MODELING AND SIMULATION OF LONG-TERM PERFORMANCE OF NEAR-SURFACE BARRIERS

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ABSTRACT

Society has and will continue to generate hazardous wastes whose risks must be managed. For exceptionally toxic, long-lived, and feared waste, the solution is deep burial, e.g., deep geological disposal at Yucca Mtn. For some waste, recycle or destruction/treatment is possible. The alternative for other wastes is storage at or near the ground level (in someone’s back yard); most of these storage sites include a surface barrier (cap) to prevent migration of the waste due to infiltration of surface water. The design lifespan for such barriers ranges from 30 to 1000 years, depending on hazard and regulations. In light of historical performance, society needs a better basis for predicting barrier performance over long time periods and tools for optimizing maintenance of barriers while in service. We believe that, as in other industries, better understanding of the dynamics of barrier system degradation will enable improved barriers (cheaper, longer-lived, simpler, easier to maintain) and improved maintenance. We are focusing our research on earthen caps, especially those with evapo-transpiration and capillary breaks.

Typical cap assessments treat the barrier’s structure as static prior to some defined lifetime. Environmental boundary conditions such as precipitation and temperature are treated as time dependent. However, other key elements of the barrier system are regarded as constant, including engineered inputs (e.g., fire management strategy, irrigation, vegetation control), surface ecology (critical to assessment of plant transpiration), capillary break interface, material properties, surface erosion rate, etc. Further, to be conservative, only harmful processes are typically considered. A more holistic examination of both harmful and beneficial processes will provide more realistic pre-service prediction and in-service assessment of performance as well as provide designers a tool to encourage beneficial processes while discouraging harmful processes.

Thus, the INEEL started a new project on long-term barrier integrity in April 2002 that aims to catalyze a Barrier Improvement Cycle (iterative learning and application) and thus enable Remediation System Performance Management (doing the right maintenance neither too early nor too late, prior to system-level failure). This paper describes our computer simulation approach for better understanding the relationships and dynamics between the various components and management decisions in a cap. The simulation is designed to clarify the complex relationships between the various components within the cap system and the various management practices that affect the barrier performance. We have also conceptualized a time-dependent 3-D simulation with rigorous solution to unsaturated flow physics with complex surface boundary conditions.

INTRODUCTION

The Department of Energy (DOE) and the world face tough challenges in assuring that contaminated materials are isolated and that risks to humans and the environment are as low as achievable, over long time periods. Removal and treatment of wastes at many contaminated sites is technically difficult, expensive, and hazardous, exposing workers and the environment to chemical and radiological contamination. Alternative approaches that incorporate “robust containment and stabilization technologies will be a key factor in the success of DOE’s strategy to manage subsurface contamination… DOE’s management commitment potentially extends for many thousands of years.”(1)

The National Research Council reviewed barrier technologies for containment of contaminants (2) in 1997 and concluded “barriers such as surface caps and subsurface vertical and horizontal barriers will be needed as important components of remediation strategies.” One of the issues they identified was the need for better knowledge to predict lifetimes of selected barrier materials and resultant barrier systems.

More recently, the Nuclear Regulatory Commission staff has stated that longevity assumptions in current barrier performance assessments “have no basis in the scientific and technical literature and experience.”(3)
The Environmental Protection Agency has studied barriers (4, 5) and concluded that data from barriers in service is often not adequate to know if the barrier is providing adequate protection; worse, rarely is there information on the internal condition of the barrier. A 1998 EPA study found groundwater contamination at 146 of 163 landfills.(4) RCRA and CERCLA caps are often designed for 30-year lifetimes, yet often the hazards will remain toxic. On what basis will cap lifetimes be extended or barriers be upgraded?

As a final example, analysts were recently forced by regulators/stakeholders into estimating time-dependent degradation.(6) A detailed study was been conducted on a proposed cap involving multiple layers of soil, a polyethylene geomembrane (1.5-mm/60-mil thick high density polyethylene HDPE membrane), a GCL (6-mm/0.25-inch), and compacted clay layer (910-mm/36-inch). They compiled information on the effects of ion exchange, wet/dry cycles, and freeze/thaw cycles. The evaluation allowed them to estimate “time-dependent, degraded hydraulic parameters” for each layer. They then estimated hydrologic behavior using Giroud’s leakage equations (7) and HELP. Giroud’s equations estimate the rate of water flow through the geomembrane/GCL barrier system from cracks, including both circular-shaped defects and infinitely long cracks (e.g. environmental stress cracks). HELP under predicted water flux through the 500-year simulation. “Results of this case study indicate that when projecting the potential long-term hydraulic performance of engineered multi-layer soil/geosynthetic caps, all of the following factors should be considered: 1) the effects of geomembrane aging and other degradation changes on long-term geomembrane hydraulic barrier efficiency; 2) the effects of progressive changes in the hydraulic properties of the various other cap layers (e.g., lateral drainage layer, GCL, etc.) on hydraulic performance; and 3) the effects of changes in hydraulic head buildup on the geomembrane component of the cap on leakage rate.”(6) We suspect that more such studies will be required; tools are needed to examine self-consistent time-dependent degradation of caps.

The barrier analytical models have focused on hydrologic models with limited evaluation of other mechanisms of contaminant transport and barrier changes over time. These hydrologic models are necessary but not sufficient to realistically estimate long-term barrier system performance and to understand how best to manage caps that have to serve for hundreds of years. We have not found a model that defines failure and associated processes and events controlling the aging of barrier systems, barrier components and materials, and resulting mobilization and transport of contaminants.

Although environmental boundary conditions (precipitation, temperature) are varied; generally other key elements of the barrier system are considered constant, including engineered inputs (e.g., fire management strategy, irrigation, vegetation control), surface ecology (critical to assessment of plant transpiration), capillary barrier interface, surface erosion, etc. However, a fully dynamic, time-dependent, multi-dimensional, interactive, simulation is necessary to:

- increase the realism in long-term performance estimation,
- provide a basis for comparing trends observed in service to those in prediction,
- optimize the behavior of barrier systems, and
- suggest the most important indicators of degradation prior to failure.

