Coupled Vadose Zone/Saturated Zone Models for Nearfield Analyses - 14289

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ABSTRACT

With continued advances in processing efficiency, over the last ten years it has become computationally feasible to solve three-dimensional combined vadose zone/saturated zone models in the context of a probabilistic assessment framework. These models are conceptually satisfying because they have no artificial boundaries separating model components. These models are also more difficult to develop, parameterize, and evaluate. This paper discusses several approaches to boundary conditions for combined models and their strengths and weaknesses. It also considers the different approaches and tradeoffs associated with calibration. The third major topic is the model structures that are required to report groundwater concentrations that are meaningful in regulatory and permitting contexts. Application of the combined model to sites of varying complexity and comparison with other model approaches allows site managers and modelers some general rules to determine under what conditions the additional detail and complexity of combined models are worth the increased costs associated with development and parameterization.

INTRODUCTION

A traditional approach to local-scale groundwater modeling has been to use separate models for the vadose zone and saturated zone. The separation of vadose zone and saturated models introduces an artificial boundary that does not exist in the field. In addition, the traditional approach does not easily allow investigation under transient water table conditions.

An alternate approach is to analyze the fate and transport of water and solute through the vadose zone and saturated zone in one “combined” model, without specification of time-dependent boundary conditions that serve as the interface between separate models. This combined approach was implemented for several local source areas at the Hanford Site in Richland, Washington, and compared to the traditional separate model approach. This paper describes some of the issues of implementing combined models and discusses the circumstances in which the additional fidelity to the field characterization is worth the additional cost and complexity of the combined approach.

Conceptualization

There are several different arrangements of boundary conditions for a combined vadose zone/saturated zone model that simulates groundwater flow and transport of solute. A depiction of the boundary conditions that were used for local-scale source areas at the Hanford site is shown in **Figure 1**.
The top surface of the model domain allows natural and anthropogenic recharge through the ground surface. The bottom surface of the model domain is located deep in the aquifer (e.g.,

sufficiently deep such that the presence of this artificial surface does not influence the model results). The vertical faces parallel to groundwater flow are also located far enough from the center of the model domain to avoid influences on plume development. The upgradient vertical face of the model domain allows water to enter the model domain beneath the water table, while the downgradient vertical face allows water to leave the model domain beneath the water table. This conceptualization was designed to optimize implementation of models with discharge onto a fluctuating water table and reporting of near-field concentrations.

