

VADOSE/W 2D Tutorial

1 Introduction

This example illustrates the basic methodology for simulating soil-climate interaction of an engineered soil cover system placed over a waste. The primary objective of the simulation is to assess the inflow of water and oxygen through the base of the cover into the waste. A commentary on various aspects of VADOSE/W modeling is also provided.

2 Feature highlights

GeoStudio feature highlights include:

- Transient flow
- Vegetation and oxygen diffusion analyses
- Climate coupling
- Surface region meshing

3 Numerical Model

Figure 1 shows the model domain and Figure 2 shows the details of the surface mesh. The Surface Layers (Draw | Surface Layers) are drawn on top of a conventional region. The use of Surface Layers, in combination with a structured and dense mesh, is numerically advantageous in cases where large spatial variations in pore-water pressure might exist. In this case, the cover is designed to promote a capillary break at the base of low conductivity materials (i.e. the compacted (orange) material). As such, large spatial variations in pore-water pressure are expected to exist at the base of the cover.

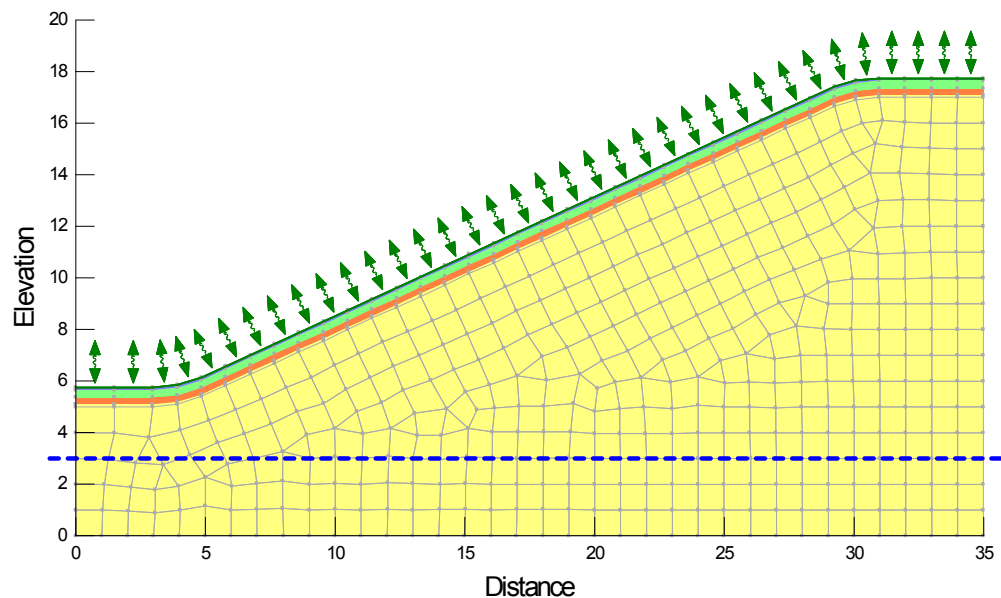


Figure 1. Model domain for the simulated soil cover over waste

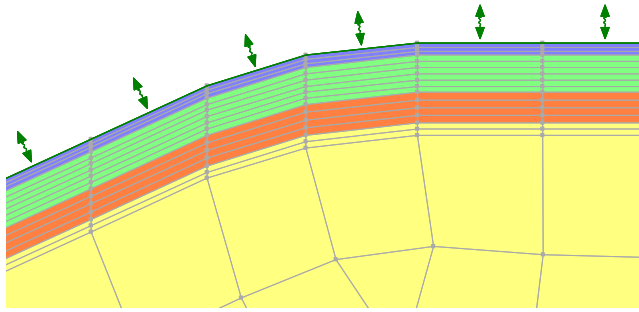


Figure 2. Detail of the surface mesh.

The bottom most surface layer was assigned the waste material (Draw | Surface Layer Materials). The cover comprises three materials. The orange layer represents a low conductivity compacted clay layer that is supposed to remain near saturation, which in-turn limits gas diffusion thereby preventing various chemical reactions within the waste. Two growth layers exist above the compacted unit (green and purple).

There are a number of attributes of the problem definition that should be explored in the KeyIn Analyses menu:

1. The initial water pressures are obtained from a water table that was drawn using the command Draw | Water Table. The pore-water pressures vary hydrostatically below and above the water table but are truncated above the water table at the specified maximum negative pressure head.
2. The initial temperatures are specified as none because the temperature are activated according to the values specified in the definitions for the material models (KeyIn | Materials).
3. The diffusion of oxygen is being simulated and the initial gas concentrations are obtained via activation as specified in the definitions for the material models (KeyIn | Materials).
4. The simulation includes ground freezing (KeyIn | Analyses | Control) if the temperatures drop below the phase change value (Set | Units and Scale). Latent energy storage and a decrease of hydraulic conductivity within frozen pores occur if the soil freezes and ground freezing is “on”. Otherwise, sub-zero temperatures could exist within the domain but latent energy effects will not be considered and decreases in hydraulic conductivity due to frozen pore-water will not be considered.
5. The simulation includes vegetation (KeyIn | Analyses | Control). Nodes within the surface region and within the specified root zones, as defined by the root depth function, will transpire water if the soil suctions are not above the wilting pressure. The maximum transpiration rate is controlled by the climate data but cannot exceed the potential evapotranspiration for the site.
6. Surface water is being allowed to pond on the climate boundary condition nodes (KeyIn | Analyses | Control). The algorithms accumulate (pond) water in topographic lows. The left or right sides of the model are assumed to be (enclosed) topographic lows if the ground is flat and the elevation is a low point. Water is stored on surface (nodes) and allowed to evaporate or infiltrate on later time steps if no topographic lows exist.

