Distilling Complex Model Results into Simple Models for use in Assessing Compliance with Performance Standards for Low Level Waste Disposal Facilities

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ABSTRACT

Assessing the long term performance of a waste disposal facility requires numerical simulation of saturated and unsaturated groundwater flow and contaminant transport. Complex numerical models have been developed to try to realistically simulate subsurface flow and transport processes. These models provide important information about system behavior and identify important processes, but may not be practical for demonstrating compliance with performance standards because of excessively long computer simulation times and input requirements. Two approaches to distilling the behavior of a complex model into simpler formulations that are practical for demonstrating compliance with performance objectives are examined in this paper. The first approach uses the information obtained from the complex model to develop a simple model that mimics the complex model behavior for stated performance objectives. The simple model needs to include essential processes that are important to assessing performance. These processes could include time-variable infiltration and waste emplacement rates, subsurface heterogeneity, sorption, decay, and radioactive ingrowth. The approach was applied to a Low-Level Waste disposal site at the Idaho National Laboratory where a complex three dimensional vadose zone model was developed first to understand system behavior and important processes. The complex model was distilled down to a relatively simple one-dimensional vadose zone model and three-dimensional aquifer transport model. Comparisons between the simple model and complex model of vadose zone fluxes and groundwater concentrations showed relatively good agreement between the models for both fission and activation products (I-129, Cl-36, Tc-99) and actinides (U-238, Pu-239, Np-237). Application of the simple model allowed for Monte Carlo uncertainty analysis and simulations of numerous disposal and release scenarios. The second approach investigated was the response surface model. In the response surface model approach, the temporal response of a complex model to an instantaneously-released unit mass of a conservative tracer at a defined point is calculated and stored (the response function). A separate response function is needed for each source-receptor pair. The convolution of the response function and estimated contaminant flux from the source then provides an estimate of the media concentration. The response function approach has the advantage of incorporating all processes included in the complex model into a single discrete function that requires only one run of the complex model. Limitations to the response surface model include the assumption of uniform retardation in the model domain and the assumption that radioactive progeny travel at the same rate as their parent. In highly heterogeneous environments where uniform retardation cannot be assumed, contaminant-specific response functions can be calculated. The response surface model was applied to a two-dimensional regional aquifer model to simulate multiple plumes of tritium originating from multiple sources across the Idaho National Laboratory.

INTRODUCTION

Long term assessment of engineered waste disposal facilities requires numerical simulation of groundwater flow and transport processes to demonstrate compliance with regulations. Improvements in computer speed and numerical techniques have led to the application of complex groundwater flow and transport models to address performance assessment questions. While complex models are useful for understanding system behavior, they are cumbersome when used to demonstrate compliance or address parametric uncertainty. Performance assessments are prospective and, by their very nature, the models cannot be truly validated. Therefore, it is important to quantify the parametric uncertainty to understand

the limitations of the model when addressing the assessment question. Furthermore, since prospective assessments often involve model predictions thousands of years into the future, the results of such assessments contain considerable uncertainty, and the answer from a complex model is not necessarily superior to that of a simpler model.

In this paper, two approaches are discussed for distilling the behavior of a complex model into simpler formulations. The two approaches are termed here as model simplification and response surface modeling. The methods are demonstrated using data and modeling studies from the Idaho National Laboratory. Advantages of each method and limitations are discussed.

MODEL SIMPLIFICATION

Model simplification extracts pertinent information obtained from a complex model of a waste disposal system to construct a simple model that mimics the complex model behavior for stated performance objectives. In general, there is no specific procedure used to simplify a model because of the amount of variability among groundwater systems and assessment questions. However, there are a few general steps that should be taken when constructing a simplified model.

1. Define the assessment question(s)
2. Develop a complex model of the site incorporating all known or suspected processes.
3. Examine the sensitivity of each process in terms of addressing the assessment question.
4. Apply first-order approximations to second-order processes (diffusion, dispersion, fluid head) when possible.
5. Compare the complex and simple model output for the stated assessment question. Calibrate simple model if necessary.