This type of need is further supported by the fact that the Nuclear Regulatory Commission has sponsored the development of a multi-dimensional, self-consistent computer simulation, 4SIGHT, for reinforced concrete barriers.(8). This code can estimate performance for reinforced concrete barriers, such as vaults considered for low-level waste storage with 500-year lifetime. The simulation includes a wide range of harmful degradation processes.

For earthen caps, computer models that come the closest to a full dynamic simulation of earthen caps are Hydrus-2D,(9) VADOSE/W,(10) SWIM,(11, 12) and EDYS (13, 14). However, as powerful and useful as they are, each lacks some components we believe necessary for a realistic simulation of evapo-transpiration/capillary break caps.

- Generally, only harmful processes are considered. A more holistic examination of both harmful and positive processes will provide a more realistic assessment of performance as well as provide a tool to examine how to encourage beneficial processes while discouraging harmful processes. For example, designers typically insert a bio-intrusion layer to block the harmful impacts (macro pores) of plant roots reaching a capillary interface and prevent animals from burrowing. However, data indicate that roots also have a beneficial impact in withdrawing moisture from deeper in the cap and burrows can increase evaporation. If the beneficial impact can be shown to compensate - and/or total system performance is adequate - it may be optimal to simplify the cap by eliminating the bio-intrusion layer.
None of the models consider degradation of neither a capillary interface nor changing material properties.

The 2-dimensional HYDRUS-2D finite-element model simulates movement of water, heat, and multiple solutes in saturated media such as the vadose zone, includes infiltration, soil moisture storage, evaporation, plant water uptake, and groundwater recharge. However, potential evapo-transpiration must be calculated external to the code and is therefore not time-dependent. Structural changes such as ecological components (e.g. ecological changes to evapo-transpiration) or capillary break are not included. Neither is treatment of snowmelt. And, “The program numerically solves the Richards' equation for saturated/unsaturated water flow and the Fickian-based advection dispersion equations for heat and solute transport.”(9) Yet, under some conditions (see below), a more complete hydrologic treatment may be appropriate.

The 2-dimensional VADOSE/W has two features in addition to those in HYDRUS. It incorporates snowmelt and soil freezing models. And, output from a VADOSE/W analysis can be imported into companion software to provide additional analysis: SLOPE/W for slope stability, SEEP/W for seepage, CTRAN/W for contaminant transport, SIGMA/W for stress and deformation, TEMP/W for geothermal analysis, and QUAKE/W for dynamic earthquake analysis.

The 1-dimensional SWIMv2 (Soil Water Infiltration and Movement model version 2) is a mechanistically based model addressing soil water and solute balance issues associated with both production and the environmental consequences of production. It is comparable to UNSAT-H. The model allows up to four vegetation types that help analyze issues associated with single crops, intercropping or mixed species (trees and grasses). Users must input time functions for potential evaporation for each vegetation type and root density distributions. SWIM is not a cap code per se, but offers incorporates features relevant to earthen caps.

The EDYS code is also not a “cap” code per se, but rather is a powerful ecological simulation tool. It is a critical component for evapo-transpiration caps. It does not accurate simulate the physics of unsaturated flow. “Because EDYS uses essentially all ecosystem components and processes at multiple spatial and temporal scales, complex ecological effects of almost any type of stressor can be addressed with suitable definition of parameters and calibration.”(14)

While each of these codes (and others not mentioned) is quite useful for various applications, none fully address the issues of modeling and analyzing the performance of earthen barrier caps. To assist the barrier community toward development of a fully dynamic simulation of a cap by a single model or suite of models, we are exploring two complementary additional areas in this study:

- Time-dependent 1-dimensional flexible system dynamic simulation of evapo-transpiration/capillary breaks focusing on exploring processes that may change barrier structure.
- Time-dependent 3-dimensional model with rigorous solution to unsaturated/saturated and free surface flow physics with complex surface boundary conditions. The goal of this model development is a simulation code that would be valid in both porous media and non-porous media flow regimes. The model could accurately simulate flow in macro pores and the interchange between fracture/fracture and the porous matrix, as, for example, may occur in earthen caps as fractures/fractures penetrate the cap.

The results from these models will be compared with real data, especially those from the Protective Cap/Biobarrier Experiment (PCBE) at the INEEL(15) and data generated by the larger INEEL project on long-term barrier integrity (16) of which this particular paper is only a part. The full project aims to catalyze a Barrier Improvement Cycle and thus enable Remediation System Performance Management. The Barrier Improvement Cycle is envisioned to iterate among the components to provide improved performance predictions, designs with more robust dynamics, and maintenance neither too late nor too early:

- Field data specifically looking at microbial behavior, which is central to ecology.
- Tests at multiple physical scales to bridge the gap between field and benchtop tests. This meso-scale regime allows examination of coupling among effects, control of those effects, and sometimes acceleration of effects.
- Dynamic modeling of barrier degradation processes - building on existing hydrological models that assume the barrier structure is static (weather inputs are dynamic).
- Selected exploration of new, non-invasive monitoring techniques that may lead to field deployment. (They also help diagnose tests within the project.)
- Integration of the above parts.

These efforts, combined with other past and current work, will improve understanding of what constitutes degradation leading to failure, improve experimental capabilities of understanding of long-term degradation processes, establish a dynamic model of long-term degradation, and suggest improved ways to monitor degradation
prior to failure. The project complements other programs’ emphasis on field and bench top studies by emphasizing (a) testing at intermediate scales - the “meso-scale” - where coupling of effects can be observed and sometimes accelerated and (b) modeling of dynamic processes. The improvement cycle itself enables Remediation System Performance Management.

WHAT WE NEED: REMEDIATION SYSTEM PERFORMANCE MANAGEMENT

Most environmental remediation problems are multi-faceted and require multi-component solutions. For example, closure of even simple landfills requires design and construction of caps, liners, leachate collection systems, and monitoring systems. Remediation of more complicated contaminated sites can also require design and construction of “pump and treat” systems, vapor vacuum extraction systems, and various in situ and ex situ treatment and disposal operations. The components of a remedial system must work together to protect human health and the environment, so analysis of remedial actions must focus on the system as a whole rather than a single component.

