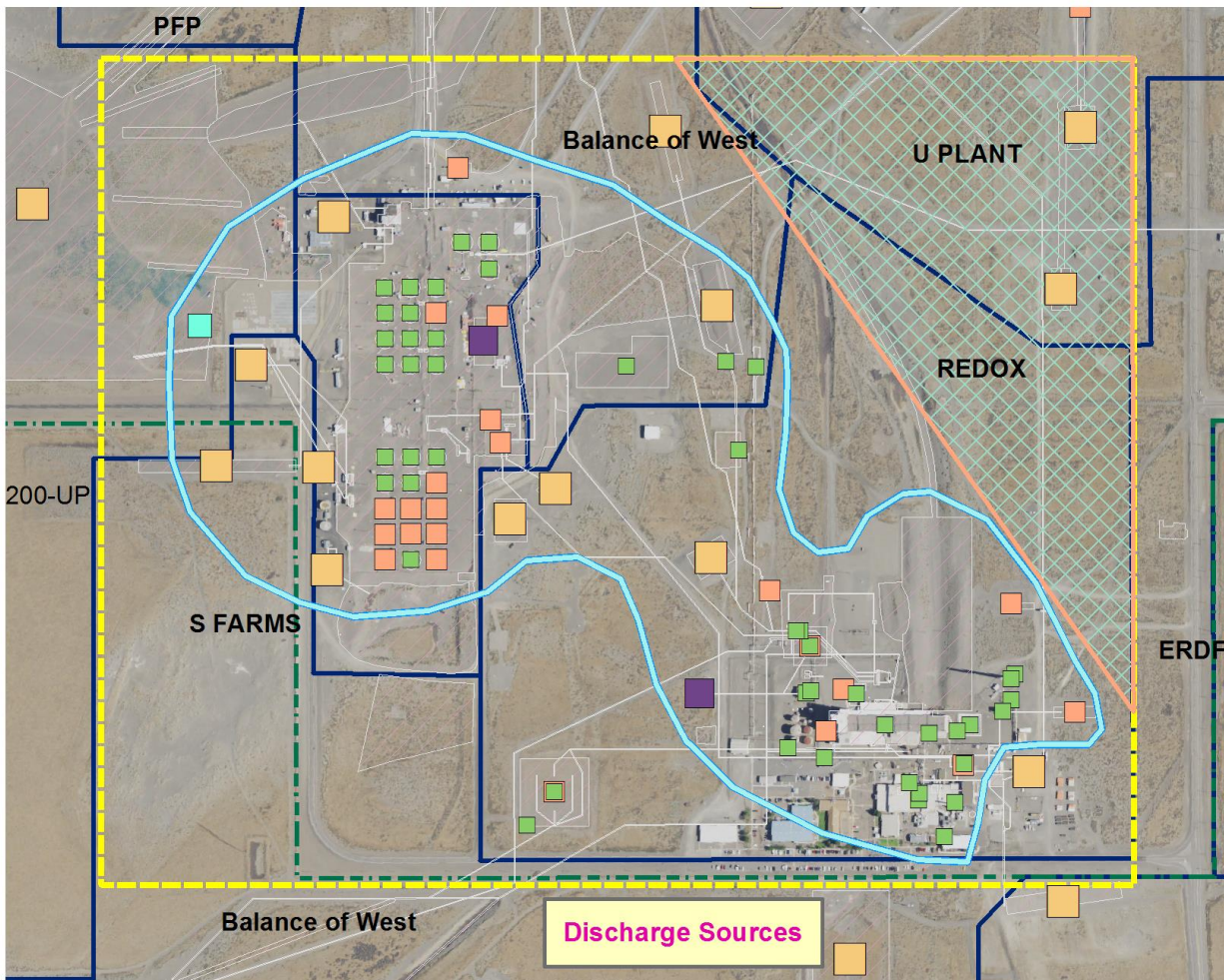


Figure 16. Example of Inner Polygon (light blue line) used for Selection of Waste Sites for a Model (the center position of the waste site is used for the selection)

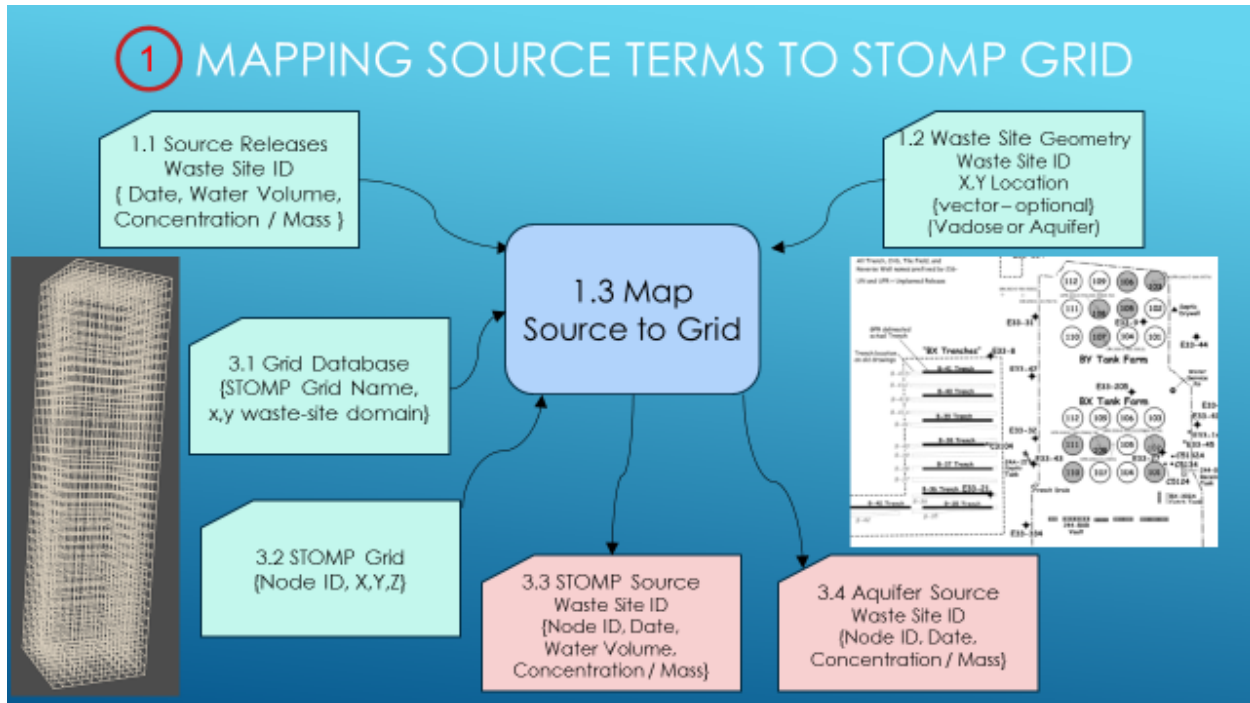


Figure 17. Example of Data Flow Diagram for Mapping Sources Terms to Vadose Zone STOMP Grid; Refer to Figure 11 for the Placement within Overall Framework (Red Numerical Identifier)



Figure 18. Plan-View of a Preliminary Model Grid with Waste Sites Superimposed for Source Term Mapping