Soil-Plant-Atmosphere Numerical Modelling of a Cover System in North-western Australia Utilizing the Moisture Store-and-Release Concept – Simulation of Seven Years of Field Performance Monitoring

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Abstract

An open-cut iron ore mining operation located in the Northern, semi-arid, region of Western Australia has waste rock material within some dumps which contain material considered to be net acid generating. Two cover system field trials, TP1 and TP2, were constructed in July 2003 consisting of a 4 m thick coarser textured run-of-mine (ROM) and a 2 m finer textured ROM, respectively. Performance monitoring of soil temperature, suction and water content within the covers has been collected continuously at the trials since construction. Consequently, a unique set of monitoring data has developed over the seven-year period as the covers evolve from bare-surface to fully vegetated conditions.

Numerical modelling was undertaken to simulate measured field responses at the two field trials. Simulating the measured field responses was challenging due to the numerous variables influencing soil-plant-atmosphere systems. Despite these difficulties, the calibrated models were able to acceptably simulate field responses, with TP1 and TP2 having coefficient of determination (R^2) values of 0.86 and 0.92, respectively, over the period.

This paper describes the methodology used to calibrate the model to accurately simulate measured field responses over the seven-year period. Field performance monitoring data is presented for the two cover system field trials.

Key Words: store and release cover, soil-plant-atmosphere modelling, field response model, model calibration, instantaneous profile method

Introduction

The development and calibration of a soil-plant-atmosphere numerical model capable of simulating measured field responses (referred to hereinafter as a field response model) is a vital component of the cover system design process. Once calibrated, the inputs from a field response model are powerful tools that can be used in performance models to evaluate long-term cover performance for an extensive variety of soil, plant and climate scenarios to aid in finalizing a cover design. However, determining a set of calibrated field response model inputs is a complex and challenging process, requiring much iteration before model results and field measurements converge.

Field response models developed for two cover system field trials located at an open-cut iron ore mining operation in the Northern, semi-arid, region of Western Australia, (referred to hereinafter as the site) provide an excellent example of the calibration process. Closure planning support studies for the operation showed that waste rock material within some dumps is potentially net acid generating. Hence, suitable cover options for the waste rock were investigated and preliminary cover system designs that utilize the moisture store-and-release (S&R) concept were recommended for further investigation. Cover systems that utilize the S&R concept rely on the ability of the cover material to possess sufficient moisture retention such that infiltrating waters are 'stored' within the cover layer, and subsequently 'released' to the atmosphere as evapotranspiration such that net percolation (recharge) to the underlying waste meets design criteria. A key aspect of achieving low net percolation rates is the ability of the cover material to manage high infiltration rates (resulting from intense and long duration rainfall events) through development of a vegetative cover that can utilize (transpire) moisture that has migrated deep into the cover profile.

Two S&R cover system field trials were constructed on site in July 2003 consisting of a 4 m thick coarser textured run-of-mine (ROM) field trial (TP1) and a 2 m finer textured ROM field trial (TP2). The two cover system field trials are immediately adjacent to each other and are designed to accept as much rainfall as possible, while minimizing runoff and associated erosion, with all infiltration remaining within the cover material. An automated Campbell Scientific Inc. (CSI) Model CS700-L tipping bucket rain gauge (with a resolution of 0.2 mm) and a CSI NR-Lite were installed at TP2 to monitor rainfall and net radiation, respectively. The remaining climate parameters required for field performance monitoring (air temperature, relative humidity, wind speed) are measured at the site's primary meteorological station located approximately two kilometers north of the field trials. *In situ* moisture conditions at each field trial are automatically measured by Sentek EnviroSCAN® capacitance water content sensors (indirect measurement of volumetric water content) and thermal conductivity (TC) sensors (indirect measurement of matric suction). One sensor nest was installed at TP1 through to a depth of 400 cm within the cover material while at TP2 one sensor nest was installed throughout the depth of the cover material and into the underlying waste rock to a combined depth of 290 cm. Each sensor nest location consists of thirty-two water content sensors and thirty-two TC sensors. Fully operational sensor locations used for the modelling presented in this paper are shown on Figure 3. Moisture conditions at each field trial are also measured with a Sentek Diviner 2000®, a portable water content sensor, to a depth of 1.6 m. These installations have been monitored continuously since construction of the field trials. As such, a unique set of cover system monitoring data have developed over the seven-year monitoring period as the covers have evolved from bare-surface to fully-vegetated conditions.

This paper describes the methodology used to determine the calibrated field response model inputs used to accurately simulate measured field responses over the seven-year period. Field response modelling results and field performance monitoring data are presented and evaluated for the two cover system field trials. The computer software VADOSE/W 2007 (Geo-Slope International, 2010) was used to complete the modelling presented in this paper.

VADOSE/W is a 2D finite element model (which can also perform 1D simulations) that predicts pressure head (suction) and temperature profiles in the soil profile in response to climatic forcing (such as evaporation) and lower boundary conditions (such as a water table). A key feature of VADOSE/W is the ability of the model to predict actual evaporation and transpiration based on potential evaporation and predicted soil suction, as opposed to the user being required to input these surface flux boundary conditions. The actual evapotranspiration rate is generally well below the potential rate during prolonged dry periods because the suction, or negative water pressure, in the soil profile increases as the surface desiccates. In addition, VADOSE/W is a fully coupled (through the vapour pressure term) heat and mass transfer model which is capable of predicting water vapour movement (Geo-Slope International, 2010).

Methodology

The calibration process for a field response model is deceptively simple: make preliminary estimates of model inputs, run a simulation and compare model results to field measurements. If the model results accurately simulate measured conditions then the model is calibrated. If not, adjust a model input and repeat the process until an accurate simulation is obtained. However, it is difficult to know which input to adjust, and by how much, to improve the simulation. Without knowing the proper procedure for adjusting model inputs the calibration process is frustrating, time-consuming and near impossible.

In general, the model inputs can be placed in four groups, which are focused on in the following order:

1. Initial, lateral, and lower boundary conditions
2. Climate
3. Material properties and layering
4. Vegetation

The following sections describe how model inputs for each group were developed for the TP1 and TP2 field response models.

Initial, lateral, and lower boundary conditions

Initial, lateral, and lower boundary conditions are defined so that they do not substantially influence the model results being compared with field conditions. As a result, little calibration is required for these inputs. Therefore, these inputs are dealt with first during the calibration process.