We need remediation system performance management,(16) with the following elements:

- Determine how remedial systems will degrade and eventually fail. For our purposes, system failure occurs only if/when regulatory dose limits are exceeded.
- Identify the indicators of degradation.
- Designing a monitoring system that is guaranteed to detect the degradation indicators.
- Incorporating positive feedback loops that will allow systems to self-heal to the maximum extent possible, i.e., beneficial dynamic processes compensate for harmful processes to the extent possible.

This project is working toward such an integrated system. However, we caution that this project does not have the objective (nor resources) to substantially increase data monitoring, collection, and analysis of field data for the hundreds of caps already in service. However, we see this project as encouraging and enabling such a development.

GETTING THERE: UNDERSTANDING DYNAMIC PROCESSES

We define “failure” only for the total protective system, namely not meeting regulatory/societal exposure limits. Individual parts of the system can, and do, degrade but the system has not failed as long as the total system performance is acceptable. Standard engineering practice is to allocate various functions and performance requirements to system components. In service, components may perform better or worse than expected. If it is possible to observe (and validate) better than expected performance in one part of the system, that can compensate for worse-than expected performance elsewhere. In-service observations and understanding of the beneficial and harmful dynamic processes are required to know what maintenance to perform and when - neither too late nor too early - and treating the right problems.

We start by defining some terminology, with the following relationships:

Stressors → Mechanisms → Effects → Consequences to barrier → Consequences to overall protection system

Stressors are inputs or boundary conditions that influence the performance of the system. They can be either natural or engineered. Typical categories include fluid (water, wind, upward gas), temperature (incl. fire), mechanical, biochemical, and radiation (UV, ionizing).

Mechanisms are the ways that stressors can influence the system. A total system performance assessment must consider all possible mechanisms for relative importance (short and long term) to the system on the basis of experience and models. For potentially important mechanisms, need empirical or “first principle” models that allow estimation of effects.

Effects are how elements of the system respond to stressors via one or more mechanisms. Effects can feedback to the influence the existence or importance of mechanisms. Effects can be grouped by categories of system characteristics or elements (state variables): hydrology, structure, and biological.
**Consequences** are the *outputs*, i.e., how the performance of the system is changed by the accumulation of effects. Consequence performance metrics can be specific to the barrier system (e.g. water getting through a surface barrier) or the entire protective system (e.g. health effects to humans). The latter requires assessment of non-barrier aspects (e.g. institutional controls, atmospheric transport, vadose zone, saturated zone) to determine *exposure* and then estimation of *health effects* from the estimated exposure.

To facilitate further discussion, we further define:

**State variables** are the important variables or characteristics that describe the condition of the system. Categories include hydrology, structure, and biological.

**Observables** are those variables (stressors, mechanisms, effects, consequences, state variables) that can be observed in the field.

**Indicators** are the subset of observables that provide valuable information on the changes in state variables.

Fig.1 shows a generic surface barrier conceptual dynamic model that illustrates how we see the boundary conditions, key categories of state variables, and outputs relate. For simplicity, the only output is downward contaminated flow to the vadose zone and ultimately to groundwater. Some problems involve other key outputs.

![Surface Barrier Conceptual Dynamic Model](image-url)

**Fig. 1. Surface Barrier Conceptual Dynamic Model**

One of the challenges in barrier performance simulation is incorporating various effects, mechanisms, and consequences that operate at different time scales. Consider Table I. As an example, the relevant mechanisms, effects, and consequences to 1-meter of additional water depend on whether that additional water is applied in a single abnormal precipitation event, over 1 year (as supplemental irrigation), a 4-year period of abnormally wet year (which would be about a doubling of normal precipitation at the INEEL), or a 40-year mild climate change (about 10% precipitation increase at the INEEL). Same stressor - water - but totally different system responses.
Table 1. Stressors Exhibit Different Time Scales (a)

<table>
<thead>
<tr>
<th>Stressors</th>
<th>Fluid (water, wind)</th>
<th>Temperature</th>
<th>Mechanics</th>
<th>Biology</th>
<th>Radiation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Normal or routine</td>
<td>Normal daily and seasonal wet/dry cycles from precipitation and snowmelt</td>
<td>Normal daily and seasonal temperature cycles</td>
<td>Normal loads and shaking</td>
<td>Normal ecological processes</td>
<td>Normal exposure to UV and ionizing radiation</td>
</tr>
<tr>
<td>Short-term (&lt;&lt; 1 year)</td>
<td>Flood</td>
<td>Fire, prescribed burns</td>
<td>Seismic</td>
<td>Engineered changes, e.g., introduce new species</td>
<td></td>
</tr>
<tr>
<td>(~years)</td>
<td>1 or more wet (or dry) years; prescribed irrigation</td>
<td>1 or more cold (or hot) years</td>
<td>Seismic</td>
<td>Invading species; ecological changes due to climate change</td>
<td></td>
</tr>
<tr>
<td>(&gt;&gt; years)</td>
<td>Climate change</td>
<td>Climate change</td>
<td>Settling, subsidence</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

a. Not all feedbacks are shown, e.g., ecological change leading to difference in vegetation mix leading to changes in erosion resistance.

Another key challenge is that only some of the elements implied in fig. 1 are readily observable. Worse, component degradation may have to be severe before system degradation is observable. The worst case, which is actually common practice, is to monitor system performance by only checking groundwater contamination. In this case, the system has failed much earlier - or at least seriously degraded - well before contaminants can be detected in groundwater. Earlier indicators of degradation are needed; identification of such indicators requires understanding the dynamics of degradation.

The long-term objective is to develop a suite of models that incorporate stressors and indicators that assess and predict barrier risk as a function of time. The models need to be able to assess uncertainties in a probabilistic sense and provide insights to the value of information, e.g., by reducing the uncertainty in parameter X, we reduce the uncertainty in calculated risk by Y at a future time period Z. Often the nature and amount of uncertainty change with time as the barrier evolves and the relative importance of stressors/effects/indicators therefore changes. This will guide both R&D and operational management of barriers and complement and enhance existing risk/uncertainty analyses.(17, 18)

The next two sections describe our approach and progress toward a preliminary evapo-transpiration/capillary break dynamic model and a full 4-D treatment.

**PRELIMINARY EVAPO-TRANSPIRATION/CAPILLARY BARRIER DYNAMIC MODEL**

We have developed a very flexible system dynamic model to explore the dynamics of barrier performance. The model provides a tool to map out the underlying feedback loop structure of the system and explore the relationships between the various components. This modeling is designed to explore the structure and behavior of the system whereas more sophisticated models are strong tools for exploring sensitivities to parameter uncertainties.