These steps are illustrated in the following application to the Radioactive Waste Management Complex (RWMC) Performance Assessment at the Idaho National Laboratory (INL) located in southeast Idaho.

Application to the Radioactive Waste Management Complex

The Radioactive Waste Management Complex (RWMC) encompasses 70 ha and is located in the southern part of the INL. It began disposing of radioactive waste in shallow trenches in 1952. Some of the early waste disposed contained transuranic waste and later retrieved, repackaged, and either sent to Waste Isolation Pilot Plant or stored above ground. Active disposal continues in a 3 ha area of the RWMC called the Subsurface Disposal Area (SDA) and in 6 meter deep soil borings called soil vaults. The site is slated for closure in the year 2010. The Low Level Waste Performance Assessment (LLWPA) covers the waste disposed in the active pits from 1984 to the present [1].

The assessment question for the LLWPA was "what are the groundwater concentrations as a function of time from present to the time of maximum, 100 m from the SDA at the RWMC?" A detailed three-dimensional multiphase unsaturated model was constructed that incorporated heterogeneous unsaturated zone, spatially and temporally variable infiltration rates and waste emplacement rates, and initial conditions that include historical episodic flooding events was constructed. The multiphase model of the unsaturated zone was coupled with a three-dimensional aquifer model to compute aquifer concentrations. The TETRAD [2][3] finite difference model was used to simulate fluid flow and contaminant transport in the unsaturated zone and aquifer. The DUST model [4] was used to incorporate time and space-dependent waste emplacement and simulate release of radionuclides from the waste to the backfilled soils.

The unsaturated zone at the INL is characterized by fractured basalt interrupted by primarily horizontal sedimentary units referred to as intebeds. Unsaturated water travel times are controlled by the presence of

sedimentary interbeds because water travels very quickly through fractured basalt. The three dimensional modeling indicated that infiltrating water from outside the SDA cover spreads horizontally along the interbeds, resulting in higher water contents in the interbeds underlying the SDA than would otherwise be estimated by one-dimensional flow through the SDA. This physical feature of the system reduces the effectiveness of an engineered cap because the vadose zone does not dry out underneath the cap. During active disposal infiltration was estimated to be significantly higher compared to infiltration through undisturbed soil which was estimated to be ~1 cm yr^{-1}. The cap was designed to reduce infiltration to one tenth the undisturbed soil infiltration rate (0.1 cm yr^{-1}).

Waste is disposed in either steel containers or wooden crates. Waste forms included surficially-contaminated trash, activated metals, activated beryllium reflector blocks, and ion exchange resins. Important radionuclides identified in a screening process included the mobile fission and activation products (I-129, C-14, Tc-99, Cl-36 and H-3) and actinides (U-238, Pu-239, Np-237). DUST modeled the failure of steel containers, corrosion of activated metals, leaching from ion exchange resins, and subsequent release of radionuclide to the soil column.