Initial conditions are defined by the field measurements on the first day of the simulation period. However, it is the authors' experience that a model needs to run for a long enough period of time so that initial conditions are not influencing model predictions and to allow field sensors to acclimate to their installation conditions. If the model is calibrated and the initial conditions reasonably defined, this period will show the model and field results converging. For TP1 and TP2, the field response models converged with field measurements after a high rainfall event on March 2, 2004. Hence, March 2, 2004, was used as the start date for comparing model results to field conditions as it was assumed that the initial field and model conditions were not substantially influencing results after this date.

Often, cover system field response models can be adequately simulated one-dimensionally. Hence, lateral boundary conditions do not need to be defined. Exceptions exist, for example, when there is a large lateral flow component. However, TP1 and TP2 were constructed in flat locations to minimize lateral flow components and simplify the modelling process.

The lower boundary of a model needs to be far enough from the monitored depth of the field trials so as to not influence the model predictions. The lower boundary is usually defined as a unit gradient unless there is a phreatic surface within close proximity to the base of the monitored field trial depth. A unit gradient boundary condition simulates the water table to be well below the base of the cover system. A unit gradient boundary condition assumes that at the lower boundary the soil suction (and, as a result, water content and hydraulic conductivity) are constant with depth. When this is the case, the total head equals the gravitational head causing a unit hydraulic gradient. In other words, a unit gradient boundary represents a location in the modelled profile where water movement is controlled primarily by gravity driven drainage at the hydraulic conductivity defined by the negative pore-water pressure (suction) condition. TP1 and TP2 used a unit gradient lower boundary placed 10 m below the surface.

Climate

The VADOSE/W model requires daily inputs of precipitation amount and duration, maximum and minimum air temperature, maximum and minimum relative humidity, average wind speed, and net radiation. All of these variables were measured onsite for the period simulated by the field response models. This is extremely advantageous as it removes most of the uncertainty in these inputs. However, these inputs must still be critiqued to ensure that inaccurate measurements have not been overlooked. Hence, all climate data was compared with other site and regional measurements available to ensure accuracy.

Based on historic data from the region, the average annual rainfall anticipated for the field trials is approximately 360 mm/year.

Material Properties and Layering

The material properties required to define moisture movement within the material profile are moisture retention curves (MRC) and hydraulic conductivity functions (k-functions). These inputs are the most crucial to calibrate correctly so that performance models using these inputs will be accurate. However, these inputs are also the most difficult to measure directly, especially *in situ*. Hence, a large amount of time and effort is focused on this calibration step.

The best way to calibrate material properties is to simulate periods with no, minimal or dormant vegetation so that any divergence between the model results and field measurements can be attributed to errors in the estimated properties without having to consider potential vegetation influences. This method provides the additional benefit of indicating when vegetation begins influencing the flow patterns within the material profile once the material properties have been calibrated.

An MRC is a continuous function relating energy and the state of water, and hence describes the volumetric water content of a material as a function of soil suction, or negative pore-water pressure. Field measurements of volumetric water content and pore-water pressure measured at similar depths within a field trial are plotted together to provide an estimate of a portion of the MRC. This portion of the MRC should be considered as known initially during the field response modelling process and only be adjusted during later iterations if deemed necessary. The parts of the MRC outside the operational range of the field sensors (such as above 1,000 kPa and below 10 kPa for the sensors used in TP1 and TP2) and, therefore, not accurately defined by field data should be systematically adjusted to determine their influence on the simulated field responses. However, it is the experience of the authors that measurements outside the operational range of the field sensors provide an indication of curve shape and location, so while they cannot be considered accurate they are still useful to aid estimates and reduce calibration time.

Figure 1 provides an example of field moisture retention data fitted with a calibrated MRC, in this case at a depth of 1.8 m below the surface of TP2. The figure shows that the field data prior to the high rainfall event on March 2, 2004, does not conform with the data after the event, which indicates that the field sensors did not acclimate to site conditions until this large wetting event and verifies the use of March 2, 2004 as the start date for comparisons of model results to field measurements.

The authors discourage using a closed-form solution, such as van Genuchten (1980) or Fredlund and Xing (1994), to define the MRC during initial field response model iterations. These solutions create an excellent fit for unimodal MRC, however, many materials have heterogeneous pore systems that cannot be correctly described with a unimodal MRC (Durner, 1994). To this end, Durner (1994) suggested superimposing multiple unimodal curves to define a multimodal MRC. However, even though a multimodal MRC can be defined to represent moisture retention properties for most materials, it is difficult to fine-tune such an MRC during the calibration process. Hence, the use of spline functions is recommended during the calibration process as they are more easily adjusted. A spline function is a mathematical technique to interpolate data points with curved line segments. Closed-form solutions are recommended to define MRCs near the end of the calibration process if it is determined that the materials conform to a definable curve shape.

