



SoilCover Reference Guide

**SoilCover Software Ltd.
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Warranty and Waiver

SoilCover is distributed without warranty and As Is. It is up to you, the end user, to ensure that the features you are using in the project you set up result in solutions that you deem reasonable. While SoilCover Software Ltd. tries to validate the software, it is possible there are unknown issues that may result in erroneous computed results. If you identify a potential issue, please bring it to our attention at Support@SoilCover.ca and we will try to validate the issue and document it. If necessary we will issue an updated version or provide a temporary “work around” solution.

In using this software, you accept all risks and you are responsible for ascertaining that your model outputs are acceptable for your specific application. When you installed the software you were given the opportunity to read the End User License Agreement, which you accepted prior to completing the installation.

1.0 SOILCOVER OVERVIEW

1.1 Introduction

Water movement through soils can be thought of as a three-component system consisting of the soil-atmosphere interface, the near surface unsaturated zone, and the deeper saturated zone. In the past, groundwater modelling has primarily focused on saturated zones. This focus creates a discontinuity in the natural system as the unsaturated zone and the soil-atmosphere interface are typically not represented. Advances in unsaturated soil technology over the past few decades have led to the development of routine modelling techniques for saturated/unsaturated soil systems. However, modelling techniques for the third component involving the evaluation of the flux boundary condition imposed by the atmosphere is not routinely considered. SoilCover is a soil-atmosphere flux model that links the subsurface saturated/unsaturated groundwater system and the atmosphere above the soil to represent the soil-atmosphere continuum.

Predicting the flow of water between the soil surface and the atmosphere is a critical issue in the design of soil covers for mine tailings, acid generating waste rock, and other land based disposal systems. The flow of moisture between the soil and the atmosphere is a complex process in which three factors dominate (Wilson, 1990). These factors do not function as independent variables, but rather as a closely coupled system. The first factor is the supply of, and demand for, water imposed at the soil surface by atmospheric conditions such as total precipitation, all net radiation, wind speed, and air temperature. The second factor is the ability of the soil to transmit water and the associated water regime. Hydraulic conductivity and storage characteristics of the soil control the flow of soil moisture. The final factor involves the influence of vegetation. The type and density of vegetation affects evaporation through the consumption of water through root uptake but also along with runoff rates and surface retention. An additional factor to consider within the soil profile is the redistribution of water towards an advancing freezing front during winter in cold climates. This manual describes the computer model SoilCover that can be used for the analysis of the flow of water between the soil surface and the atmosphere based on the issues discussed above.

1.2 Model Description

SoilCover is a one-dimensional finite element package that models transient conditions. The model uses a physically based method for predicting the exchange of water and energy between the atmosphere and a soil surface. The theory is based on the well known principles of Darcy's and Fick's Laws which describe the flow of liquid water and water vapour, and Fourier's Law to describe conductive heat flow in the soil profile below the soil/atmosphere boundary. SoilCover predicts the evaporative flux from a saturated or an unsaturated soil surface based on atmospheric conditions, vegetation cover, and soil properties and conditions. A modified Penman formulation (Wilson, 1990) is used to compute the actual rate of evaporation from the soil / atmosphere boundary. A freezing and thawing formulation (Newman, 1995) is used to allow year-round modelling of soil behaviour where climatic conditions result in seasonal ground freezing and thawing.

1.3 Features and Capabilities

The primary features and modelling capabilities of SoilCover are as follows:

- Up to 100 years of simulation,
- Saturated/unsaturated transient liquid and water vapour flow,
- Soil-atmosphere flux boundary that can be specified as either a positive or negative flux (i.e. infiltration or evaporation), or calculated intrinsically based on the input climate data and the Penman Wilson (1990) or Modified Penman Wilson (Tran et al 2016) formulations,
- Soil suction, soil temperature, and water flux, and unit gradient boundary conditions,
- An option to allow for surface ponding or have excess water “run off”,
- Specification of initial soil pressure profiles and initial soil temperature profiles,
- Vegetation influences including water stress, canopy, and root depth effects,
- Moisture redistribution due to ground freezing and thawing,
- Specification of detailed climate data including minimum and maximum air temperature, net radiation, minimum and maximum relative humidity, and windspeed,
- Specification of reduced climate data including air temperature, relative humidity, and potential evaporation (windspeed is optional),
- Multi - layered soil profiles,