System Dynamics (19) is an analytical approach that examines complex non-linear feedback loop systems through the study of the underlying system structure. A thorough understanding of the structure of these complex systems can lead to an explanation of their performance over time and in response to both internal and external perturbations. By understanding a system's underlying structure, predictions can be made relative to how the system will react to change.

A System Dynamics model is a visual representation of a system. This visualization of the components and connections is one of the assets of this modeling technique. The visual model defines, through a graphical interface,
a series of differential equations that define the behavior of the system over time. For this effort, we have used commercial software packages, STELLA (20) and VENSIM (21). STELLA is somewhat easier and more flexible to use; VENSIM is more numerically powerful. The calculations are performed using numerical integration. Although the interface makes the modeling look superficial and almost trivial, there is a very sophisticated mathematical engine that does the calculations. Using this modeling technique it is possible to model very complicated systems.

System Dynamics models are descriptive in nature. All the elements in the model must correspond to actual entities in the real world. The decision rules in the model must conform to actual practice and real world phenomenon. Thereby, adjusting an element in the model corresponds to a physical change in the real system. The purpose of the model is threefold: 1) A visual diagram of the system from which to engage discussions on the various elements of the model and elicit input from interested parties; 2) To gain insights into the dynamics of the movement of moisture in the soil and to identify core structure of the system; and 3) To develop a tool for the analysis of long-term performance.

System Dynamic models are based on four basic components, stocks, flows, constants/auxiliaries and connectors.

The **stocks**, \( \square \), accumulate quantities of material, in this case, moisture. The **flows**, \( \rightarrow \), physically change the quantities of the stocks. The direction of the arrow defines whether it is an inflow into the stock or an outflow from the stock. Inflows would include precipitation, irrigation and run-on. Outflows would include runoff, deep drainage, evaporation and transpiration. **Auxiliaries/Constants**, \( \bullet \), contain information that feeds into the stocks or flows. The **Connectors**, \( \rightarrow \), symbolize a relationship between two elements in the model and the direction of the arrow indicates the direction of the influence.

Our first illustrative barrier model is a simple soil cap with a vegetative cover and underlying capillary break. The model tracks the soil moisture content in the cap as well as deep drainage into the waste level. The change in moisture in the cap layer is dependent on the inflow of moisture from precipitation, run-on and irrigation, field capacity of the soil, current moisture level of the soil, and extraction from evapo-transpiration and deep drainage.

The model precision depends on the exactness of the data and equations used to simulate the physical phenomena as well as the ability to capture the relationships that are important to the behavior of the system. The basic model provides a focal point to begin to discuss the physical components (inflows, outflows, evapo-transpiration, etc.) and how they are connected. Our initial model has the following characteristics:

- Time-dependent precipitation (rain, snow) based on historical data from southeastern Idaho.
- Runoff based on slope and amount of precipitation.
- Evapo-transpiration is estimated using the FAO Penman-Monteith equations. Transpiration is governed by root density. The higher the root density, the more transpiration occurs up to the point where the soil moisture reaches the lower limit of extraction; whereby transpiration from that zone ceases to occur. The root density will increase if there is sufficient moisture in the soil to sustain the current amount of plant life. If the moisture levels drop below the necessary amount to sustain the current amount of plants, then there is a decrease of plant root density and thus a lower capacity to remove moisture from the soil. The FAO Penman-Monteith equations estimate the potential evapo-transpiration that could occur based on available sunlight, temperature, elevation, humidity, longitude and crop type. The potential evapo-transpiration is used with plant available water and soil type to estimate actual evapo-transpiration.
- The storage level is split into 10 layers/nodes for tracking the water down and up through the storage layer. The layers or nodes can have the same soil properties or can be varied if the cap has non-uniform layers.
- Downward movement of moisture through the soil is governed using the Green-Ampt equation.
- Capillary rise or wicking moves moisture from the wetter lower layers back up towards the surface as the surfaces areas dry through evaporation and transpiration. The capillary effect is affected by soil type, moisture content and height to surface. The model will use the unsaturated Darcy flow where total potential is capillary less gravity.
- Hypothesized capillary break interface degradation due to freeze/thaw, wet/dry, etc.
The following two sub-sections go into more detail on the evapo-transpiration and capillary break portions of the full model.

**Evapo-Transpiration Sub-Model**

An ET cap offers the potential to promote beneficial feedback dynamics and discourage detrimental feedback dynamics if we can identify, credibly model, and promote the important dynamic processes. Most of these are ecological – discourage plants (and animals) from doing detrimental things (intrusion); encourage evapo-transpiration from plants, and encourage stability of plant cover against perturbations (fire, drought, excessive precipitation, climate change, etc.)

It is possible that such a cap could have extremely long term functionality, only limited by water and wind erosion of the site by providing sufficient robustness against the other stressors and effects. The performance assessment system has to check the system’s stability against various perturbations; otherwise, cumulative effects will degrade the barrier. Different perturbations have different response times, for example:

- **Fires** are a natural part of most ecosystems; how fast does vegetation re-establish? Does the same vegetation mix re-establish in the absence of active maintenance or is intervention required? As the post-fire ecosystem evolves, does the barrier provide adequate storage and protection each year?
- **Droughts** are natural. During the drought, there is less stress on the barrier, but as the climate returns to “normal”, does vegetation re-establish soon enough so that the storage capacity of the barrier is not exceeded? As the post-drought ecosystem evolves, does the barrier provide adequate storage and protection?
- **Abnormally high precipitation** (relative to average) is natural. The natural ecosystem will respond to increased precipitation. The details of the response depend on whether the increased rainfall is for a month, an entire season, multiple years, etc. Basically, the ecosystem will take advantage of the increased precipitation.
- **If climate slowly changes** will barrier’s response to the net effect of precipitation, temperature, ecosystem changes continue to provide protection? These perturbations are similar to wet/dry year, except they continue for longer periods with more time for ecosystem responses.