3.1 Material properties

Figure 8 shows the volumetric water content functions for the three soils: waste, a compacted low permeability layer, and a growth layer. The waste layer has the lower porosity and the compacted clay layer the highest. The volumetric water content function characterizes the capacity of a soil to store or

release water as a result of changes in pore-water pressure. As such, these functions can have a significant effect on the performance of a soil cover subject to cycles of wetting and drying.

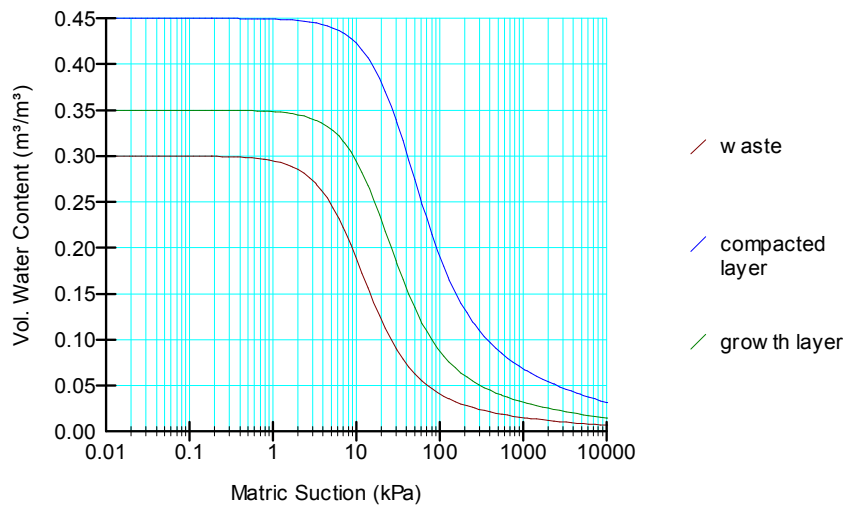


Figure 8. Water content functions.

Figure 9 shows the hydraulic conductivity functions. The hydraulic conductivity functions can be entered (from lab data) or estimated from the volumetric water content functions according to the methods of van Genuchten or Fredlund and Xing. An add-in function can also be used. In this case, the van Genuchten estimation technique was used. The upper part of the growth layer has a modified function that is truncated at a higher conductivity at large suctions (i.e. when the soil is dry). This modification to the function attempts to account for desiccation (cracking), root penetration, and alteration by other surface processes.

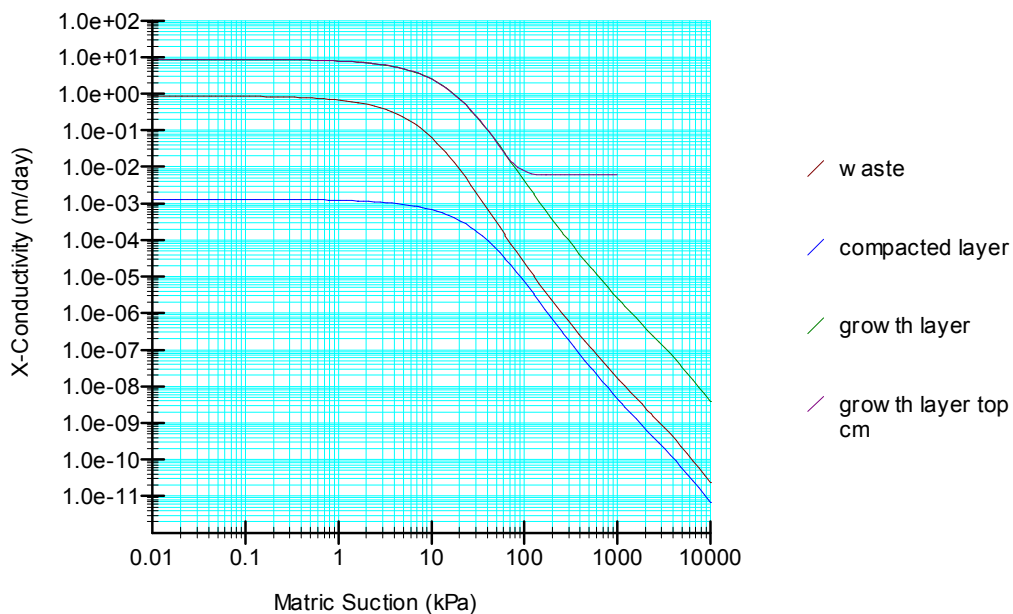


Figure 9. Hydraulic conductivity functions.

The Simplified Thermal model was used to represent all of the materials, which requires specification of the frozen and unfrozen thermal conductivity and volumetric heat capacity (Figure 10). The key simplifying assumptions of the simplified model is that thermal conductivity does not vary with volumetric water content and that all water within the pore-space changes phase instantly. The Simplified Thermal model is generally adequate if the thermal response is not of great concern and/or thermally driven vapor flow is not a dominant mechanism. Figure 10 also shows the activation temperature of the material.