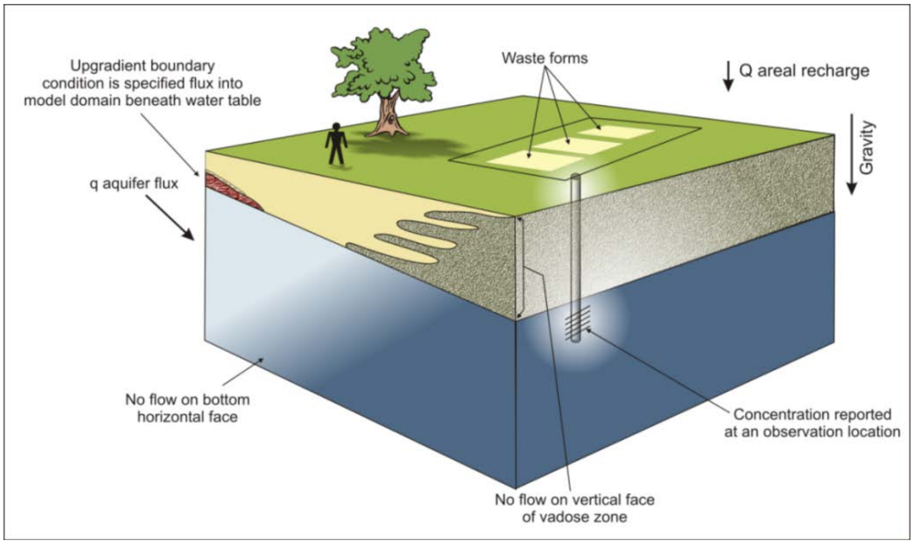

Figure 1. Combined Model - Arrangement of Boundary Conditions

Boundary Conditions

The conceptual model illustrated in **Figure 1** is implemented through a combination of no-flow, specified flux, and specified pressure boundary conditions. The sidewalls of the simulation domain that are parallel to the principle direction of flow are no-flow boundaries that are located sufficiently far from the area of interest to minimize influences from the boundary condition on the contaminant plume. The bottom of the simulation domain is also a no-flow boundary located either at an impermeable barrier (e.g., top of basalt) or deep enough in the saturated zone to minimize influences from the boundary condition on the contaminant plume. The top and up-gradient (vertical) faces of the simulation are specified flux boundary conditions. The spatial distribution of flux on the top face represents infiltration rates through different parts of the site. The spatial distribution on the up-gradient vertical face represents groundwater flow into the model domain. Both of these distributions may vary with time. In order for the problem to be well-posed, the pressure for at least one point in the model domain must be specified. For the local-scale models developed for the Hanford Site, the location of the water table across the down-gradient vertical face of the domain was specified to satisfy this condition.

The recharge through the upper horizontal face is generally obtained from site characterization data. For example, the total flux (anthropogenic and natural recharge) across the upper face could consist of known temporal sequences of discharges from specific waste impoundments in combination with a background infiltration rate for undisturbed areas. The groundwater flux entering the domain through the up-gradient face has been found to be best treated as a calibration parameter. In general, this flux can be varied to induce changes in the height and slope of the water table that allow the modeled water table to mimic the behavior observed in monitoring wells. This idea will be discussed in the next section. Finally, the down-gradient pressure distribution is most naturally specified at a location where the water table elevation is governed by some hydrogeologic feature (e.g., discharge into a river or surface water body). Such a feature may not exist near the down-gradient location of a local-scale model. In these cases, the equivalent of a generalized head boundary (GHB) at the down-gradient end of the domain with a hydraulic conductivity and specified head determined by calibration could be implemented. In the context of the STOMP numerical model, this is relatively easy to implement but adds additional parameters to the calibration process.

Gridding (Discretization):
The local-scale models developed for the Hanford site in support of the TC & WM EIS [1] used the STOMP [Subsurface Transport Over Multiple Phases] model [3] and were implemented in fully transient, three-dimensional mode. The cells in these vadose zone only STOMP models were rectangular parallelepipeds. Using this approach the vadose zone grid is designed primarily to facilitate the numerical vadose zone flow and transport solution. Achieving efficient numerical computation requires: finer grid resolution near the source to capture local-scale behaviors; a model domain that extends enough to prevent influences from the boundary conditions on the solution; and a coarse enough discretization near the outer boundaries of the model domain to stay within the computational limits.

In general, the combined model discretization process involved starting with a local-scale vadose zone model that was developed for the TC & WM EIS long-term groundwater impacts analysis. The vadose zone model was extended into the aquifer (typically with resolution fine enough to capture the local-scale water table). Additional nodes were added at the downgradient end of the model for the purposes of reporting concentration.

The discretization of the model domain must take into account the requirements for accurate numerical solution in both the vadose zone and the saturated zone; allow for accurate solution near the water table (under transient conditions) where velocity vectors change from being small and vertical to large and horizontal. The discretization must also support the objective of reporting near-field concentrations from the grid to reasonably represent monitoring wells that exist in the field. These considerations must be evaluated in the context of the overall constraint of the computational limit of the modeling equipment.

A combined model approach has additional functions and thus additional design considerations during the discretization process. There is an additional complexity of staying within the computational limits because the grid extends into the saturated zone requiring more grid elements than a separate vadose zone model. Another consideration during the discretization process is the regional-scale water table behavior and whether or not additional resolution near the water table is required to capture a representative flow solution. Discretization specifically optimized for the combined model approach at a particular site tends to minimize numeric dispersion, particularly across the water table, as well as refine and sharpen the modeled contaminant plumes as they migrate past downgradient reporting locations. Results show that the concentrations reported at downgradient locations depend strongly on the grid cell dimensions, therefore careful attention should be taken during the model discretization process.

Calibration

As discussed above, boundary conditions can be adjusted to reflect field observations, making them useful tools for model calibration. Underneath many individual source areas at Hanford, the water table fluctuates as a result of regional-scale influences (large volumetric discharges to surface impoundments) outside of the local-scale model domain. Typically the boundary conditions in the saturated portion of the aquifer are used as the primary tool to model these changes in the water table. At other source areas, anthropogenic recharge from a high discharge source (e.g., cribs and trenches) may influence the water table directly beneath the source. In these cases, the relative amounts of water coming from the top and upgradient side face governs the transient behavior of the water table.