Based on the TETRAD conceptual model a simplified conceptual model of the facility was constructed that incorporated the significant processes that control the behavior of the system relative to the assessment question (Fig. 1). The simplified model included the processes of transient infiltration in a heterogeneous unsaturated zone. Prior to cap placement, the flux through the waste and backfilled soil is controlled by the infiltration through disturbed soils (~5 cm yr^{-1}). After cap placement, water flow through the waste and backfilled soil is reduced (~0.1 cm yr^{-1}) but water fluxes in the vadose zone are only reduced to background infiltration rates (~1 cm yr^{-1}) because vadose zone water flux rates will be primarily controlled by background infiltration outside the SDA. These processes were modeled by decoupling the source and vadose zone. Governing equations for fluid flow and contaminant transport were written in terms of first-order differential equations as implemented in the Mixing Cell Model (MCM) [5][6]. Metal and beryllium corrosion could also be approximated in terms of first-order processes and was incorporated into the DUST model. Sorption coefficients and hydraulic properties of the unsaturated materials were taken directly from the TETRAD simulation. The aquifer was simulated using a semi-analytical solution to the advection dispersion equation as implemented in the GWSCREEN code [7].
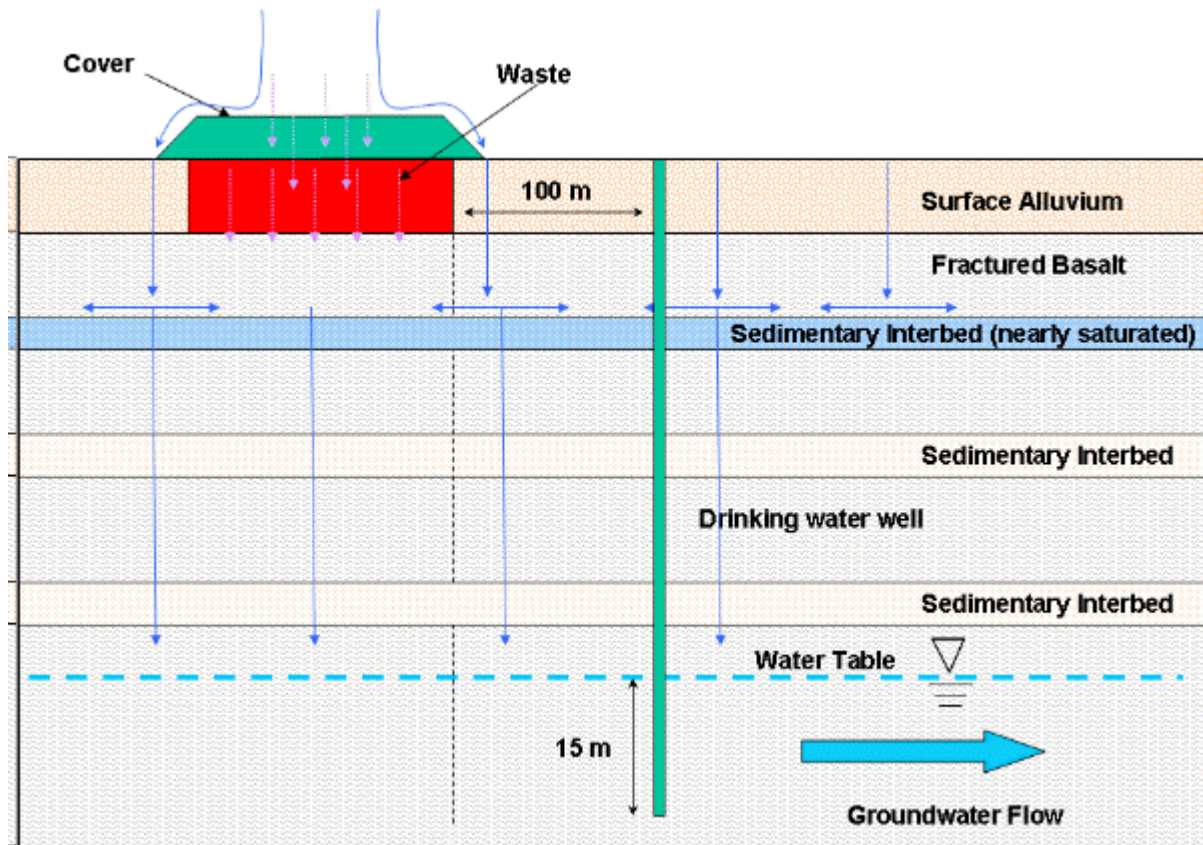
Fig. 1. Simplified conceptual model for water flow and radionuclide transport for the Radioactive Waste Management Complex. Water is diverted around the waste by the presence of the engineered cap. The nearly saturated conditions of the first sedimentary interbed is from past flooding events and is modeled as an initial condition.