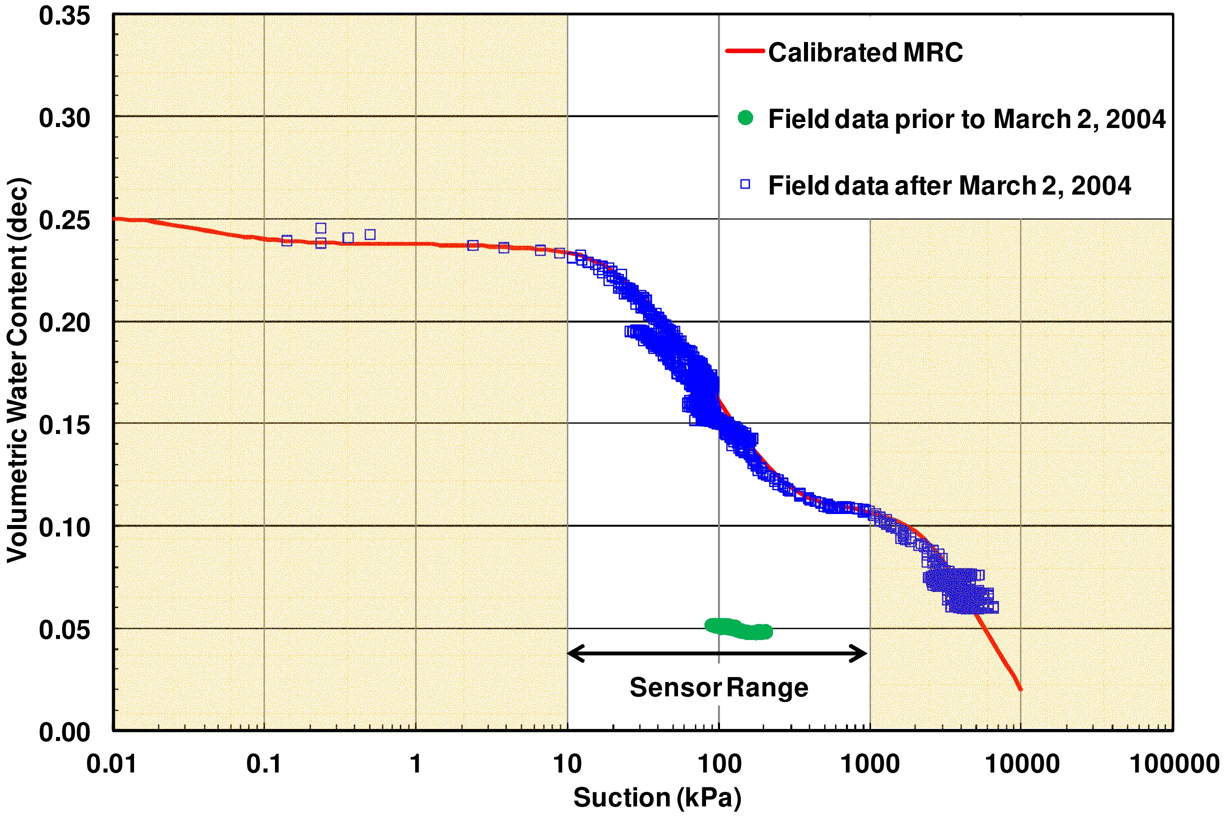

Figure 1. Moisture retention data measured 1.8 m below the surface of TP2 fitted with a calibrated MRC

Hydraulic conductivity is a measure of a material's ability to transmit water, and is a maximum for a saturated material. The k-function is one of the most difficult to measure. It can vary more than 10 orders of magnitude when considering soils that range from gravel to clay (Fredlund et al., 1994). As a result, prediction methods are frequently used to estimate the shape of the k-function from the more easily measured moisture retention data. Hence, initial estimates of k-functions for field response models are usually estimated using a prediction method such as van Genuchten (1980) or Fredlund et al. (1994).

The instantaneous profile method (IPM) (Richards and Weeks, 1953; Watson, 1966; Weeks and Richards, 1967; Daniel, 1983; Fredlund and Rahardjo, 1993; Eching et al., 1994) was used to estimate a range of unsaturated hydraulic conductivity values for each material. The IPM uses the measured changes in water content and suction to calculate an estimate of hydraulic conductivity. The resultant data points are usually disperse; leading to the initial conclusion that they are of no value. However, the IPM data points provide a range that the estimated k-function should remain within close proximity, unless all calibration efforts prove this not to be the case. Hence, this data is compared to the function created using the chosen prediction method, and the predicted function is usually adjusted to conform to the IPM range during subsequent iterations of the field response model. Figure 2 provides an example of IPM data points compared with the final calibrated k-function, in this case IPM data for 0.35 m and 0.75 m depths below the surface of TP1 compared with the calibrated k-function used to simulate the layer between these two depths.

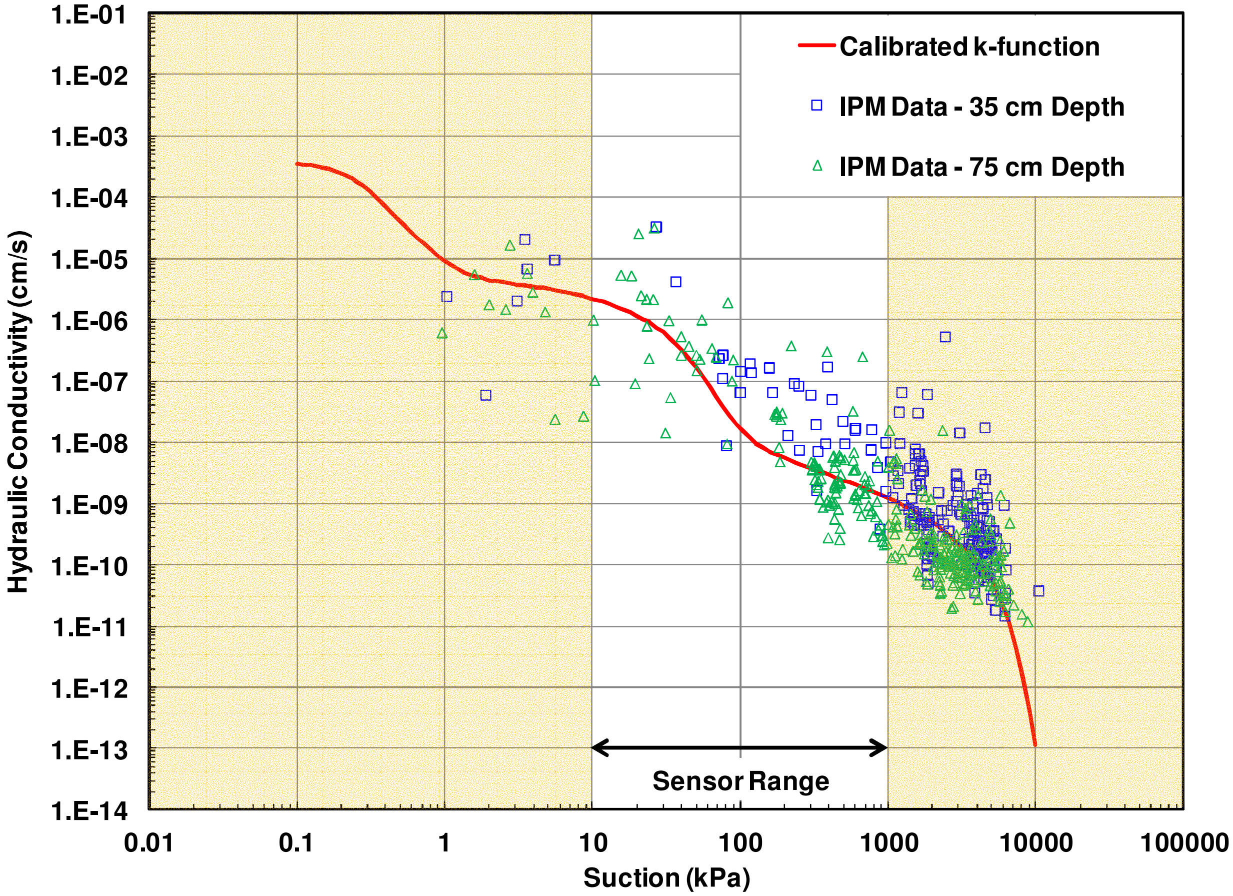

Figure 2. IPM data for 0.35 m and 0.75 m below the surface of TP1 compared with the calibrated k-function used to simulate the layer between these two depths

The data for TP1 and TP2 showed little evolution in the material properties with time, indicating little settlement and a stable system. However, if the data had shown changes in the properties with time, each change would have to be calibrated separately; essentially creating multiple field response models from the larger dataset.