Calibration of flow for a combined model in STOMP can be achieved by adjusting the aqueous flux through the inflow boundary to match water table conditions derived from field data. Field data required for calibration using this approach include data for both the water table gradient and elevation. Thus, the accuracy of the estimated inflow of the combined model can be limited by the uncertainties in the field measurements of the water table elevation and gradient near the source area. Additionally, the availability of water table gradient and elevation data is often variable based on the location and history of the area of interest. For example, a site may not have an individual well that fully captures the changes in the water table elevations over time. In this case it is necessary to derive a composite hydrograph based on data from several wells to characterize the changes in the water table elevation over time and calibrate the inflow boundary condition. **Figure 2** illustrates the application of a composite hydrograph to the calibration of a model for cribs in the Hanford 200-West Area discharging onto a fluctuating water table. In this particular case, the water table is responding to discharges from large artificial ponds outside the model domain.

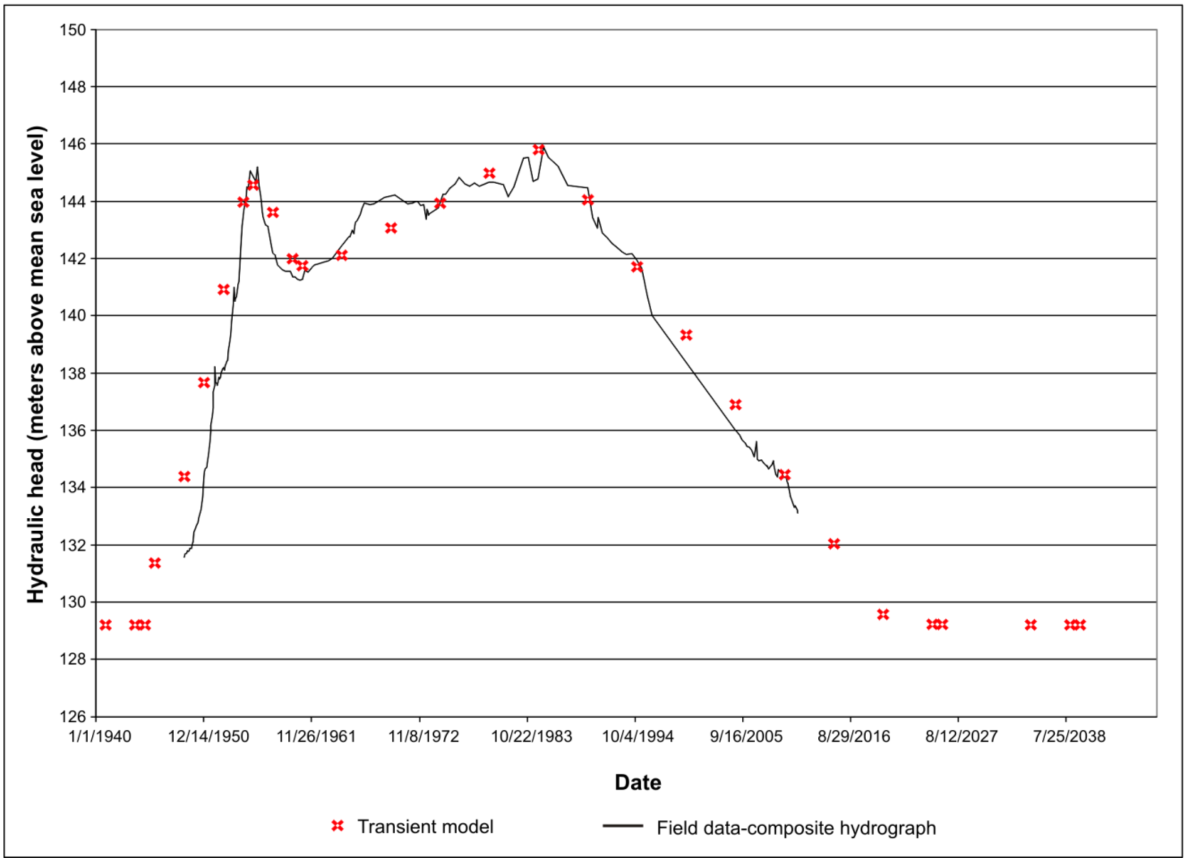

Figure 2. Results for Flow Model Calibration for the TY Cribs

When a source area has a nearby natural hydrogeologic boundary, calibration can be achieved by fixing the water table elevation at the boundary condition representative of the natural feature and selecting a set of times and inflow values representative of the water table at the other boundary condition and allowing STOMP to linearly ramp the inflow at appropriate times. For example, for sites such as the River Corridor sites at Hanford, the downgradient water table elevation can be fixed by the elevation of the Columbia River, and the inflow can be adjusted using a Neumann boundary condition. The calibration can then be refined by using a different ramp for the temporal variation in the inflow flux.

The calibration approach becomes increasing complex for sites that are not located near a natural hydrogeologic boundary because an arbitrary boundary that appropriately represents regional scale characteristics and is based on field data has to be incorporated. STOMP does not contain a boundary condition setting that is equivalent to MODFLOW's (modular three-dimensional finite-difference groundwater flow model [2]) generalized head boundary (GHB), but does allow the user to mimic the effect of a GHB by adding a vertical stack of nodes downgradient of the flow domain with an arbitrary hydraulic conductivity and specified head. This boundary condition represents a distant location where the hydraulic head is fixed as a constant value based on field data. By fixing the hydraulic head at a location distant from the downgradient location of interest, the user can then adjust changes to the inflow boundary condition naturally using a Neumann boundary condition. This allows control of the hydraulic head and gradient in the flow model domain. This approach increases the number of nodes in the model domain, and the saturated hydraulic conductivity of the vertical stack of nodes down gradient of the flow domain becomes an important and additional adjustable parameter during the calibration process.