Unsaturated fluxes and aquifer concentrations for ^{36}Cl (Fig. 2) show that the simplified conceptual model utilizing MCM yielded aquifer fluxes and concentrations that were within a factor of two of the complex model that utilized TETRAD. Improved agreement could be achieved through model-to-model calibration. However, it should be recognized that even complex models are subject to great uncertainty and they do not necessarily provide the "correct" answer for prospective assessments. Computer run times for TETRAD were on the order of several weeks while MCM run times were no more than several minutes. Model simplifications allowed for an evaluation of numerous closure options and exposure scenarios, and a Monte Carlo parametric uncertainty analysis for the endpoint of All Pathway Dose. The Monte Carlo uncertainty analysis showed that during the compliance period (year 2100–3000), the distribution of doses spanned about an order of magnitude while after the compliance period (>3000), doses spanned several orders of magnitude. The larger variability in doses after the compliance period reflects the uncertainty in actinide sorption coefficients, and cap performance and longevity.
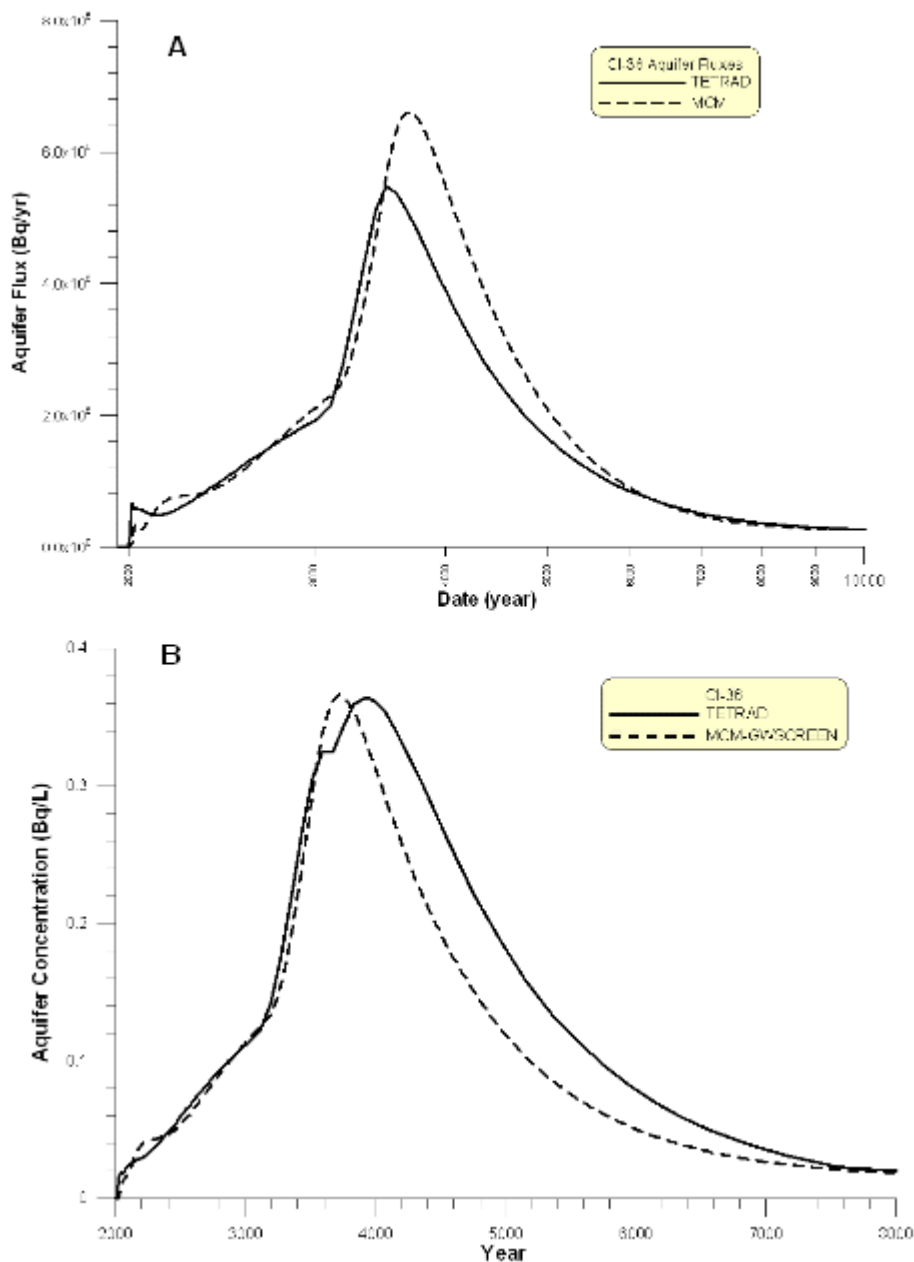
Fig 2. Chlorine-36 flux to the aquifer (A) and concentration in the aquifer at the point of compliance (B) for the complex TETRAD model and simplified MCM-GWSCREEN model. Both the complex model and simple model use the same Cl-36 release rate from waste to soil.