Thermal Properties		
Thermal Conductivity:	Volumetric Heat Capacity:	<input checked="" type="checkbox"/> Activation Temp:
Unfrozen: 150 kJ/days/m/°C	Unfrozen: 2,500 kJ/m ³ /°C	10 °C
Frozen: 125 kJ/days/m/°C	Frozen: 2,300 kJ/m ³ /°C	
Gas Properties		
Radon Decay (Years):	0	
Eff. Reaction Rate Coef. for Oxygen:	0 /days	
<input checked="" type="checkbox"/> Activation Gas Concentration:	0 g/m ³	

Figure 10. Thermal and gas properties

The gas properties are also shown in Figure 10. Only the activation concentration and effective reaction rate coefficient are required to simulate gas diffusion. The later of these parameters copes with oxygen consumption by oxidation processes, which is not being considered. Notice that a diffusion coefficient function is not specified. VADOSE/W internally computes the diffusion function using a method proposed by Millington and Shearer. The activation gas concentration has been set to 0.

3.2 Boundary Conditions

Figure 3 shows the climate data set for Spokane WA that was imported from the database file contained on the Resources CD (KeyIn | Climate Data Sets | Add | Import). The distribution pattern selected is sinusoidal which means the temperatures, rainfall, relative humidity and sun's energy (radiation) will be distributed throughout the day based on a sinusoidal pattern. The time of sun rise is controlled by the latitude and day within the year – making it necessary to specify the Start Date – while the onset and end of a rainfall event is user specified.

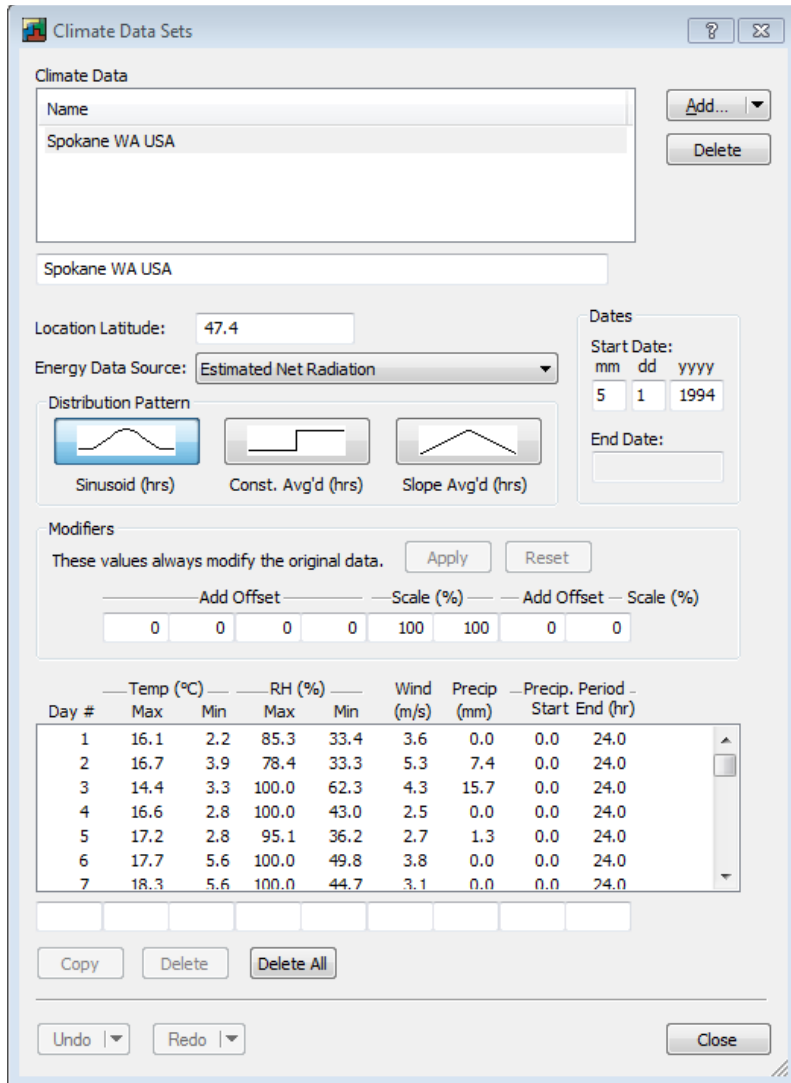


Figure 3. Climate data.

Notice that modifiers can be applied to quickly amend the climate data. For example, a Scale (%) modifier value of 150% can be specified for the Precipitation to simulate 50% more precipitation in every event of the climate record. Similarly, an Offset of 1.0 can be specified for the Maximum Temperature to increase all of the maximum daily temperatures by that value.

Vegetation has been toggled on, making it necessary to define the appropriate functions and associate the functions with the climate boundary condition. There are three related functions: the leaf area index (Figure 4), the moisture limiting function (Figure 5), and the root depth function (Figure 6). The leaf area index function was estimated based on a standard shaped function for a “good” quality grass (KeyIn | Climate Functions | Leaf Area Index). The LAI function can be cycled during a multi-year analysis by selecting the Cycle Function option.