- Optional specification of an internal mesh node that SoilCover will automatically monitor and report cumulative fluxes at,
- Optional specification of an internal liquid source / sink nodes that are constant fluxes or functions of time (up to two functions and one constant flux),
- Optional specification of oxygen diffusion coefficients for monitoring steady state oxygen flux and concentration between soil surface and 2nd user specified node,
- Specification of hydraulic soil properties including hydraulic conductivity versus suction and water content versus suction relationships,
- Specification of thermal soil properties including thermal conductivity versus gravimetric water content and specific heat versus gravimetric water content relationships,
- User defined or SoilCover predicted thermal and hydraulic soil property functions,
- Internal adaptive time stepping scheme for daily simulations,
- Relative convergence criteria for suction and temperature applied at every node,
- Output data files providing daily profiles of volumetric and gravimetric water content, degree of saturation, matric suction, total head, temperature, ice content, hydraulic conductivity, oxygen concentration, and vapor pressure,
- Daily reporting of potential evaporation, surface flux, base flux, total evaporation, total runoff, root flux, user selected internal node flux, and,
- On-screen tabular output during program execution showing continuous daily or cumulative fluxes.

1.4 Model Application

SoilCover can be used to model one-dimensional movement of water in a cover/waste system which is subjected to infiltration and evapo-transpiration at the soil surface. Precipitation is specified by the user, while evaporation can be either user specified or calculated by SoilCover. Profiles of water content, suction, temperature, and so on can be viewed to evaluate the performance of the cover system.

1.5 SoilCover Input

The input requirements are categorized into soil type, climate parameters, vegetation parameters, boundary conditions, initial conditions, and modelling details. Examples of these input requirements are as follows:

Soil Parameters:

- soil porosity and specific gravity
- soil water characteristic curve and hydraulic conductivity data
- thermal conductivity and specific heat versus water content data
- unfrozen water content versus freezing temperature data (for freezing analysis)
is computed internally based on the Soil Water Characteristic Curve and thermodynamic equilibrium physics.

Climatic Parameters (required for detailed weather data option):

- net radiation or potential evaporation
- precipitation and rainfall start / stop hour
- minimum and maximum relative humidity
- minimum and maximum daily air temperature
- windspeed
- latitude

Vegetation Parameters:

- moisture limiting / moisture wilting point
- leaf area index – built in or user supplied
- depth of root centroid functions of time, for two root zones, a fixed depth zone and a triangular pattern zone

Boundary Conditions:

- pressure
- temperature
- Unit gradient
- Climate
- Snow melt is accumulated during winter and applied over a specified thaw period

Initial Conditions:

- water pressure
- temperature
- Or copy results from prior models and use them as initial conditions

Modelling Details:

- mesh geometry - computed automatically based on user specified soil layer data.
- convergence parameters
- time step parameters

1.6 SoilCover Output

SoilCover creates an output file that contains daily results for the following (if selected):

Actual evapo-transpiration	Matric suction profiles
Potential evapo-transpiration	Total head profiles
Surface and base flux	Temperature profiles
Root uptake fluxes	Hydraulic conductivity profiles
Total runoff	Oxygen concentration
Vol. and grav. water content profiles	Nodal ice content
Degree of Saturation profiles	Vapour pressure profiles