Concentration Reporting

The concentration calculation is largely based upon the dimensions of the concentration grid cells used in the calculation. The programmatic objective of the TC & WM EIS required presentation of the maximum concentration within 100 meters of the reporting location. The EIS approach for contaminant fate and transport utilized multiple models starting with release to vadose zone models, followed by a vadose zone flow and transport model (STOMP), followed by a particle tracking approach which used outputs from the local-scale vadose zone models and a regional-scale MODFLOW-generated flow-field. The groundwater concentrations were then predicted using the results from the regional-scale groundwater transport analysis. The calculation used a concentration grid cell depth equal to 40 meters or the top of basalt with a grid cell width of approximately 100 meters in each horizontal direction. This approach allowed for a regional-scale comparison of groundwater concentrations for several alternatives and met the programmatic objective of reporting concentrations within 100 meters of the reporting locations.

The combined model approach has a conceptual advantage of using STOMP to calculate local-scale groundwater concentrations. A vertical stack of nodes can be used as an analog to a monitoring well and takes advantage of STOMP's internal concentration calculation. Similar to the EIS approach, the horizontal grid cell dimensions near the observation location and vertical extent of the stack of grid cells that represent a well-screen interval need to be considered because they are a primary factor in the concentration calculation.

In situations where a vertical stack of nodes is used to represent a monitoring well, there are several options for producing a single concentration for that well from the constituent values. One method is to search through the vertical stack of nodes and find the maximum concentration value. A second method is to average all of the concentrations using the cell volumes as weights. A third method is to average the concentration values using the hydraulic conductivities as weights. Choosing among these methods requires an understanding of the programmatic objectives and regulatory requirements that guide the modeling study. **Figure 3** illustrates the influence of the reporting method on the results for one of the cribs in the Hanford 200-West Area. In any case, the finer-scale concentration reporting of the combined model will result in concentrations that are less influenced by averaging than those calculated using a regional-scale transport model.