The timing of the processes is critical to cap performance and subsequent failure. At semi-arid cold sites like the INEEL, precipitation typically exceeds evaporation for most of the year. Thus, ET caps must be able to remove sufficient moisture during the few hot months via evapo-transpiration to balance precipitation; they must have storage capacity (soil depth) to avoid water breakthrough into the waste at the transition between precipitation and hot months (spring after snow melt). The yearly dynamic is further complicated by the fact that infiltration into the soil is relatively rapid in the hot months and negligible during snow season. “Snow accumulation from numerous precipitation events can result in a significantly greater amount of infiltrating water when thawing occurs than individual precipitation events may indicate. Evaporation and transpiration during and immediately following periods of thaw are likely to be low, thus putting greater stress on the barrier system than during summer or fall.”

The depth of the topsoil layer is essentially a buffer against perturbations. “In semiarid or arid regions, the mostly likely cause of such failures is simply an inadequate depth of soil.” At the INEEL, about 1.8-2.0 meter of soil is needed to store precipitation during “exceptionally wet years” and have “sufficient moisture storage capacity to sustain a healthy stand of perennial plants.” For long-term performance prediction, one must know not just whether precipitation increases or decreases (yearly fluctuations, climate change) but *when* during the year.

Consider the increased precipitation case further. A brute force design approach is for regulators to stipulate that a barrier has to withstand say 3x normal rainfall for a given number of years and then add storage capacity (soil depth) accordingly. This begs the question of how much increased rainfall for how many years. The further out in time one is trying to estimate performance, the less certain such numbers will be.

A more dynamic approach is to consider how the ET cap would respond over months and years - with more moisture available there would be more vegetation to take advantage of the increased moisture. The more vegetation responds to the increased moisture, the less additional storage capacity has to be added to the design. (One would have to check the severity of a fire – and subsequent ecosystem response - that might occur at a time of increased vegetation.)
For example, at Hanford, it has been hypothesized and studied that wetter climate, trees and other deeper-rooted plants could invade to take advantage of the increased moisture. They should have the beneficial impact of increasing ET, but a possible negative impact of deeper roots stressing the capillary barrier.(25)

The INEEL Protective Cap/Biobarrier Experiment (PCBE) provides 8 years of data on how ET caps behave in a relatively cold, semi-arid environment. Its objectives “are to examine the effects of placing an intrusion barrier in a soil cap on water infiltration, water storage capacity, and plant rooting depths and to determine which species of plants, if any, will grow roots through an intrusion barrier and extract water from the soil below it (which would be necessary if the intrusion barrier were placed at a shallow soil depth).”(24) This experiment was started in 1993 and a major report has recently been released (15). We are using these data to develop and calibrate the model.

Fig 2. illustrates key features of our evapo-transpiration sub-model. Starting on the left of the diagram, we note that inflows to the cap include:

- Surface run-on
- Precipitation
- Irrigation

Currently, all precipitation and irrigation is assumed to move into the top layer of the cap.

Fig. 2. Illustration of part of the evapo-transpiration sub-model (Portions of the model in green are sometimes included dynamically in current hydrological models, black portions are included but only statically, red portions are generally not included.)

Similarly, on the right of the diagram, we note a primary outflow, surface run-off. The model has a runoff component based on the slope and amount of precipitation. The current model has a slope component that can be adjusted, but for current analysis the slope is set at zero.
At the top of the diagram is evapo-transpiration, which is governed by the root density component of the model. The higher the root density and plant biomass, the more transpiration occurs up to the point where the soil moisture reaches the lower limit of extraction, whereas transpiration from that zone ceases to occur. The root density will increase if there is sufficient moisture in the soil to sustain the current amount of plant life. If the moisture levels drop below the necessary amount to sustain the current amount of plants, then there is a decrease of plant root density and thus a lower ability to remove moisture from the soil.

At the bottom of the diagram are upward and downward flows deeper into the cap. The capillarity effect (wicking) would move moisture from the wetter lower layers back up towards the surface as the surface areas are dried by evaporation and transpiration. The capillary effect is affected by soil type, moisture content and height to draw soil back up.

The model keeps track of current moisture content in each of the different layers as well as total drainage from the bottom of the cap into the waste zone. Graphs are used to display the moisture levels throughout the simulation period. The user can track the inflow of moisture and see the effects on the moisture content in the various layers and see the effect of the drying cycle through the evapo-transpiration process.

The system operates on a system of feedback loops. For example, fig. 2, illustrates both beneficial and harmful effects from animal burrows. In the upper right we include the beneficial effect that animal burrows have been shown to have to increase evaporation. “During the summer months, more water is lost from plots with animal burrows than from plots where no animal burrows are present. During the winter months, both the animal burrows plots and the control plots gain water. In addition, water does not infiltrate below ~1 m, even though burrow depths always exceed ~1.2 m. The lack of significant water infiltration at depth and the overall water loss in the lysimeter plots is occurring despite the following worst-case conditions: 1) No vegetative cover (no water loss through transpiration), 2) no water runoff (all incipient precipitation is contained), 3) The burrow densities in the lysimeters are greater than the burrow densities found in “natural” settings, 4) Extreme rainfall events are applied frequently (three 100-year storm events in 3 months), and 5) Animals burrow deeper in the lysimeters than in “natural” settings. … “The overall water loss from soils with small-small burrows appears to be enhanced by a combination of soil turnover and subsequent drying, ventilation effects from open burrows, and high ambient temperatures.”(26)

Thus, in this case, animal intrusion had a net positive effect. Indeed, earlier Hanford work shows that soils were dryer beneath burrows than elsewhere.(25, 27) Link reports that the increased moisture in burrows facilitated vegetation response that increased plant transpiration as plants took advantage of the moisture, sent roots to use it, leading to dry zones under the burrows. “Ecologically, it is expected that a local abundance of a limiting resource, in this case soil moisture, would be rapidly used and therefore depleted.”(25)

To further increase the challenge, note that the different effects can occur at different time scales. And, the ability to test individual effects differs at different physical scales. One needs, for example, a certain minimum scale to investigate animal and plant intrusion. On the other hand, the expense increases and practicality decreases for testing of shaking and subsidence effects at larger and larger scales. Thus, a complete understanding would seem to require tests at different physical scales and conditions, especially if we want to understand long-term phenomena at times shorter than service life - and then combining the mechanistic understanding in a computer code (or codes).