TP1 and TP2 data does exhibit hysteresis. However, the computer software used for the modelling presented in this paper does not have the capability of including hysteresis in the analysis. Hence, curves were estimated to account for both the wetting and drying curves. This is a weakness in the model and does account for some of the divergence between the model results and field measurements.

In the past, field response models developed by the authors assumed that each defined layer of the waste material and cover system design is a homogeneous block of material. That is to say, that no unintentional sub-layering occurs during placement, or following a period of settlement and weathering. Sub-layers were only added when it became obvious that field conditions could not be simulated unless additional layers were added to the model. Although this process seems to follow the proper modelling procedure of starting a model as simplistic as possible and then adding complexity, it actually adds complexity to the model calibration process as it 'glazes over' measured field material properties that can be used as known variables that usually require little or no adjustment during the calibration process (Shurniak and O'Kane, 2009).

The procedure now used by the authors for calibrating field response models, including those for TP1 and TP2, is to estimate a unique set of material properties for each monitored depth of the soil profile; referred to hereinafter as a discrete model. Once a discrete model is calibrated the estimated material properties for each sensor depth are compared to determine the general layering of the cover system and underlying waste rock. Figure 3 shows the layering for the discrete and general field response models developed for TP1 and TP2. The figure shows that both discrete models were simulated with 8 layers (one for each sensor depth location) but after comparing the calibrated material properties for each layer, it was found that the TP1 cover material could be simulated using one set of general material properties but that the TP2 cover material requires a surface layer with differing properties from the remaining underlying cover material. TP2 requires a surface layer because the hydraulic properties required to simulate the sensor depths nearer the surface with the discrete model showed a difference in material behaviour from the remainder of the cover (Figure 4).

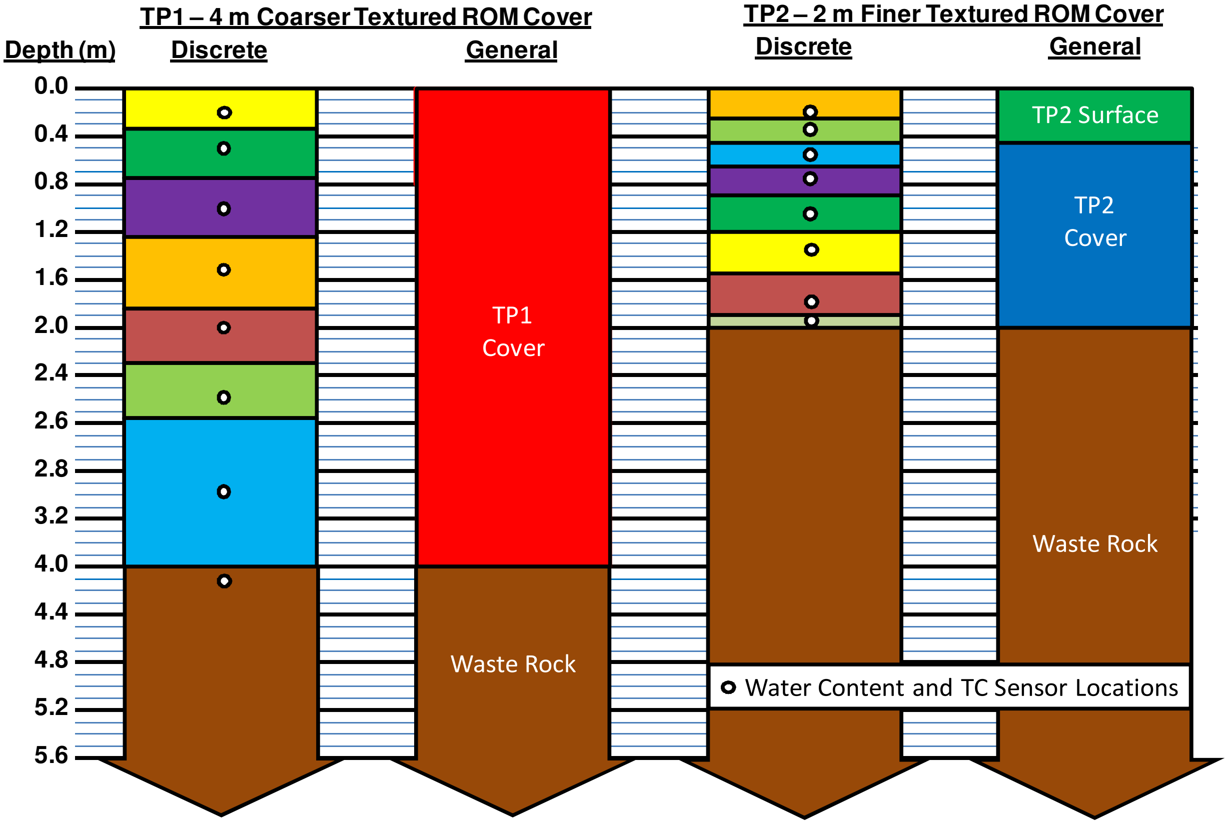

Figure 3. Layering used to simulate the discrete and general field response models for TP1 and TP2. Locations of Sentek EnviroSCAN® capacitance water content and TC sensors also included on figure.