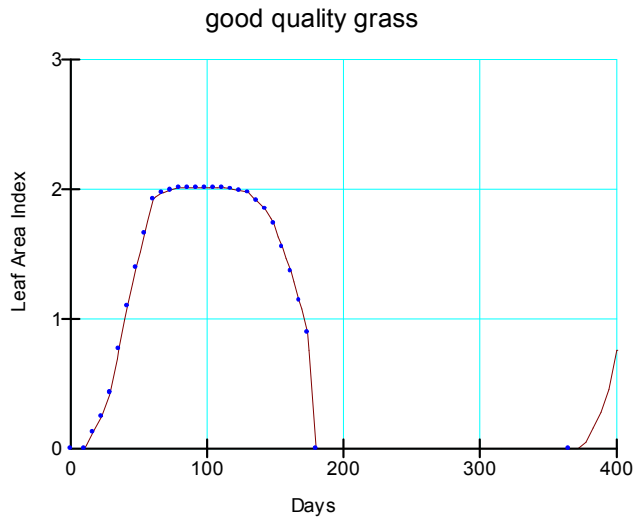


Figure 4. Leaf area index function

The moisture limiting function indicates that the plants will start to have uptake limited at a soil suction of 100 kPa and will shut-down at 1500 kPa.

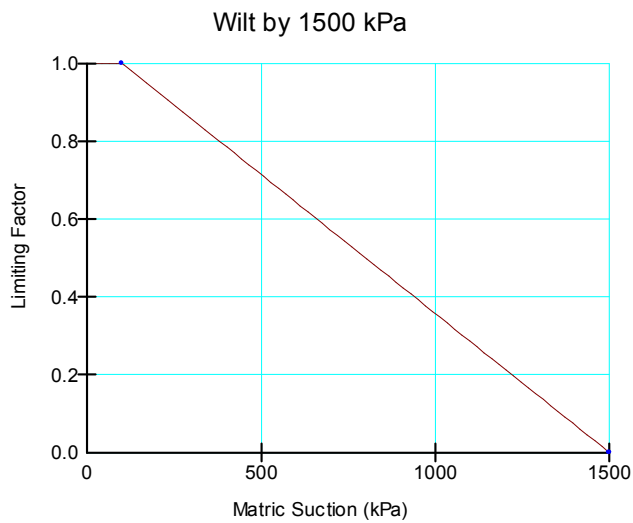


Figure 5. Moisture limiting factor function

The roots are assumed to be at a depth of 10 cm on the first day of the analysis and then grow to a depth of 40cm by the 3rd month. The maximum root depth must be less than the thickness of the surface regions.

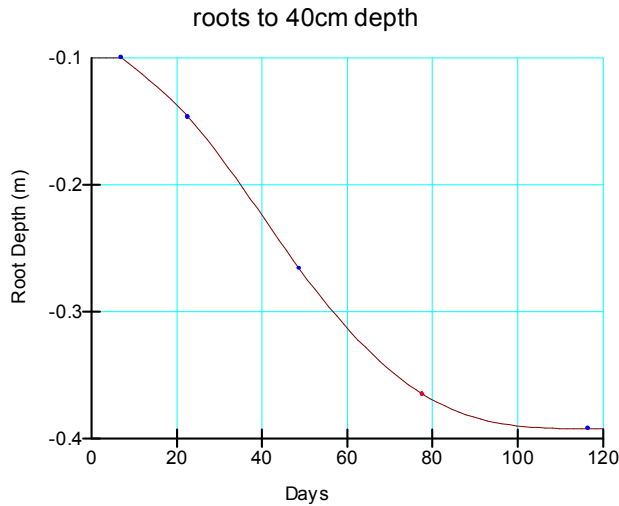


Figure 6. Root depth function

Figure 7 shows how the functions are associated with the climate data within the climate boundary condition definition. A rectangular root distribution has been selected. Many climate boundary condition definitions can be created to facilitate such things as sensitivity analyses or climatic/vegetation variations on slopes facing certain directions. It is also worth noting again that the Modifiers can be used to alter the climate data for these purposes (e.g. cooler on shaded slope).

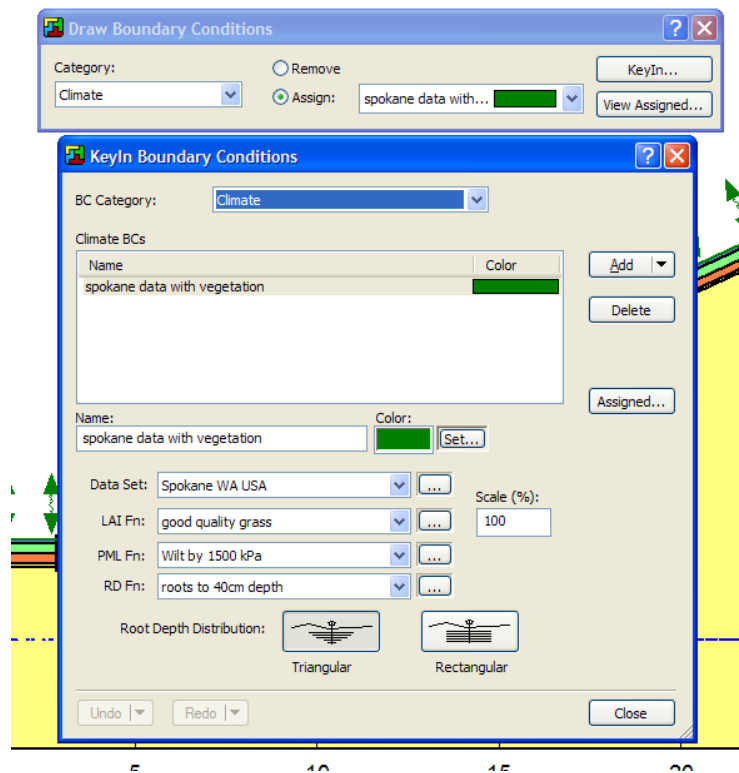


Figure 7. Climate boundary condition definition.