RESPONSE SURFACE MODELING

A response surface model distills the behavior of a complex model into a simple function. Applying the principles of convolution and superposition allows for rapid simulation of numerous contaminants and release scenarios while retaining most of the complexity of the underlying model.

The response function is essentially the breakthrough curve at a receptor to a unit mass pulse input of a conservative tracer from each source. The response surface model requires a response function for each source-receptor pair, and contaminant loading rates (i.e., contaminant mass flux) as a function of time for

each source. The computational endpoint (concentration or flux) at a given receptor is obtained from the convolution of the contaminant loading rates and the response function. The convolution can be thought of as a series of "pulses" where the magnitude of the pulse is a function of the product of the contaminant-loading rate at a given time, the response function at some time thereafter, a decay and retardation factor, and a time step. When summed together, the individual pulses form a continuous function over the time period of interest.

The contaminant concentration is given by the response surface model as:

$$C_{i,j,k(m)}(t) = \frac{1}{Rd_m} \int_0^t RF_{i,j}\left(\frac{t-\tau}{Rd_{m=1}}\right) S_{i,k(m=1)}(\tau)\, DIF_m(t-\tau)\, d\tau \qquad \text{(Eq. 1)}$$

where

$C_{i,j,k(m)}(t)$	=	concentration of decay product m at time t for source i at receptor j (M L^{-3})
$RF_{i,j}((t-\tau)/Rd_{m=1})$	=	response function for source i at receptor j at time $(t-\tau)/Rd_{m=1}$ (L^{-3})
$S_{i,k(m=1)}(\tau)$	=	source-loading rate of parent ($m=1$) for source i at time τ (M T^{-1})
Rd_m	=	the retardation factor for product m, [$m=1$ for parent] (unitless)
DIF_m	=	decay-ingrowth factor (see below) for decay product m at time $t-\tau$ (unitless)
$k(m)$	=	decay product index [$m=1$ for parent] for contaminant k.
i	=	source index
j	=	receptor index
k	=	contaminant index

To account for the decay and sorptive properties of different contaminants, and decay and ingrowth of radioactive progeny, several simplifying assumptions are made:
1. Retardation is uniform throughout the medium,
2. Porosity is constant throughout the medium,
3. Parent and progeny radionuclides travel at the same rate in the medium.

For a single decay species with no progeny, the decay-ingrowth factor is simply e$^{-\lambda tage}$ where *tage* is the age of the pulse (i.e., $t-\tau$). For a decay product other than the parent, the decay-ingrowth factor is given by [8]

$$DIF_m(tage) = \frac{\lambda_m}{\lambda_{m=1}}\left[\left(\prod_{i=1}^{m-1}\lambda_i\right)\sum_{i=1}^{m}\frac{e^{-\lambda_i tage}}{\prod_{\substack{j\neq i\\j=1}}^{m}(\lambda_j - \lambda_i)}\right] \qquad \text{(Eq. 2)}$$

where

$\lambda_{m=1}$	=	decay constant for the parent (T^{-1})
λ_m	=	decay constant for the mth progeny (T^{-1})
tage	=	age of pulse (T).