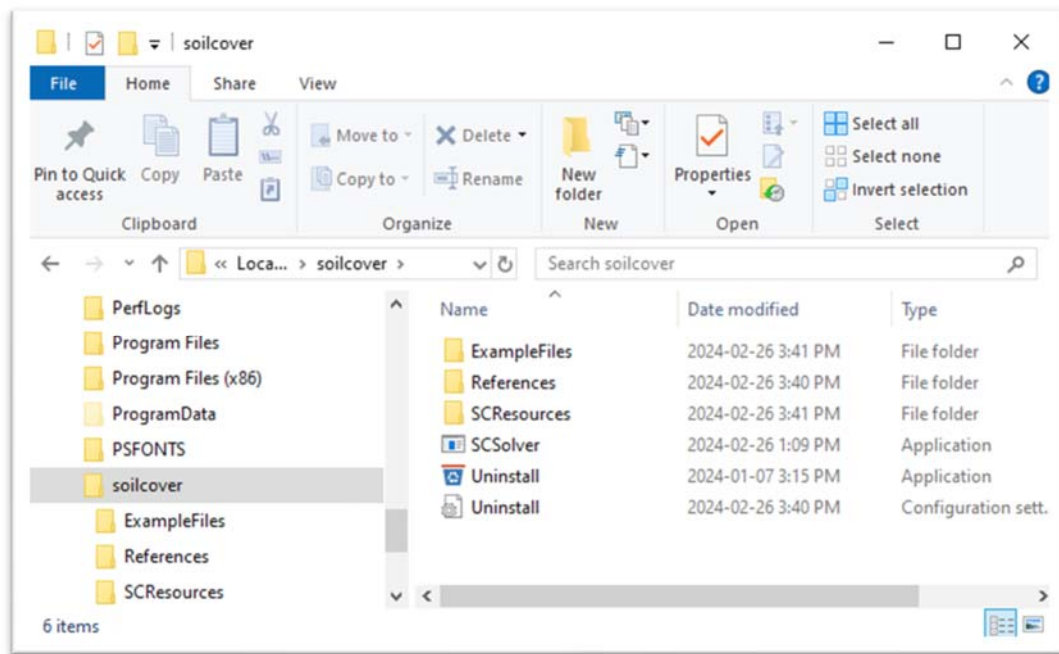
All graphs are generated automatically but you can use the power of Excel to filter data, format axes etc.

1.7 Language and Code

The processing component of SoilCover was developed and compiled with Microsoft Visual Studio Fortran and will run on 32 or 64 bit systems. The Excel program menus and dialogue boxes were created using Microsoft Visual Basic compatible with Microsoft 365.

1.8 Installation

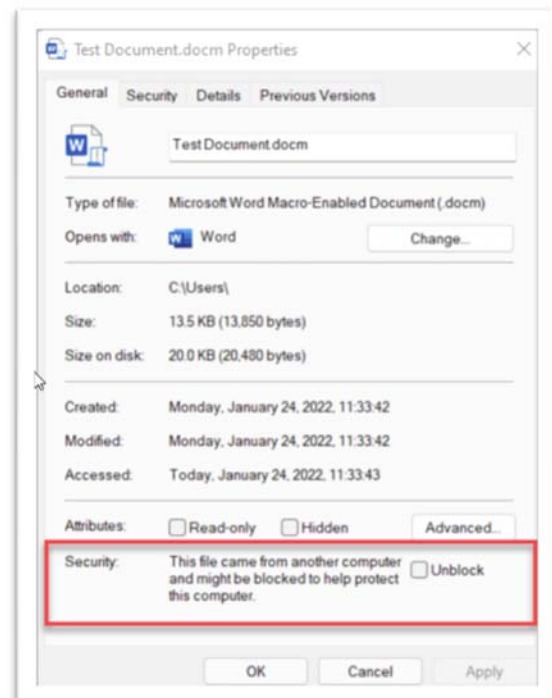
SoilCover is distributed using an installation executable file that will create the necessary file folder structure on your C:\ drive. You may need Administrator Rights to install the program. The software MUST remain in the C:\SoilCover folder, created as part of the installation. The folder structure created at the time of installation looks like:



It consists of the main folder on the C: drive plus sub folders and the solver and uninstall files. There are a few example files included that can be opened and reviewed. You can save your own projects anywhere on your computer **as long as** there are no blank spaces in the folder structure path or project file names.

The project workbook file extension is *.xlscov. These are macro enabled workbooks. The new version of Windows blocks this type of file if it is emailed to you so depending on what version of Windows/EXCEL you have installed, you may need to manually unblock them. Right click the filename in Windows Explorer, and check the security box as shown on the right.