In the bottom right we include the harmful effect of burrows on percolation, namely increased downward water movement due the presence of holes in the cap.

Another feedback in the model (not shown in the figure to preserve readability) relates to excess soil moisture above transpiration capacity. Excess moisture in the soil causes an increase in plant growth thus plant root density which in turn increases transpiration which reduces the excess moisture in the soil until the two elements (transpiration, moisture) are in equilibrium. The amount of moisture the soil will be able to hold will depend on the type of soil and the depth of the cap. Both of these parameters will be adjustable to test the performance levels of different soils as well as cap depth. In addition, different plant species have different transpiration rates and capacities and will affect the performance of the cap. The model will allow for the user to select the variety of plants on the cap. In addition, some plants will send roots down very deep where others will keep their roots relatively close to the surface. This difference would change the performance of the ET component in terms of transpiration performance as well as rooting into waste zone.
Another set of feedbacks that are only partially in the model relate to vegetation response against various perturbations. ET caps require a stable mix of plants that uses as much water as possible (at least as much as assumed in the design). “Stability” has to be judged against various perturbations. If plant mix evolves toward plants that use less water, the cap may not function adequately.

- Soil depth must be sufficient to provide for stable and health vegetative cover and adequate storage for “wet” years.
- Plants have to re-establish after drought.
- Plants have to re-establish after fire. The fire concern is highest late in the growing season when soil moisture is low, above ground vegetation is maximum and become dormant (Fig. 3). “If vegetation on an ET cap includes a diverse mix of species and life forms, including healthy populations of perennial grasses, cover on the cap can be expected to recover to pre-fire levels within two growing seasons (S. Buckwalter and J. Anderson, unpublished data). It is likely that there would be sufficient cover in the first post-fire season to use most of the precipitation received, but additional research is recommended to confirm this.”(15)

Accordingly, we are currently formulating models for soil erosion, plant regrowth after a fire, plant and animal intrusion, GCL degradation, etc. Rate parameters and submodels will be adjusted as additional experimental data becomes available.

Fig. 3. The sequence of graphs illustrates the effects of fire on an ET cap. The vegetation on the ET cap develops until it reaches equilibrium. Equilibrium is established when the amount of transpiration from the vegetation matches the amount of moisture available in the cap. The effect of a fire is to decrease the amount of vegetation thereby decreasing the amount of transpiration, which then increases the amount of moisture in the cap. The cap recovers but it takes time. The time scales and magnitudes of moisture and biomass depend on the ecological and environmental conditions of the local area.

Capillary Break Sub-Model

Fig. 4 illustrates part of the capillary interface sub-model. A capillary barrier (or the capillary portion of a multi-layer barrier such as an ET-capillary cap) uses the change in hydraulic conductivity between an upper layer of fine material and a lower layer of coarse material to increase water storage capacity and inhibit downward water movement. The performance of such a barrier depends on maintaining a sharp gradient at the interface. Some capillary barriers also include slopping of the barrier to promote lateral flow in the fine layer to further inhibit downward water movement.

Fig 4 contains two stocks. One is the soil moisture in the layer just above the capillary interface; the other is a simplified attribute, “capillary interface effectiveness.” The figure shows several of the factors that could degrade the effectiveness of the barrier; note that “effectiveness” only flows outward. That is, the model has no provision for processes that could improve the interface effectiveness. (Were such processes to be observed or hypothesized, they could be easily added to the model.)

There are limited data regarding interface degradation processes acting individually and no known data regarding any coupling or synergistic interactions. For example, consider a class of scenarios that start with one or more of the
following effects that increase the amount of moisture getting into the coarse layer: excessive rainfall/snowmelt, animal/plant intrusion, mechanical effects, and microbial effects on capillaries. Normally, plants have no incentive to send roots into the coarse layer because it is dry; similarly, there should be little moisture to foster microbe communities. (This stimulates the question of how much moisture for how long a time?) If roots impact the capillary layers, the barrier could be subject to a cascading or propagating failure. Similarly, water breaking through the capillary interface can carry fines into the coarse zone, weakening the interface. The processes and the coupling of these processes must be understood to have confidence in the long-term robustness of capillary barriers. The model provides a way to conceptualize relationships; data from the rest of the project will clarify the relationships and underlying processes.

At the top is the effect of freeze-thaw cycles. We hypothesize that freeze-thaw cycles and associated expansion/contraction can promote migration of fines into coarse, degrading the interface. Similarly, when GCLs are used at the interface, freeze-thaw cycles over decades may slowly degrade performance.
Below freeze-thaw is wet-dry. The recovery of capillary barriers following abnormally high precipitation has been (and is being) studied at the INEEL Engineered Barrier Test Facility (EBTF). The facility has 10 cells, each with concrete walls and floor and measuring 3.05-m wide, by 3.05-m long by 3.05-m deep. The top is open to the atmosphere. An access trench runs between the cells and houses instrumentation and data acquisition systems.

Throughout a previous two-year experiment, vegetation was prohibited to maximize the effect of increased (simulated) precipitation. Thus, the water loss from the surface was only via evaporation, not transpiration. Replicates of both a capillary barrier and a thick soil cover were irrigated in 1997 to induce breakthrough of water to the bottom of the cells. The objective was to study the dynamics of recovery. The dominant water infiltration both years was snowmelt in March. The thick soil design also showed additional infiltration during short-term rain periods in 1998 (May, 11 days, 43.7-mm water) and FY1999 (June, 10 days, 49.5-mm water). The capillary barrier recovered faster, partially in year-1 and almost completely in year-2. The capillary barrier stored more water in the upper portion of the cap. “Within two years of intentionally induced breakthrough, evaporation alone (without transpiration) restored the capability of the capillary barrier covers to function as intended, although water storage in these covers remained at elevated levels.” Thus, the capillary barrier can recover from abnormally wet conditions leading to breakthrough. However, the study showed that there could be significant delay in stopping water breakthrough (1-2 years in this case) and a residual effect of increased water content in the “fine” layer of the barrier, which would presumably return to “normal” in another year or two. These response times would be expected to be faster with vegetated capillary caps because of the increased water removal via transpiration.