The contaminant concentration at a given receptor location from multiple sources is the sum of the concentration from each individual source.

$$C_{j,k}(t) = \sum_{i=1}^{n} C_{i,j,k}(t) \qquad \text{(Eq. 3)}$$

Where

n	=	number of sources considered in the model domain
j	=	receptor index
i	=	source index

k = contaminant index

Application of a Response Surface Model to the Snake River Plain Aquifer

The response surface model was applied to the Snake River Plain Aquifer (SRPA) system underlying the Idaho National Laboratory (INL) located in eastern Idaho. Response functions for instantaneous unit inputs of a conservative tracer were developed with a two dimensional MODFLOW/ MT3DMS [9] simulation. Tritium (^{3}H, half-life = 12.3 years) fluxes to the SRPA from sources at the Idaho Nuclear Technology and Engineering Center (INTEC) and the Radioactive Waste Management Complex (RWMC) were used with the response functions and the convolution integral to calculate aquifer concentrations at six downgradient receptor locations (Fig. 3 and 4). Injection well releases of tritium at INTEC occurred from 1952 to 1986 and significant quantities of tritium have been disposed of at the RWMC. However, tritium fluxes to the SRPA from INTEC and RWMC sources were only used to demonstrate the model and do not necessarily represent the current or best understanding of tritium releases from INL facilities. The MODFLOW domain encompasses the INL in the eastern Snake River Plain and occupies and area of roughly 7,770 km^2. The aquifer model was calibrated to water-level data collected in June of 2004 [10].