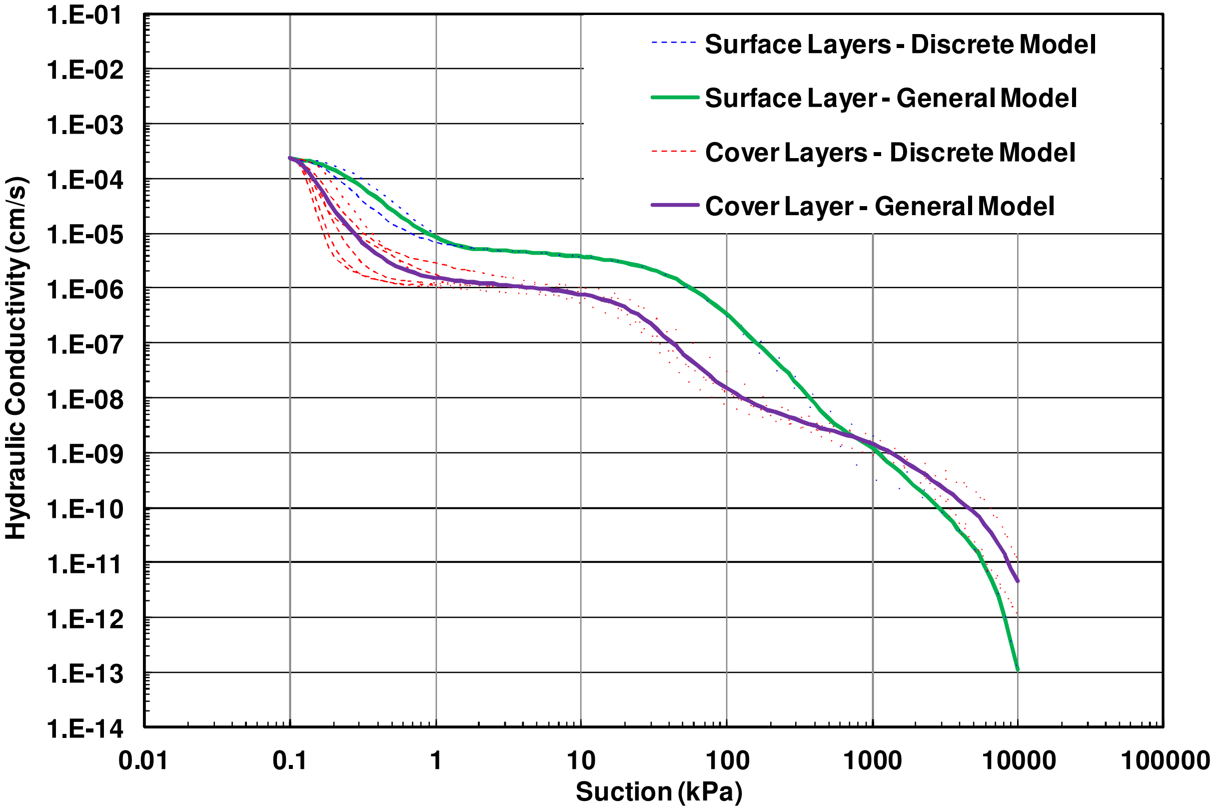

Figure 4. K-functions estimated for each layer of the TP2 discrete and general field response models.

Vegetation

Once the model has been calibrated during bare-surface or dormant vegetation conditions, it can be extended to simulate times of active plant growth. In fact, the model itself will indicate these times when field data measurements and model results diverge. This is shown in the results for the TP1 and TP2 field response models (Figures 5 and 6, respectively). Without vegetation it is impossible for the covers to desiccate as much as the field responses show without plants removing stored water from depth. Hence, vegetation was simulated to start development on January 1, 2006, and reach maturity (i.e. have a simulated rooting depth of 2 m) by July 20 of the same year. After including vegetation the discrete field response models for TP1 and TP2 R^2 values of 0.86 and 0.92, respectively, for the period of March 2, 2004 to March 31, 2010; just over 6 years.

Figures 5 and 6 were compiled by multiplying water content results by the profile volumes they were estimated to represent and adding these water volumes together to come up with an estimate of total cover water volume. Hence, it could be argued that these results may not be as accurate as presented. For example, if there were higher water volumes than measured at surface and lower at depth the overall result would still look accurate even though the model would not be calibrated. However, as shown in Figure 7, the model results presented in this paper are accounting for water movement near surface and at depth.

No field response model can be calibrated to perfectly predict all field responses. Furthermore, it must be kept in mind that there is no single unique calibration. Not every nuance of the soil-plant-atmosphere flow regime can be (or likely will ever be) accounted for, and different models may lead to equally acceptable representations of field responses; a condition referred to as equifinality (Beven and Binley, 1992; Beven and Freer, 2001; Beven, 2006). Hence, at some point, no additional changes will enhance the model predictions. At this point the model can be considered reasonably calibrated and its inputs can be used as a basis for evaluating long-term mine waste cover system performance. This being said, comprehensive testing of the potential range of input parameters (alone and in concert) must be undertaken to determine how sensitive (or insensitive) the model is to changes in each model input. The calibrated model should also be completed and compared to measurements at multiple monitored locations on a cover system to enhance understanding with regards to spatial variations in cover performance. As written by Ebel and Loague (2006), "…the equifinality problem becomes tractable when both integrated and distributed response data are used to assess model performance".