What about repeated cycles? Stormont conducted column experiments with silty sand (25% fines) and clay (85% fines). “The silty sand apparently has enough cohesion for it to bridge over the voids of the coarse layer and remain stable. The clay was initially stable, but eventually failed. The clay would crack during drying, and progressively erode during rewetting. Eventually, swelling of the clay was not sufficient to prevent a continuous crack to develop.” “These results indicate that conventional criteria are not necessarily applicable to capillary barrier configurations. Further, the stability of the capillary barrier may be jeopardized if the cover is susceptible to large volume changes in response to wetting and drying.”

Below wet-dry in fig 4 is root intrusion. The fear is, of course, that roots can create flow paths that defeat the interface. The classic approach to the problem is to guard against such an occurrence by inserting a bio-intrusion layer. However, what is the likelihood that this occurs, how bad would it be? If we have to guard against it, are there simpler, longer-lasting ways?

Plants will not grow in soils with water content below the “wilting” point. “Because coarse materials drain to low water contents, typically below the wilting point, they can serve as barriers to root penetration. To be effective as a root barrier, fines must be kept out of the coarse layer. This suggests the size of the coarse layer either has to be limited so that overlying fines do not penetration into it, or an intermediate layer has to be used to retain the overlying soil.”

Root channels, animal burrows, and cracking in the fine zone (significantly above the interface) should not compromise a capillary barrier because the storage layer is unsaturated and water is held in the soil matrix - just as a hole cut in a sponge will not cause the sponge to lose its water. Thus, such penetrations that do not approach the interface should not compromise the barrier because the water will eventually be drawn into the soil matrix.

As the penetrations approach the interface, the situation becomes more complex. A partially penetrating hole could provide a water path (e.g. rapid snowmelt, thunderstorm or other large infiltration event) that could cause locally saturated conditions at the interface, causing localized leakage.

If root channels or animal burrows penetrate to the coarse layer and a large infiltration event occurs, water could flow down the pathways (short circuiting the barrier interface) instead of being drawn into the soil matrix or running off the barrier.

Thus, plants and animals have little incentive or ability to get into the coarse zone as long as it stays dry. The coarse zone tends to stay dry as long as intrusion (or penetrations or beyond-design basis precipitation) does not occur. It remains to be shown how much moisture (breakthrough) into the coarse zone, for how long, for how many times creates enough of a perturbation that the system cannot recover and plant and animal intrusion becomes a problem.
On the other hand, roots have observed to have a beneficial effect - remove water.(15) Thus, the model includes both harmful and beneficial effects of plant roots on the capillary interface. As we calibrate the model with data, we will have a tool to explore the interplay between harmful and beneficial effects.

Model Status

This is a simple preliminary model. It does not yet include all the components needed to evaluate the long-term structural integrity of a cap design. It is included here to trigger discussion about the different components already captured in the model as well as the components that are not in the model but should be included. Furthermore, the model, even in this simplistic stage, can test some simple cap designs and give insight as to the complex behavior of ET-capillary Caps.

We are calibrating the model with existing data (15, 23, 29) and data generated from the rest of the larger project.(16)

The model will eventually allow simulations such as the following:
- Time-dependent balance for animal intrusion burrows between harmful open porosity versus beneficial increased evaporation.
- Time-dependent balance for plant intrusion between harmful macropores versus beneficial increased wicking and evapo-transpiration.
- Time-dependent system response as the water storage layer thickness changes due to soil erosion.
- Response to fire - plants providing evapo-transpiration are destroyed, cap is initially less protective, time and water allows plants to reestablish.
- System response to fluctuating precipitation (one or more abnormally wet or dry years will cause plant changes, thereby changing evapo-transpiration; long-term wet or dry periods will cause ecosystem changes).
- Hypothetical long-term capillary break degradation.
- Hypothetical long-term GCL degradation.

4-D HYDROLOGY PERFORMANCE ASSESSMENT MODEL DEVELOPMENT

Here, we look beyond the preceding preliminary dynamic model, toward an all-inclusive dynamic barrier simulation code (or suite of codes) for evaluation long-term performance. The code will be developed using modularity and will potentially incorporate all barrier degradation mechanisms identified as significant.

The approach includes the following: a) survey the available barrier simulation codes; b) survey the “state-of-the-art” computational techniques used in hydrology and other fields such as computational fluid dynamics; c) identify the “state-of-the-art” computational techniques amenable to unsaturated/saturated groundwater flow and contaminant/energy transport simulation in near surface barriers and select a preferred method; d) develop the simulation code using this method in a progressive sequence starting with a one dimensional code and continuing to 2 and 3 dimension; and e) verify, validate, and benchmark the code with analytical models, experimental results, and comparisons with other codes, respectively.

There are currently no multi-dimensional codes available to simulate the full range of physics occurring in barriers. The current codes available for simulating evapo-transpiration and the physics of unsaturated flow (capillarity) are two-dimensional and only valid for flow in a porous media continuum (Darcy flow assumption). The model review identified two 2D models, Vadose-W (10) and Hydrus 2-D (9) that can be used to simulate capillary barriers. There are numerous multi-dimensional models available that rigorously solve the unsaturated flow problem, but they only offer simple surface boundary conditions and do not include atmospheric energy and water transfer at the surface from continually changing atmospheric conditions. Furthermore, the current two-dimensional barrier and multi-dimensional unsaturated flow codes use the Darcy flow assumption, which neglects the convective components in the momentum equations. They neglect the momentum equation altogether and only solve the continuity (mass balance) equation. The validity of Darcy flow is questionable for many subsurface environments such as fractures/macro pores and surface water/subsurface interactions.
Currently, the barrier models for water, energy, and contaminant transport in unsaturated porous media are based on Richard’s equation, which describes unsaturated liquid water flow; Fick's Law, which describes water vapor movement; Fourier's Law, which describes conductive heat flow in the soil profile; the convection-diffusion equation, which describes energy movement with the pore water; and the advection-dispersion equation, which describes contaminant transport in the subsurface.

Alternatively, the conservative form of the Navier-Stokes equations can describe water movement in a porous medium. These equations will reduce to Richard’s Equation when the convective components are neglected. This is the case for most flow in a porous medium because the velocity is very small and inertial forces play a very minor role. The advantage of employing the Navier-Stokes equations is that the code will have a wider range of applicability and could include overland water flow, flow in fractures and macro pores and atmospheric conditions into the computational domain. The main strength of this approach will be barrier simulation code that valid in both porous media and free surface flow regimes.