The response surface model was implemented in a Microsoft Access Database via a Visual Basic Module. The convolution integral was solved using a Simpson Rule integration routine described in Press et al. [11]. Liner interpolation was used to generate function values at any point from a discrete representation of the response function and contaminant loading rates.
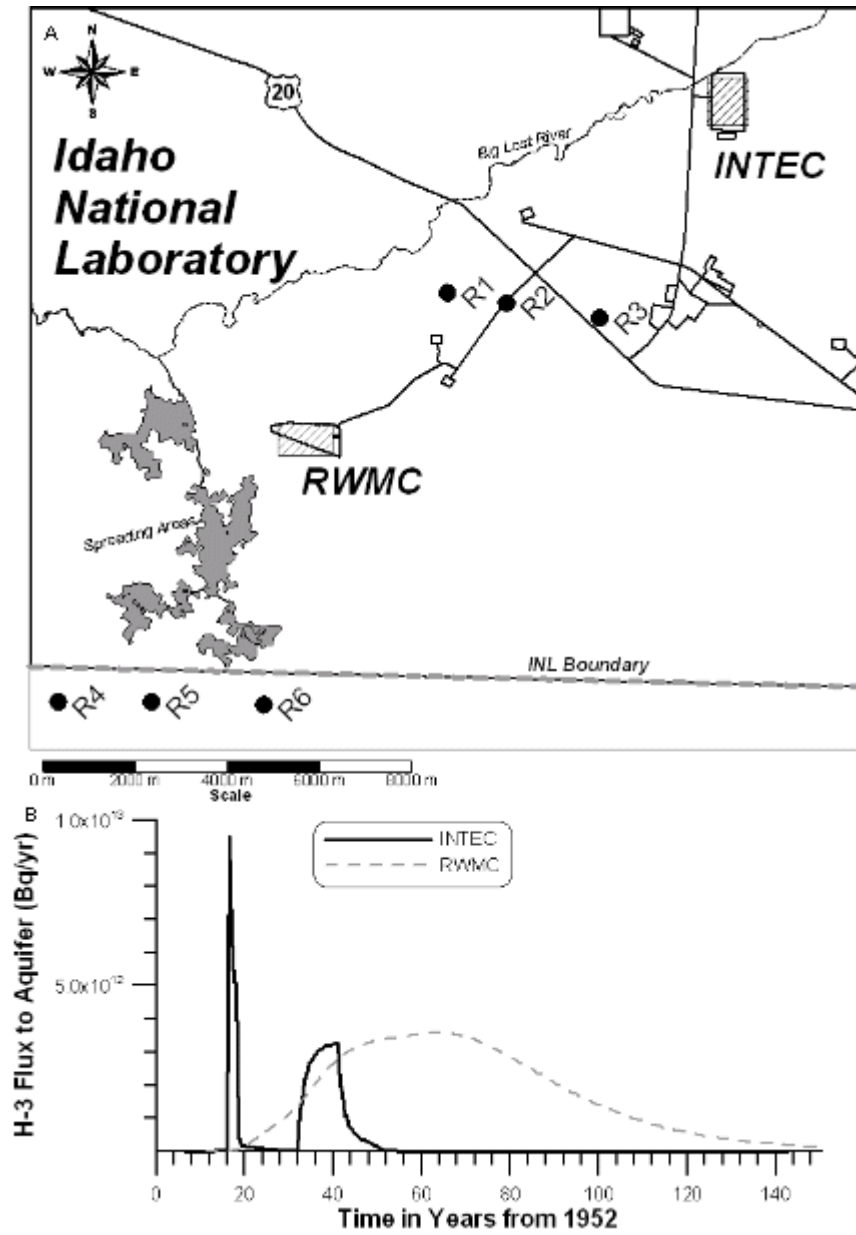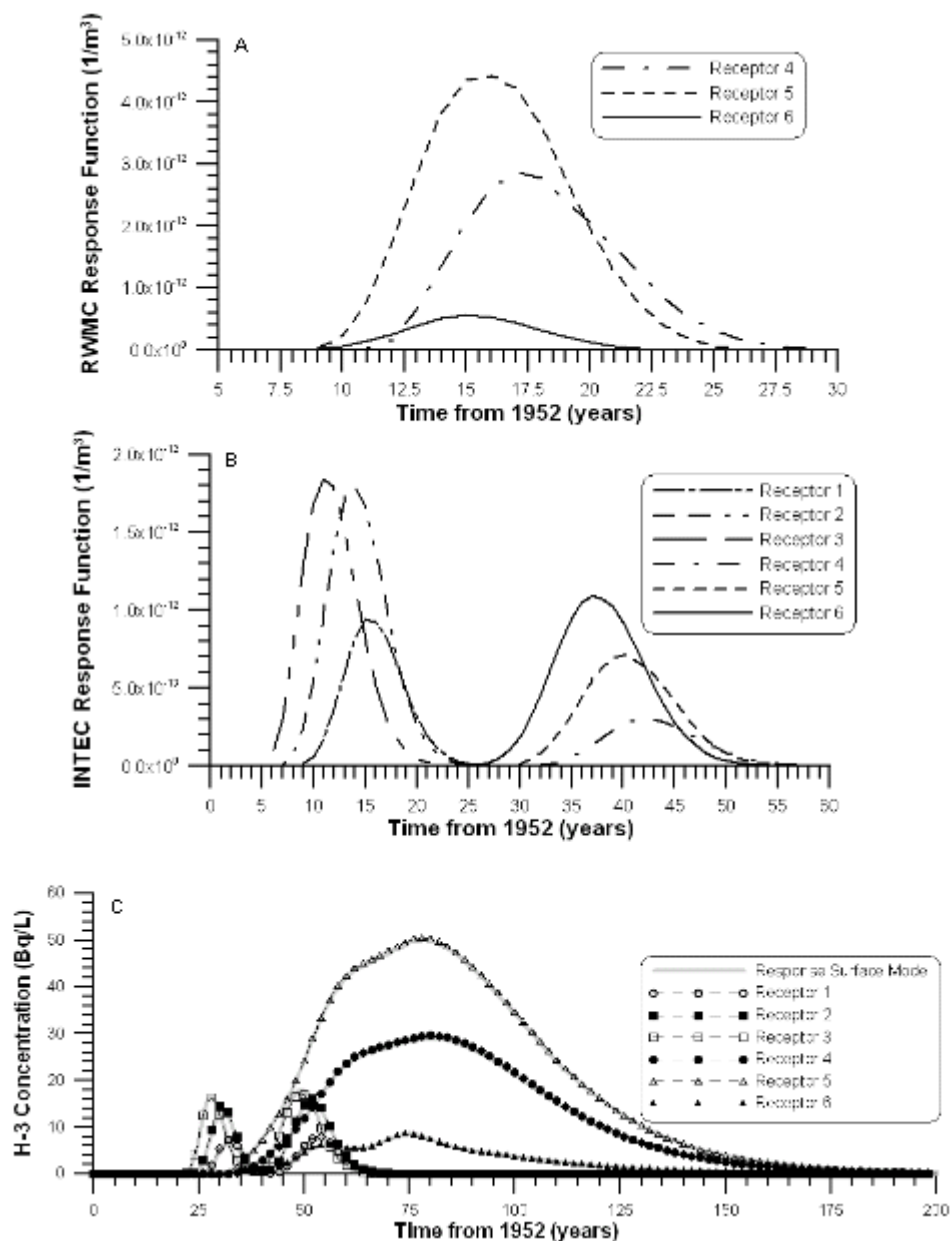
Fig 3. Response surface model domain showing the INTEC and RWMC sources and receptors (R1, R2, R3…R6). The lower graph shows the H-3 flux the aquifer from each source.