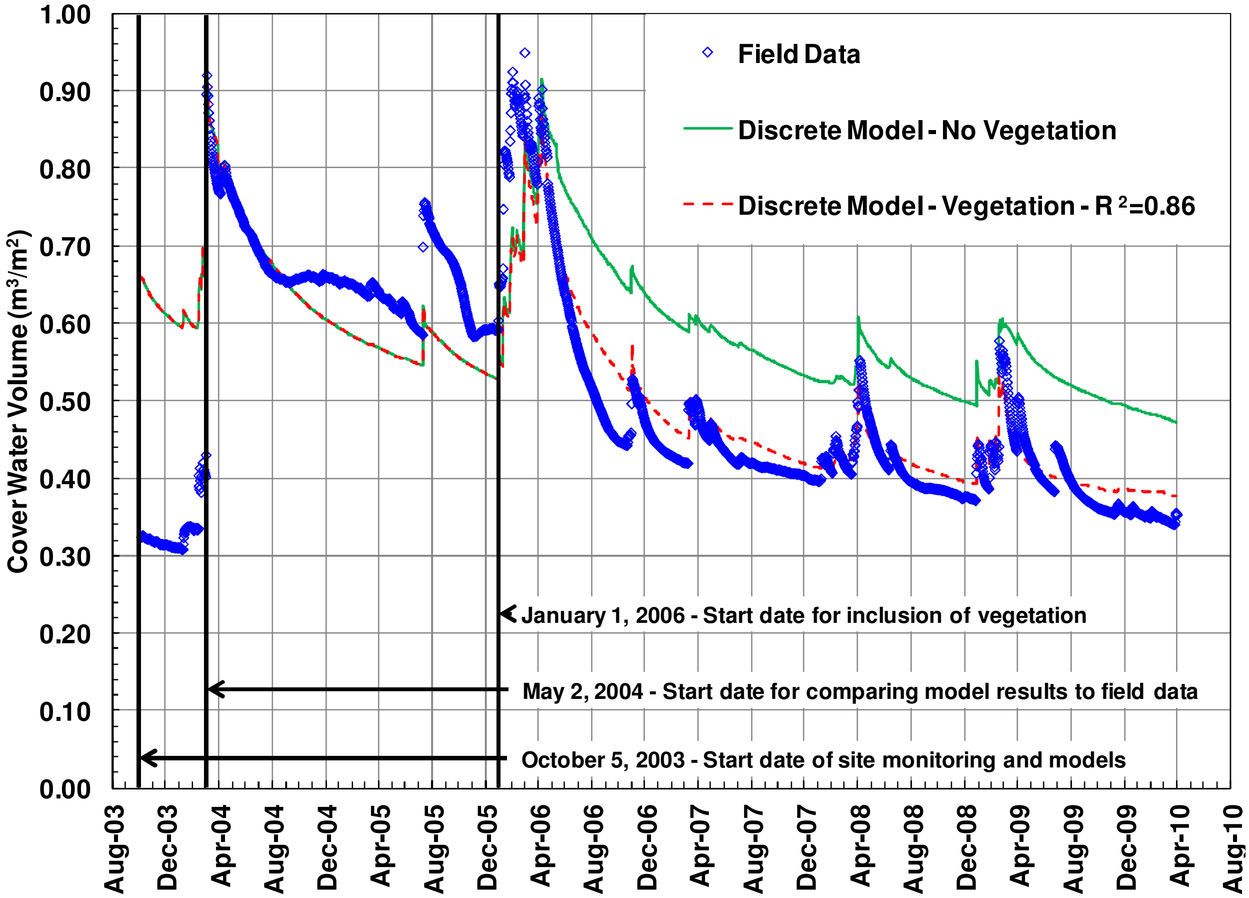

Figure 5. Comparison of TP1 field cover water volumes to results obtained from the TP1discrete model, with and with vegetation simulated

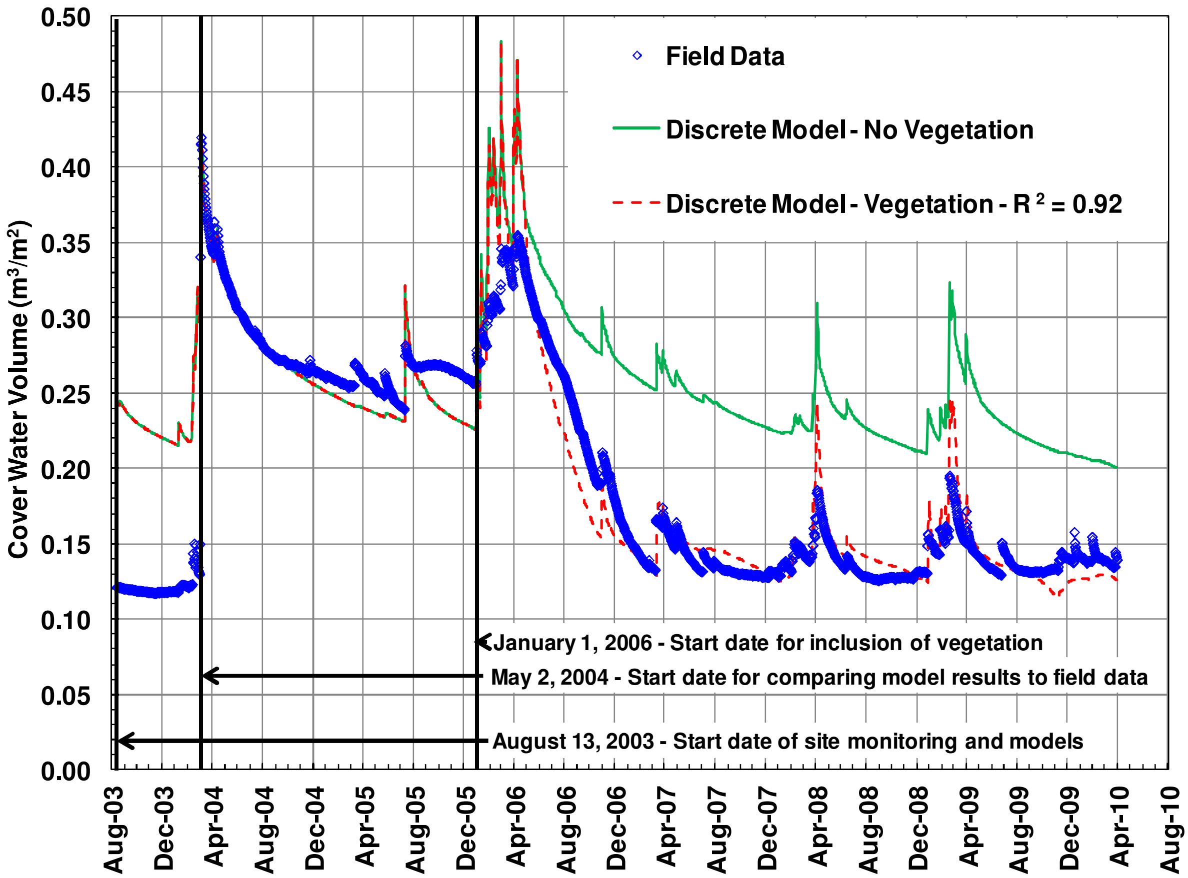

Figure 6. Comparison of TP2 field cover water volumes to results obtained from the TP2 discrete model, with and with vegetation simulated