The governing equations for fluid flow are solved by simulation codes using one of three general methods: 1) Analytical; 2) Finite difference; and 3) Finite element. Analytical techniques use classical mathematical methods to obtain explicit solutions to the partial differential equations and often can only be applied to simplified cases. Finite difference methods replace the partial derivative in the governing equations with a quotient of two finite differences resulting in a series of algebraic equations. Finite element methods use a technique similar to the finite difference method in that the governing equations are reduced to a series of algebraic equations upon discretization. However, the finite element method uses an integral form of the governing equation and use interpolation functions for estimating variable values across discrete elements.

Groundwater simulation codes cannot be used as tools with confidence until they are thoroughly tested. Three types of analysis are being used in testing a newly developed code. These are verification, validation, and benchmarking. Verification is accomplished by comparing simple analytical solutions to those predicted by the simulation code. This verification process has two main objectives. The first objective is to verify that the computational algorithms can accurately solve the governing equations and the second objective is to determine if the code is fully operational and no major programming errors persist. Often the analytical solutions available for comparison exist for very simple problems. Thus, even if the numerical model successfully duplicates the analytical model, the code still may fail in complex “real world” situations. Field experiments can be used to determine how well the code will handle complicated boundaries and soil heterogeneities. However, the data from appropriate field experiment may not be available. In this situation, the code may be bench marked by comparing the results to another code that has already been carefully tested.

Computational fluid dynamics (CFD) from the mechanical engineering discipline has made much progress in developing new numerical techniques in the past few years and groundwater models are often a decade or more behind the current “state-of-the-art.” One very interesting technique used within CFD is adaptive mesh refinement. Adaptive mesh refinement is most useful for physical problems, which have variations in scale. When solving these problems numerically, high grid resolution is needed to adequately solve the equations. However, there are also often large portions of the domain where high levels of refinement are not needed at different simulation times. Using a highly refined mesh over the entire simulation region and over the entire simulation time may represent a waste of computational effort. By locally refining the mesh only where needed at any time during the simulation, adaptive mesh refinement allows concentration of effort where it is needed in local high gradient areas. The progression of an infiltration event into dry soil is an example of a variable scale problem. At the leading edge of the infiltration front, the matric potential gradient is very large and requires a very fine mesh to adequately solve the problem. However between infiltration events, the gradient can be very uniform and a very fine computational mesh is not needed. Furthermore, new computational meshes will be needed if erosion processes have changed material layer thickness.

A new groundwater model employing the conservative form of the Navier-Stokes equations is under development to simulate subsurface and near-surface flows. It would be an “all-phase” model that would be composed of three basic phases: 1) Liquid; 2) Gas; and 3) Solid porous matrix. Multiple components could exist in each of the phases such as water vapor and air in the gaseous phase. The Navier-Stokes equations would govern all three phases. The solid porous matrix can be viewed as an unmovable third phase. However in the solid porous matrix, the Navier-Stokes equations reduce to a thermal energy equation. The proposed model would extend beyond the current
groundwater models by full inclusion of overland water flow and atmospheric conditions into the computational domain. The model will contain the following features.

- Governing equations are multi-phase, multi-component variable density Navier-Stokes equations in multiple spatial dimensions.
- Model will employ the Pressure-Corrected Implicit Continuous Eulerian-Finite Element Method (PCICE-FEM) scheme developed here at the INEEL. This scheme is a semi-implicit, pressure-based algorithm capable of high-order accurate transient and steady-state simulations.
- Reactive physics capable of simulating an arbitrary number of components and phases (liquid and/or vapor reactants).
- Extensive phase change physics for the liquid water-water vapor and air mixture to include evaporation, condensation, and freezing at the free surface and in the solid porous matrix.
- Model capability includes simulating the atmosphere near the free surface to include barometric pressure, temperature, absolute humidity (water vapor-air mixture), and heat flux.
- Full thermal energy resolution in the liquid, gaseous, and solid porous matrix phases to include energy transport due to the fluid mass transport, reactive heat generation, and atmospheric conduction and radiation.
- The model incorporates the Ergun drag model for porous material. Whereas Darcy’s approximation assumes that the pressure gradient is proportional to velocity (permeability coefficient), the Ergun model combines permeability with the nonlinear inertial effects (velocity-based).

SUMMARY

This project will benefit the DOE and the world by improving confidence in existing barriers, providing an improved technical basis for managing existing barriers, and improving the basis for designing and testing new barriers. DOE is quickly driving toward achieving as much cleanup as possible by 2012. At many DOE facilities, caps and barriers will play a major role in cleanup strategies and need to be designed with maximum integrity to minimize future risk. Often the duration of hazards is long. This project will help provide the basis for managing and improving performance of these barriers.

The development of previous analytical models have mostly focused on hydrologic models with limited evaluation of other mechanisms of contaminant transport and changes to the barrier over time. A peer reviewed conceptual model, validated against data, that defines the important features, processes, and events controlling the aging of barrier, their materials, and the transport of contaminants, has not been developed. Therefore, we have initiated a preliminary system dynamic model of evapo-transpiration/capillary break caps. The model is starting to help us envision the dynamics of barrier degradation. Once complete and validated with relevant data, it will improve barrier performance prediction and will guide the experimental portion of the project.

The survey of available barrier simulation codes as part of the 4D modeling activities identified a multi-dimensional code that has recently been released. Some models simulate the interaction of the meteorological conditions, the ground surface, the vadose zone, and the local groundwater regime. However, these models are limited to 2-D and based on Richard’s equation. The Richard’s equation formulation limits the code to only simulating fluid movement in a porous medium only. The modeling literature search revealed a growing trend to model subsurface flows with multi-phase governing hydrodynamic equations because the Darcy assumption's validity is questionable for many flow features in near surface environments. A Darcy formulation is only valid for flow through a porous medium. This formulation is not valid for individual fracture or macro pore scale simulations. Free surface influences, such as the atmosphere or surface water must be simplified and treated as a boundary condition in the Darcy formulation. A groundwater model employing the conservation of mass, momentum, and energy equations would be valid for simulating porous medium and non-porous medium and the interaction between the two domains.

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