Fig 4. Response functions for the RWMC (A) and INTEC (B) and H-3 concentrations at the six receptor locations (C).

Concentration time histories (Fig. 4C) show that receptor 5 had the highest tritium concentration, which is consistent with what would be expected based on the response functions for INTEC and RWMC and the tritium fluxes to the aquifer (Fig. 3). The relatively small response at receptor 2 and 3 to the high release of ^{3}H between years 16 and 20 from INTEC reflects greater dispersion in the aquifer in that region compared to the region between the RWMC and receptors 4, 5, and 6. Receptors 4, 5, and 6 are also impacted by both the INTEC and RWMC sources.

For comparison, tritium concentrations were also calculated directly using MODFLOW/MT3D, and these results are plotted alongside the response surface model results (Fig. 4C). Differences between the *maximum* tritium concentrations estimated with the response surface model and those estimated with MODFLOW were no greater than 6% and typically were less than 3%. Computer run times for the Response Surface Model were typically less than a few seconds.

SUMMARY AND CONCLUSIONS

Complex models of the unsaturated zone and aquifer are useful for understanding system behavior, but are cumbersome to use in risk assessment and Monte Carlo uncertainty analysis because of prohibitively long simulation times, voluminous code output, and results that may be difficult to interpret. Furthermore, without detailed and relevant measurements with which to compare model estimates to, it is difficult to assert that the results from a complex model are any better than a simple model. This is especially true for simulations that extend far into the future where no measurement data exist.

Two methods for distilling complex model behavior into simpler model formulations are presented in this paper (model simplification and response surface modeling). Simple models must incorporate significant processes that drive system behavior for a particular assessment question. The output from the simple model should be compared to the output of a complex model for the stated assessment question. In some cases, it may be desirable to calibrate the simple mode to the complex model using parameter estimation software such PEST [12].

The response surface model is a viable method of condensing detailed groundwater flow and transport models into an assessment framework that considers arbitrary source-loading rates for numerous sources and contaminants. The method is particularly attractive for the composite analysis requirement of LLW performance assessment. Additionally, it provides a tool for assessment and management of groundwater resources.

It should not be construed that complex modeling is unnecessary. The complex model is the tool used to improve system understanding and evaluate sensitivity to different flow and transport related mechanisms. It is the basis for defining the simple conceptual model and defines the response function used in the response surface model. The objective is to better utilize complex modeling to address assessment questions. Simpler models that are based on complex modeling provide a practical computational tool to demonstrate compliance with performance objectives.

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