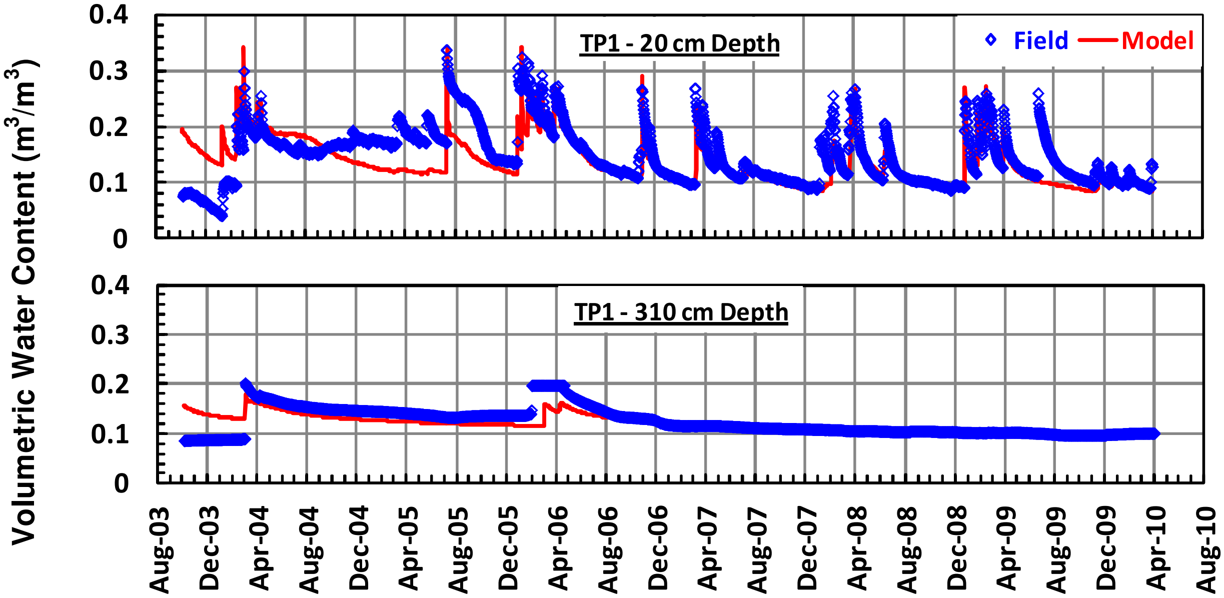

Figure 7. Comparison of TP1 volumetric water content field and model results near surface and at depth

Application

Once the field response models are calibrated they can be used to determine estimates of variables not directly measured in the field and evaluate overall cover performance. One of the most important variables and indicators of cover performance is the amount of water which permeates the waste material underlying the cover (i.e. net percolation). Net percolation into the underlying waste rock is not directly monitored for TP1 and TP2. However, due to the confidence with the field response modelling results, one can use the models to gain understanding for net percolation rates over the same period. Figures 8 and 9 show the amount of net percolation simulated to enter the waste rock during the monitored period for TP1 and TP2, respectively. The figures show that TP1 and TP2 had estimated cumulative net percolation amounts of 172 mm and 223 mm, respectively, during the monitored period. It must be noted that these amounts discount any net upward fluxes, which cause water to move from the underlying waste rock back into the cover material.

All the net percolation for both field trials occurs within the first 1000 days (i.e. August 13, 2003, to May 6, 2006, inclusive) of the simulation. The reasons for this are as follows:

- Rainfall during the first 1000 days is over 1500 mm, 50% higher than the amount of rain anticipated for the same 1000 days during average rainfall conditions (i.e. 1000 mm).
- A one-day rainfall event of 178 mm (or half of the average annual rainfall) occurred on March 2nd, 2004, corresponding to the first spike in net percolation.
- Over 750 mm of rainfall occurred during the 120 days from December 20, 2005, to April 18, 2006, inclusive. The 'normal' rainfall for this time period is only 236 mm, or over three times less than what actually fell. Hence, the second spike in net percolation occurs during this time period.
- Minimal vegetation develops at the sites until mid-2006. Hence, there is no deep root biomass present during the first 1000 days to remove any water infiltrating to depth. Therefore, this water is allowed to enter the underlying waste rock unabated. Plants are highly beneficial to the performance of a cover system that relies on the moisture S&R concept as they extract water from depth that could not be removed by evaporative forces alone; thus, reducing net percolation.

In summary, for the first 1000 days the field trials experienced what could be argued as extreme conditions from the perspective of a net percolation rates and having the cover system limit net percolation rates. However, even with high rainfall events and a complete lack of the advantages gained from vegetation, the net percolation rates for TP1 and TP2 during the first 1000 days are only 11% and 15% of rainfall, respectively (or 8% and 12%, respectively, if net upward fluxes from the waste rock are included). Including the full simulation period, net percolation rates for TP1 and TP2 are 8% and 12% of rainfall, respectively, but 6% and 8%, respectively, if net upward fluxes from the waste rock are included.