There are some additional boundary conditions applied to the model that can be explored using commands such as View | Object Information. It should be noted that the surface gas concentration boundary condition is assumed to be that of oxygen in air (280 g/m³). A user specified concentration is not necessary.

3.3 Convergence and Under-Relaxation

VADOSE solves the finite element equations using a repeated substitution technique. The solution for a particular time step is deemed converged if the primary variables – pore-water pressure head and temperature – are equivalent within a tolerance on two successive iterations. For this example, the maximum iterations was set to 25; that is, after 25 attempts to attained convergence the program will accept the solution and move onto the next time step. The key convergence criterion for determining equivalency is the number of significant figures, which was specified as 2 for this example. The significant figure is used to determine a tolerable difference. For example, values between 0.950 and 1.05 would be deemed equivalent to 1.0 and values between 95 and 105 would be deemed equivalent to 100 when the significant figure tolerance is set equal to 2.

The settings for the under-relaxation technique and additional details on the convergence criteria can be found in the VADOSE Engineering Methodology documentation.

3.4 Time Definition

A time step definition is required in a transient analysis (KeyIn | Analyses | Time). The starting time has been defined as 100 days. As such, the first climate data entry to be used will correspond to day 100. Only 30 days of the climate record are simulated, but this can be modified by changing the starting time to 0 and the duration to 365 days (or more). Incidentally, VADOSE will cycle back through the climate record if the duration exceeds the number of climate days. The results are being saved at every second day, but this value should be increased proportionally as the duration to prevent saving excessive amounts of data (and slowing down the solve time).

The time steps must align with one day increments if climate data is being used. For example, the time increments must be 1 day or 0.5 day or 24 hours or 12 hours depending on the time units. The program will produce a verification error if the time definition is incorrect.

Adaptive time stepping should generally be used when a climate boundary condition is applied. The program will insert additional time increments between the defined steps in order to promote convergence and track large variations in the boundary conditions, as indicated by changes of the primary variables within the domain. For example, the adaptive time stepping method will insert additional steps in order to capture the start and end of a rainfall event and variations in net radiation during the day (which promotes drying). The VADOSE Engineering Methodology documentation provides additional details on the techniques available.

4 Discussion of results

4.1 Water Balance

Figure 11 shows the water balance graphs which are generated at every time step, not just the saved time steps. Each water balance graph is a summation of the parameter for all nodal or gauss values within the entire domain. The following observations can be made from this graph:

- a. Approximately 0.684 m³ of rain accumulated during the simulation;

- b. There was 0.0 m³ or runoff (not shown)
- c. Approximately 3.0 m³ of water was extracted from the domain (within the growth layer) due to plant transpiration (AT);
- d. Approximately 1.41 m³ of water left the domain due to plant evaporation (AE);
- e. Approximately 0.063 m³ of water entered the domain at the boundary nodes (BF; the boundary nodes refer to all nodes except those to which the climate boundary condition was applied).
- f. A storage change of approximately 3.65 m³ of water occurred within the domain.

The final water balance is approximately given by (using more precision):

$$\text{change in storage} = \text{Precp.} + \text{Runoff} + \text{AE} + \text{AT} + \text{BF}$$

$$- 3.65 \text{ m}^3 \cong (0.684 + 0.0 - 1.41 - 3.0 + 0.063) \text{ m}^3$$

The water balance error is calculated as the summation of all terms, which is a near-zero number when calculated with more precision.

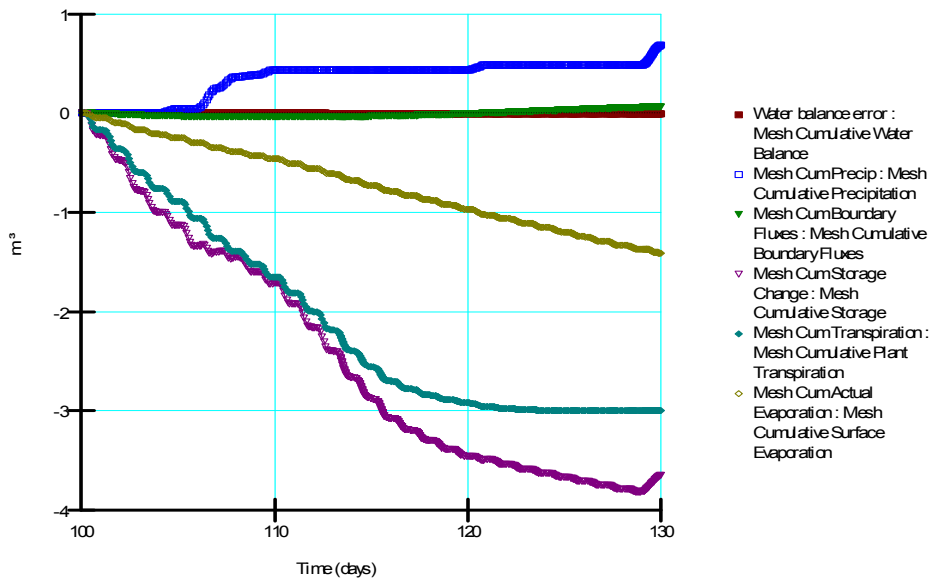


Figure 11. Water balance data

4.2 Cover layer flows

There are some insightful graphs that can be generated in VADOSE by obtaining Data from:

1. Surface Region Nodes: plots at individual nodes in time, position or distance of:
 - a. Liquid water, vapor, or total (liquid and vapor) water volume (referred to as Cumulative Flux); or,
 - b. Liquid water, vapor, or total (liquid and vapor) water volume rates (referred to as Flux).