You may still need to enable Macros in your version of Excel which you can do from inside Excel using the File-Options menu stream.



To get started with a project file it is easiest to open the NewProject.xlscov template file located in the ExampleFiles folder. Alternatively, a SoilCover icon has been installed both on the computer desktop, as well as the Quick Start menu. The menus and commands are created by an Add-In file that is loaded with the project file. When you close out of Excel, the Add-In will self-uninstall.

You can work through the menu commands in SoilCover to change a project file, give it a new name or import one of your old SoilCover projects.

SoilCover requires a valid license to save and solve files. A license can be purchased from www.SoilCover.ca or by emailing support@SoilCover.ca. We will send you a valid digital key that you will be asked for the first time you try to save and solve a project file. You must have a working internet connection for licenses to be validated at the time you try to save or solve a project file.

1.9 About SoilCover

The theory that forms the basis of the SoilCover program was developed at the Department of Civil Engineering, University of Saskatchewan, as part of G. W. Wilson's Ph.D. dissertation entitled, "Soil Evaporative Fluxes for Geotechnical Engineering Problems" completed under the supervision of Dr. D. G. Fredlund and Dr. S. L. Barbour. The computer program documented here was initially formulated as an explicit finite difference scheme (Wilson, 1990). The original program was subsequently developed into a more rigorous finite element formulation by Joshi (1993). Modification of the original formulations to include a modified Penman method (Wilson, 1990) which calculates the evaporative flux from an unsaturated soil surface using typical climate data were performed by Machibroda (1994). Swanson (1995) added the oxygen diffusion algorithm, Tratch (1995) continued development of the vegetation algorithm, and Newman (1995) added the freeze/thaw capabilities. Newman (1996) also developed the DOS Version 2.0 and Windows Version 3.0 pre and post processors as well as the revised soil property function algorithms and executable code. Versions 4 and 5 were developed by Geo-Analysis 2000 Ltd. The current SoilCover is maintained and distributed by SoilCover Software Ltd. (www.SoilCover.ca).

Initial funding for the development of the SoilCover program was through a research contract with the Government of Canada's MEND (Mine Environment Neutral Drainage) program. Dr. G. Ward Wilson was the principal investigator leading the project.

2.0 THEORY

2.1 Heat and Mass Transfer Equations

The heat and mass transfer equations derived by Wilson (1990) are used to model coupled one-dimensional transient heat and mass flow in the soil profile. The flow of water vapour and liquid water are described on the basis of Fick's Law and Darcy's Law as follows:

$$\frac{\delta h_w}{\delta t} = C_w^1 \frac{\delta}{\delta y} (k_w \frac{\delta h_w}{\delta y}) + C_w^2 \frac{\delta}{\delta y} (D_v \frac{\delta P_v}{\delta y}) \quad (2.1)$$

where:

h_w	=	Total head (m)
t	=	Time (s)
C_w^1	=	Coefficient of consolidation with respect to the liquid water phase
	=	$\frac{1}{\rho_w g}$
ρ_w	=	Mass density of water (kg/m ³)
g	=	Acceleration due to gravity (m/s ²)
y	=	Position (m)
k_w	=	Hydraulic conductivity (m/s)
C_w^2	=	Coefficient of consolidation with respect to the water vapour phase
	=	$\frac{(P + P_v)}{P \rho_w^2 g m_2^w}$
m_2^w	=	Slope of the moisture retention curve (1/kPa)
P	=	Total gas pressure in the air phase (kPa)
P_v	=	The partial pressure due to water vapour (kPa)
D_v	=	Diffusion coefficient of water vapour through the soil (kg•m/kn•s)
	=	$\alpha \beta (D_{vap} \frac{W_v}{RT})$
α	=	Tortuosity factor of soil
	=	$\beta^{2/3}$
β	=	Cross sectional area of soil available for vapour flow
D_{vap}	=	Molecular diffusivity of water vapour in air (m ² /s)
	=	$0.229 \times 10^{-4} (1 + \frac{T}{273.15})^{1.75}$

T	=	Temperature (°K)
W _v	=	Molecular weight of water (0.18 kg/kmole)
R	=	Universal gas constant (8.314 J/mole/°K).