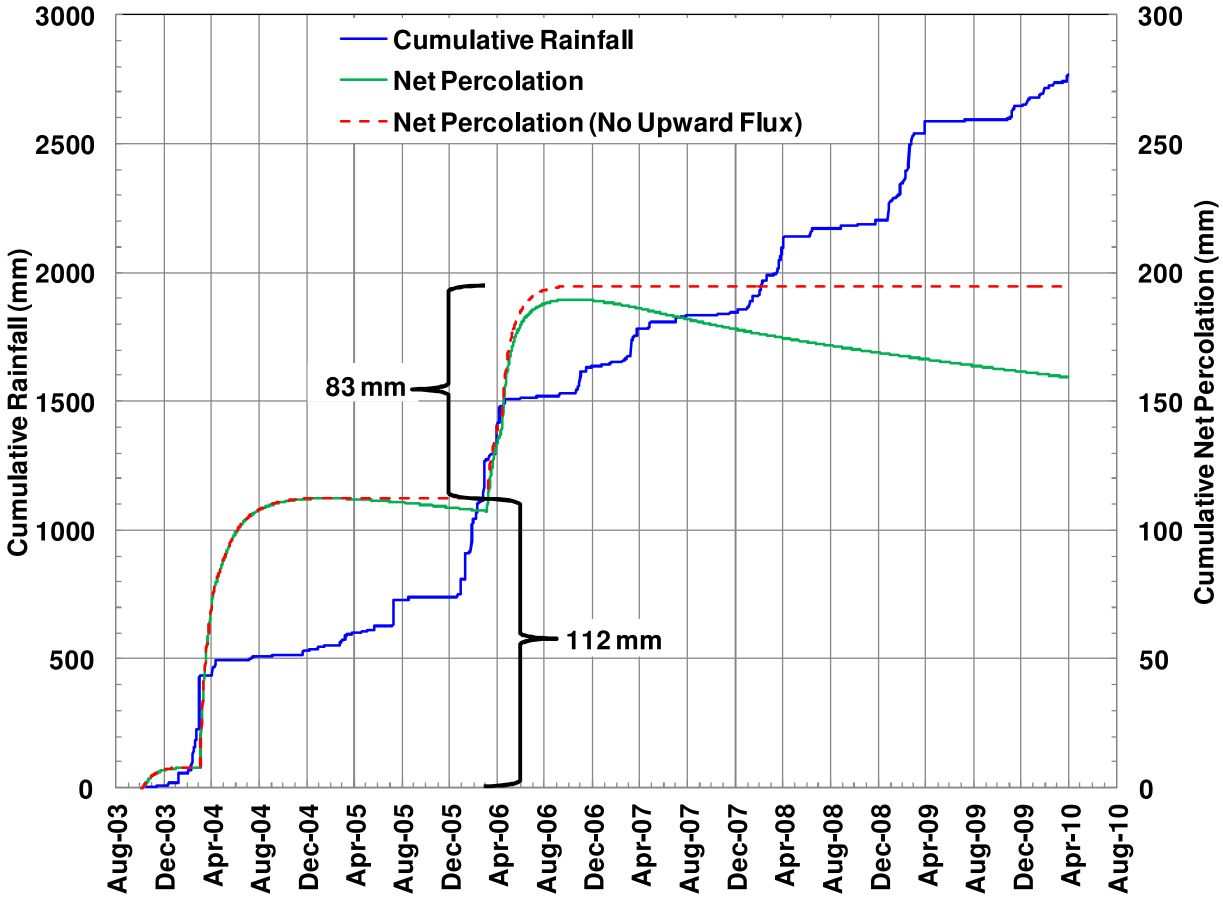

Figure 8. Net percolation estimate for TP1 using calibrated field response model

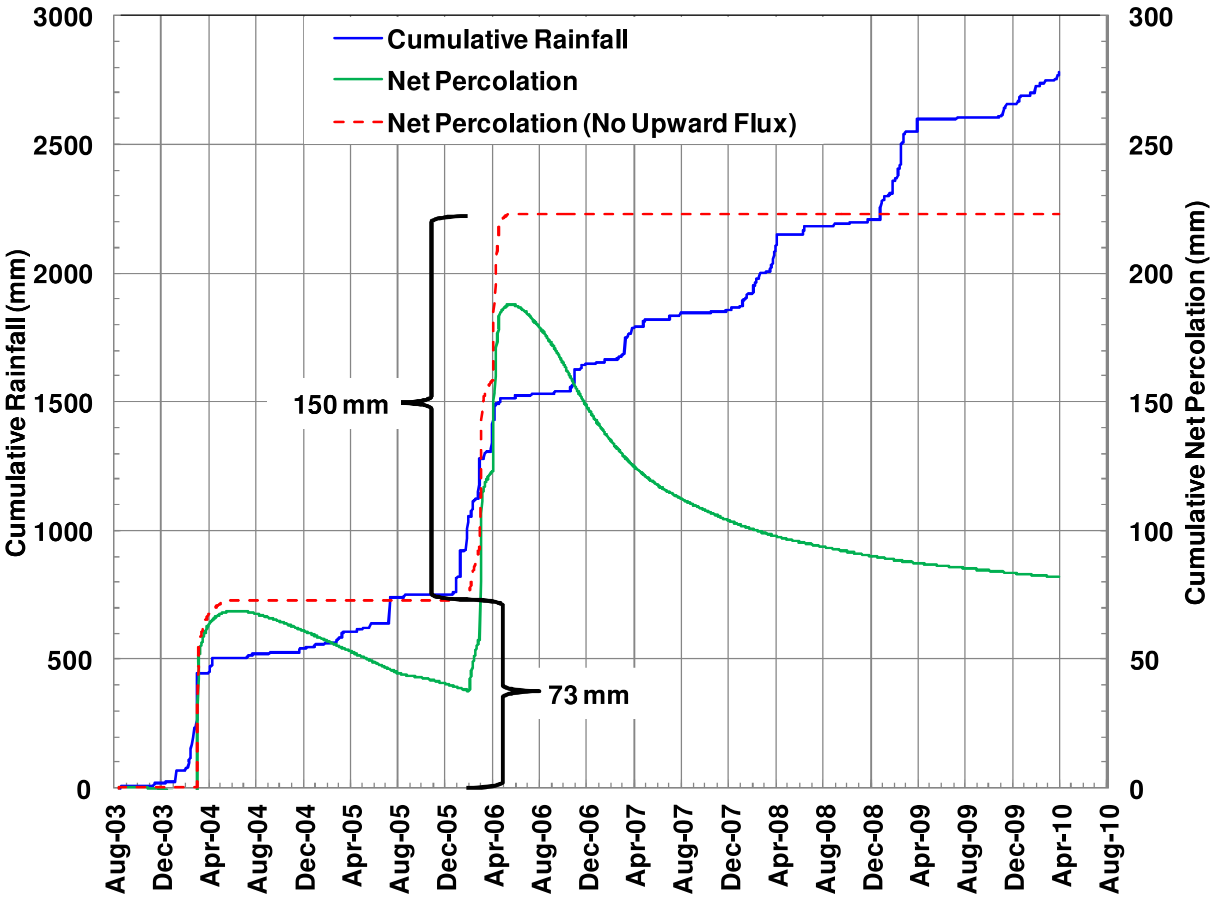

Figure 9. Net percolation estimate for TP2 using calibrated field response model

Summary

Field response modelling is the most effective way to estimate cover parameters (i.e. material properties, layering and vegetation) that can be used to evaluate cover performance. However, the work required to develop a calibrated field response model is complex and near impossible without knowledge of the proper procedure for adjusting model inputs.

This paper puts forth a general procedure for adjusting the model inputs in the following order:

1. Initial, side, and lower boundary conditions
2. Climate
3. Material properties and layering
4. Vegetation

By following this procedure the authors were able to develop a pair of calibrated field response models for two monitored field trials that were able to adequately simulate field conditions over a 6 year period. These models could then be used as a tool to evaluate cover performance with increased confidence in the results.

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Acronyms

R^2	Coefficient of Determination
S&R	Store-and-Release Cover System
ROM	Run-of-Mine
MRC	Moisture Retention Curve
k-function	Hydraulic Conductivity Function
IPM	Instantaneous Profile Method