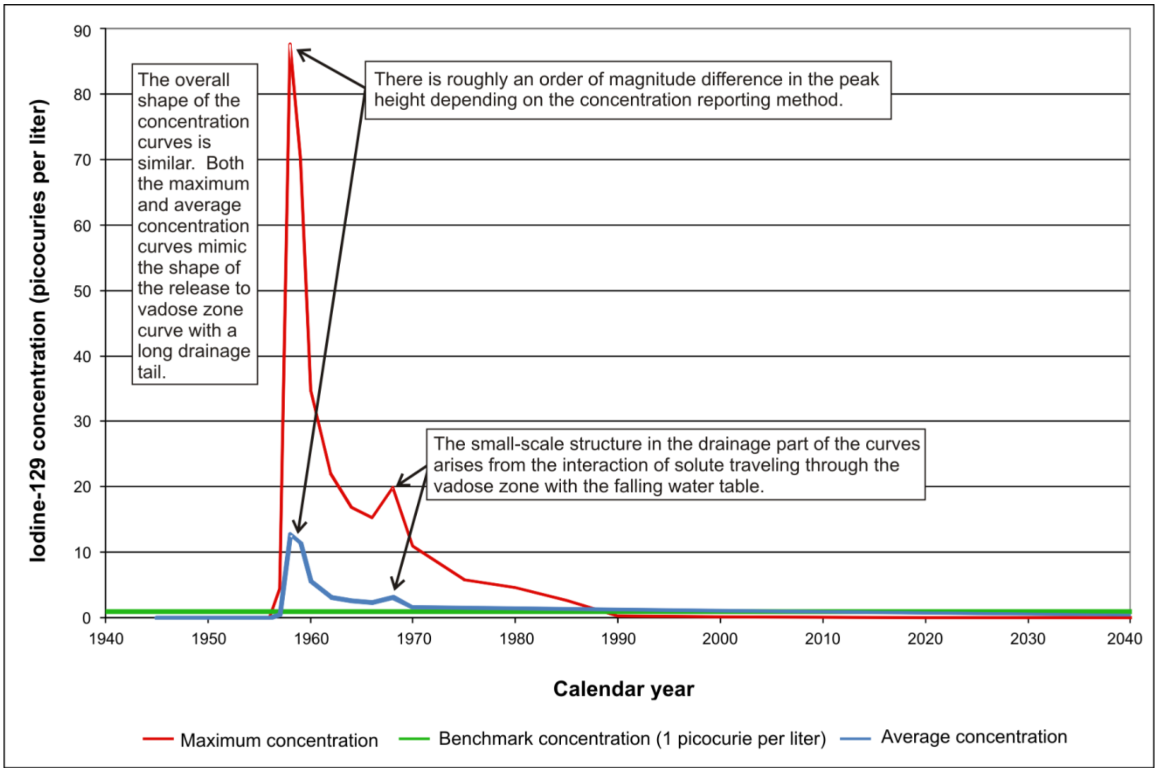

Figure 3. TY Cribs Iodine-129 Groundwater Concentration Versus Time

Evaluation

The following is a list of strengths and weaknesses that should be considered in conjunction with the programmatic objectives to determine if the circumstances of the project warrant the additional complexity of a combined vadose zone/saturated zone model.

Strengths of combined model

- Local scale results that are less influenced by spatial averaging
- File handing\management and concerns associated with configuration control are eliminated when a combined model is used because intermediate files are not needed.
- In cases where the water table is fluctuating because of influences outside of the model domain, the combined model allows direct consideration of that fluctuation.
- The vertical distribution of contaminants across and into the water table can be directly investigated from model output.
- The combined approach allows an integrated mass balance check for the transport calculation from the point of contaminant introduction to the point where contaminant leaves the model domain.

Weaknesses

- The grids are inherently more complex and take additional labor to develop.
- For a given site and horizontal resolution, the combined model tends to have more vertical nodes and consequently requires more computational resources.

- Depending upon the availability of data and complexity of the behavior of the water table, the calibration process for the combined model can require more computational and labor resources. The computational time increase is proportion to the number of nodes to the fourth power. In certain cases, the combined model is more computationally intensive than the separate vadose zone and saturated zone models.

CONCLUSIONS

Based on the considerations listed above, the additional complexities provide benefits from the resulting model simulations for studies with few source areas and sufficient water table elevation and gradient field data. The user can see the direct effect of the rise and fall of the water table on a single source or a small subset of sources using the combined approach. A combined approach is not effective for studies with large number of source areas or a regional-scale domain because the strengths of the combined model are best geared toward local-scale analyses. In cases where the rise and fall of the water table occurs at the same time as the solute in vadose zone approaches the saturated zone, the combined model approach can be used to investigate interactions that are precluded by the separation of the models. However, if concentrations are reported at the same scale, in most cases results from the separated approach and the combined approach are the same, and the additional investments in labor and resources associated with developing the combined models do not yield returns in model stability, efficiency, or accuracy.

REFERENCES

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