2. Surface Region Base Layers: cumulative time history plots of :
 - a. Liquid water, vapor, or total (liquid and vapor) water volume past all nodes along the layer; that is, summation of the volumes from all nodes (referred to as Cumulative Flux); or,
 - b. Liquid water, vapor, or total (liquid and vapor) water volume rates at all nodes along the layer; that is, summation of the volumes rates at all nodes (referred to as Flux).

Special algorithms are used to determine the flow volumes and rates at the nodes along the top or bottom of every surface layer (region). Positive volumes (or rates) for the uppermost surface layer; that is, the ground surface, indicate flow into the domain. Positive volumes for base layers within the domain indicate upwards flow (and therefore a negative value indicates downwards flow).

Figure 12 shows the cumulative total flow volumes across each surface regions base layer (Draw | Graph | Data From: Surface Region Base Layers). The Base of Layer 1 is the lowest in the profile, the Base of Layer 2 the next lowest (above the Base of Layer 1) and so on. Recall that the Base of Layer 1 is at the bottom of a thin region of waste material while the Base of Layer 2 is at the bottom of the compacted (orange) layer.

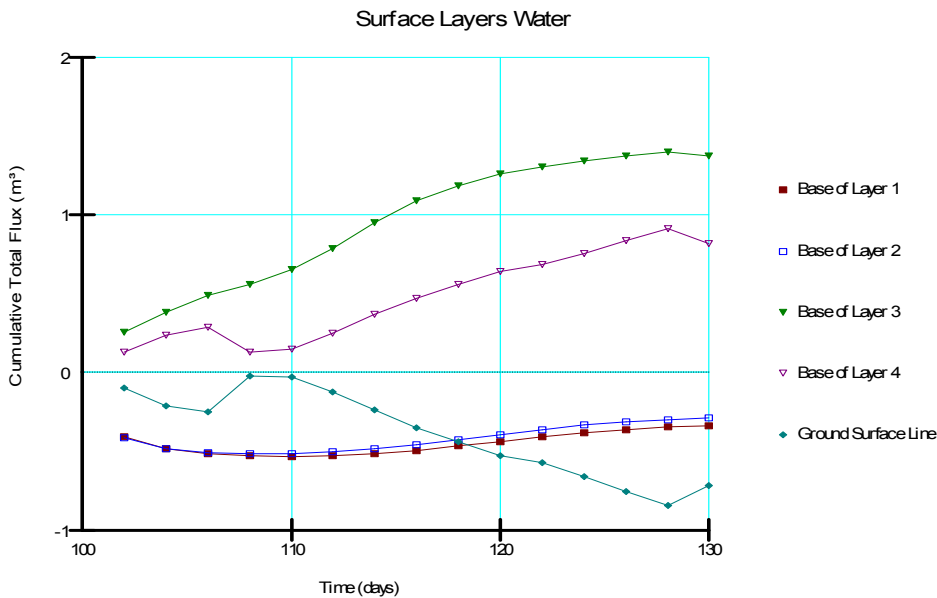


Figure 12. Time history of the cumulative flow volume of water (liquid and vapor) across the surface region base layers (summation of all nodal volumes).

Figure 12 indicates that approximately 0.72 m³ flowed up past the ground surface lines, which is in keeping with the water balance data, which indicated that (precipitation – actual evaporation) = (0.684 – 1.41) m³ = -0.72 m³. The graphs for Layers 1 (bottom of thin layer of waste) and 2 (bottom of compacted layer) indicate that water moved down past the base of these layers. The graph for Layer 3 (interface between compacted layer and growth layer) and 4 (closest to ground surface) indicate that water moved upwards towards the ground surface. From this information it can be observed that the growth layer (green and purple) dried out by water moving towards the ground surface or being extracted by transpiration. The water balance data confirms that transpiration was the dominate mechanism,

accounting for 3.0 m³ of water being extracted from the growth layer. The extraction of water from the growth layers is therefore primarily responsible for the drying of the top part of the compacted layer. In addition, the compacted layer is drying due to small amounts of water moving down into the waste.

Figure 12 provides an overall response for the base layers but provides no spatial information. Figure 13 shows the cumulative total flow volumes at each individual node plotted versus x-coordinate for the bottom and top of the compacted layer, respectively (Draw | Graph | Data From: Surface Region Base Layers; Base Layer 2 and 3). Figure 13 indicates that:

- a) there was a net upwards movement of water at every node along the top of the compacted layer, which is in-keeping with the large extraction of water within the growth layers by transpiration; and,
- b) there was a net downwards (negative) movement of water at every node along the base of the compacted layer from about x = 7 m to the right edge of the domain.
- c) there was some upwards movement of water to the left of x = 7 m, but the extraction out the top of the cover is greater, which would lead to drying of the compacted layer. The over-all upwards flow is a reflection of the greater availability of water for root uptake.

In summary, the entire compacted layer – from the left to the right of the domain – is in a drier state by the end of the analysis. Incidentally, the data corresponding Base Layer 3 could be pasted into a spreadsheet and summed for all nodes to obtain the value of approximately -0.34 m³ shown in Figure 12 at the last time step.

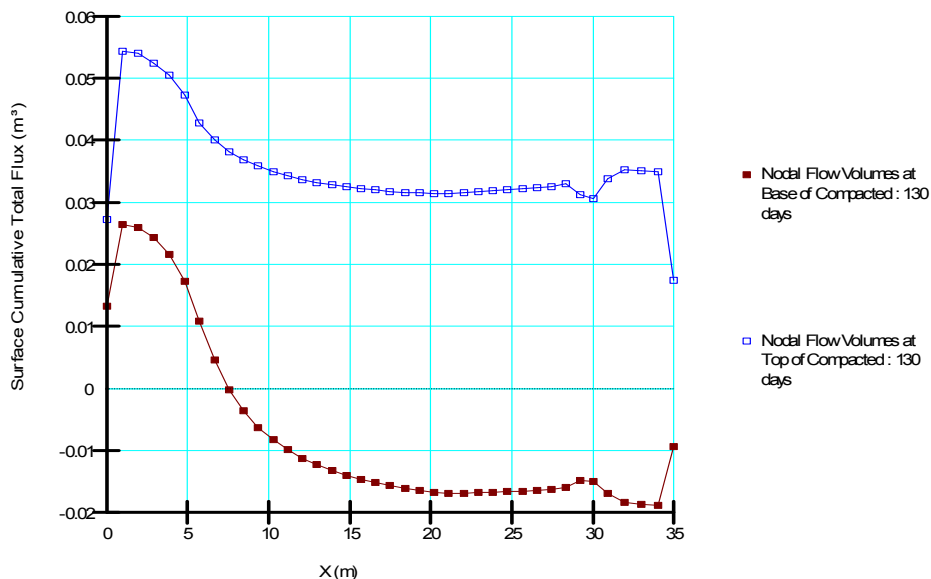


Figure 13. Cumulative total flow volumes at every individual node versus x-coordinate at the top and bottom of the compacted clay layer.

4.3 Vertical water content profiles

Figure 14 and Figure 15 show the volumetric water content profiles along the left and right edges of the model. The compacted layer extends from elevation 5.1 to 5.35 m and 17.1 m to 17.35 m on the left and right edges of the domain, respectively. The very bottom of the cover between retained most of the water; however, the top part of the cover is drying significantly by the end of the 100 day simulation. The growth layer is nearing the residual water content due primarily to transpiration. The effects of retaining water through part of the compacted layer are reflected in profiles of gas concentration (Figure 16 and Figure 17).

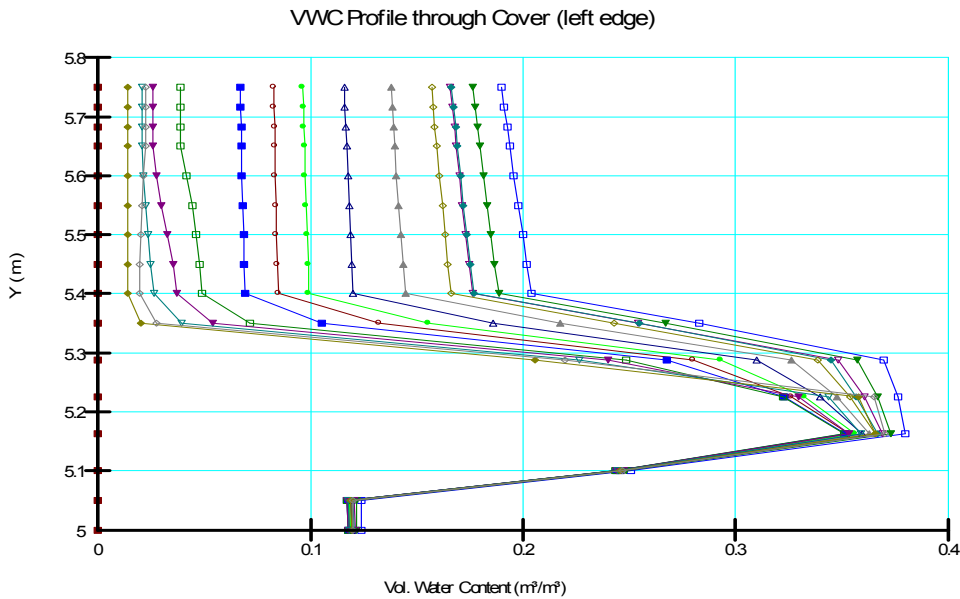


Figure 14. Volumetric water content profile through the cover along the left edge of the model

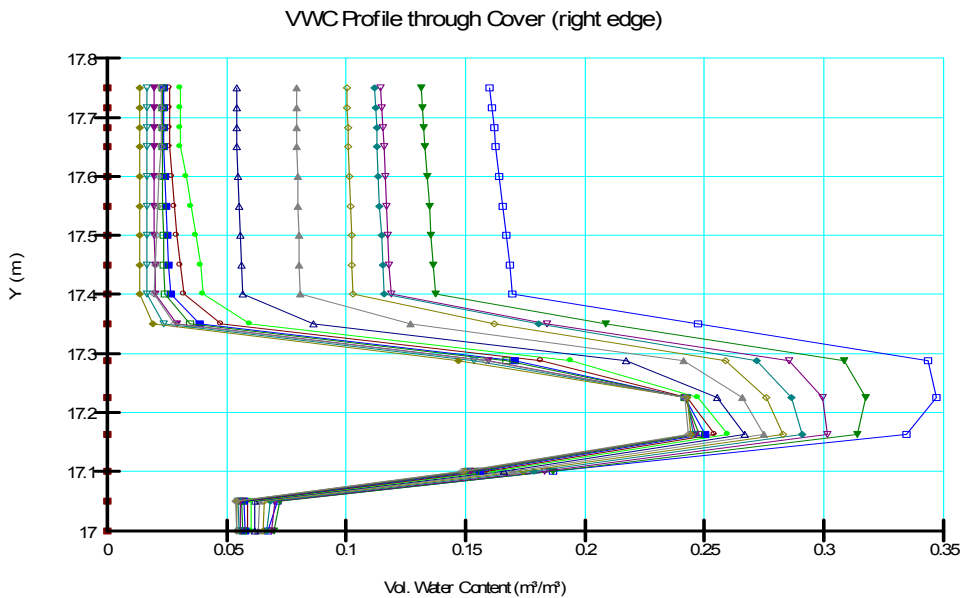


Figure 15. Volumetric water content profile through the cover along the right edge of the model

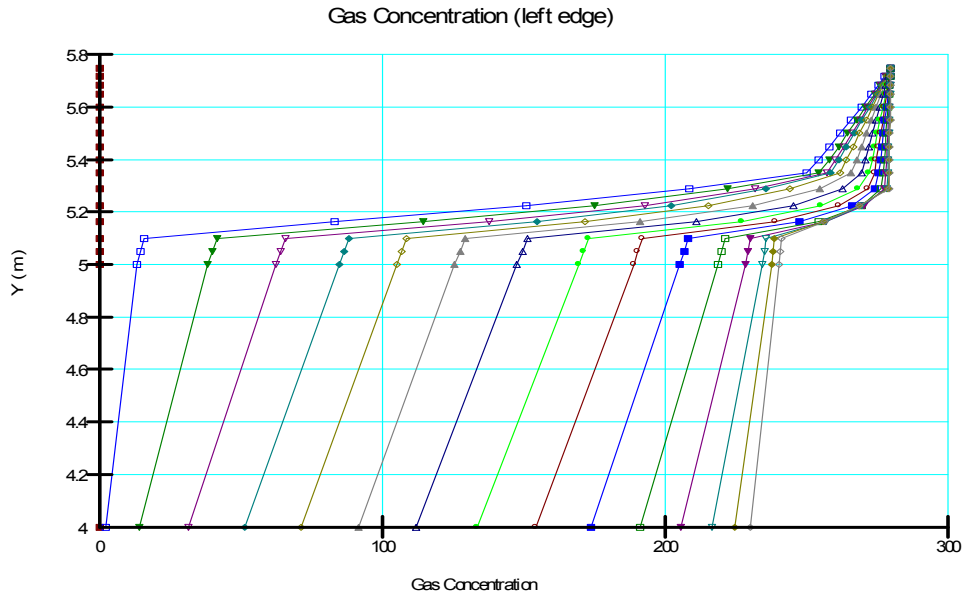


Figure 16. Gas concentration profile through the cover along the left edge of the domain.

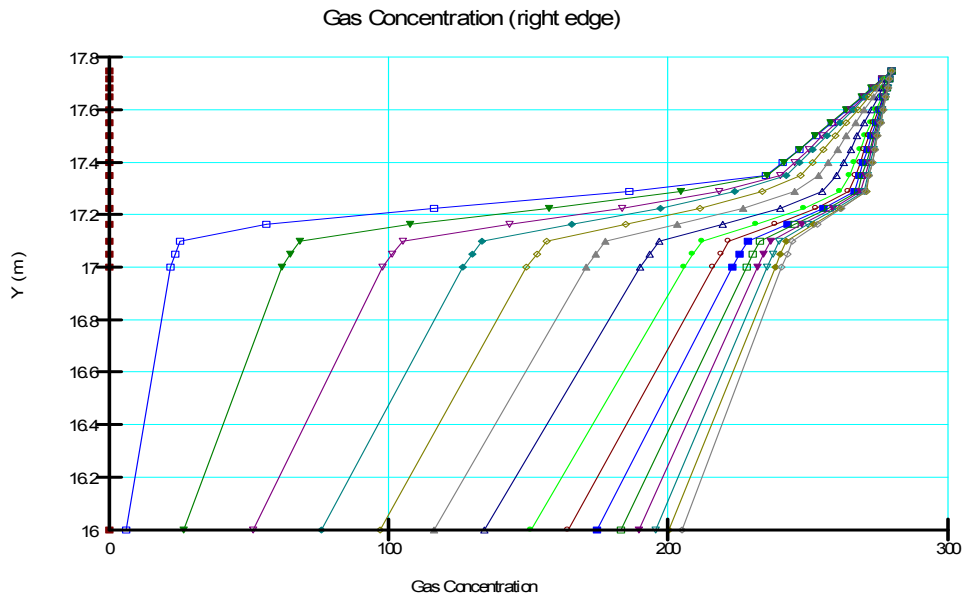


Figure 17. Gas concentration profile through the cover along the right edge of the domain.

5 Conclusion

The interpretation of soil cover systems is a rather involved process. The preceding discussion demonstrated only a fraction of the number of graphs that can be generated to assist interpretation. To highlight this point, consider that graphs can be generated with Data from: Surface Region Nodes | Climate BC. The subcategories drop down menu contains all of the important climate related data that can be plotted at individual nodes. Proper interpretation of cover systems often relies heavily of this data.