Temperature is evaluated on the basis of conductive and latent heat transfer as follows:

$$C_h \frac{\delta T}{\delta t} = \frac{\delta}{\delta y} \left(\lambda \frac{\delta T}{\delta y} \right) - L_v \left(\frac{P + P_v}{P} \right) \frac{\delta}{\delta y} \left(D_v \frac{\delta P_v}{\delta y} \right) \quad (2.2)$$

where:

T	=	Temperature (°C)
C _h	=	Volumetric specific heat of the soil as a function of water content (J/m ³ /°C)
	=	C _v ρ _s
C _v	=	Specific heat of the soil (J/kg/°C)
ρ _s	=	Mass density of the soil (kg/m ³)
λ	=	Thermal conductivity of the soil (W/m/°C)
L _v	=	Latent heat of vapourization of water (J/kg).

SoilCover calculates the vapour pressure in the soil using the relationship provided by Edlefsen and Anderson (1943) where vapour pressure is calculated on the basis of the total suction in the liquid phase.

$$P_v = P_{sv} h_r \quad (2.3)$$

where:

P _v	=	Actual vapour pressure within the soil
P _{sv}	=	Saturation vapour pressure of the soil at its temperature, T
h _r	=	Relative humidity of the soil surface as a function of total suction and temperature
	=	$e^{\left(\frac{\Psi g W_v}{RT} \right)}$
Ψ	=	Total suction in the soil (m).

2.1.1 Verification of Heat and Mass Transfer Equations

The heat and mass transfer equations were verified by comparing them to commercially available mass transfer and heat transfer finite element packages (SEEP/W and TEMP/W). The two figures below compare SoilCover and SEEP/W results for a draining column of sand that is initially saturated. The base boundary condition was set to a pressure of 0 kPa and the column was allowed to drain. The heat transfer component of

the SoilCover program was “turned off” by setting the surface and base temperatures equal to each other.

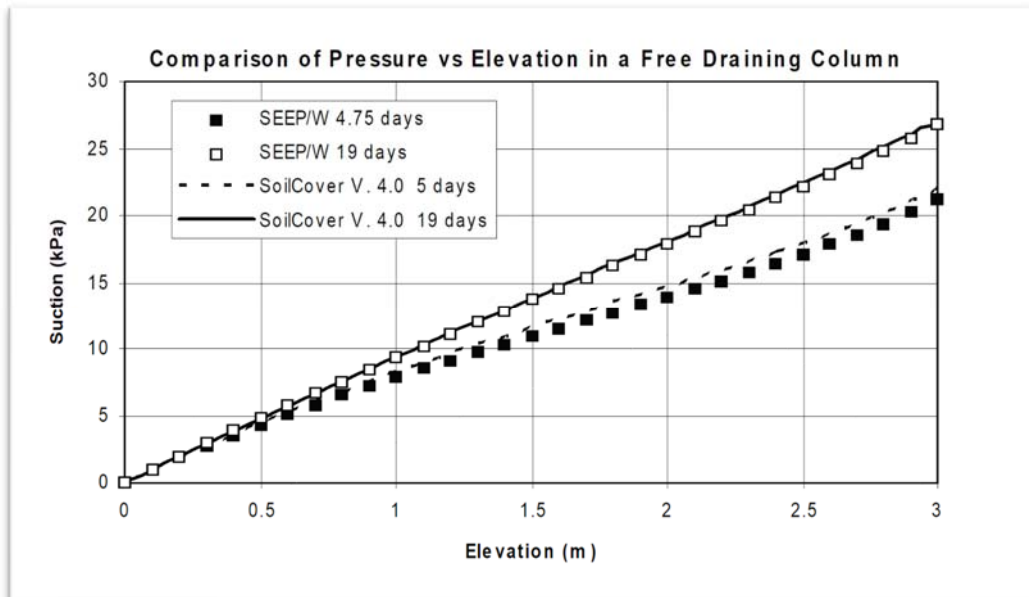


Figure 1: Verification of the Mass Transfer Algorithm (Geo-Analysis 2000 Ltd., 1997)

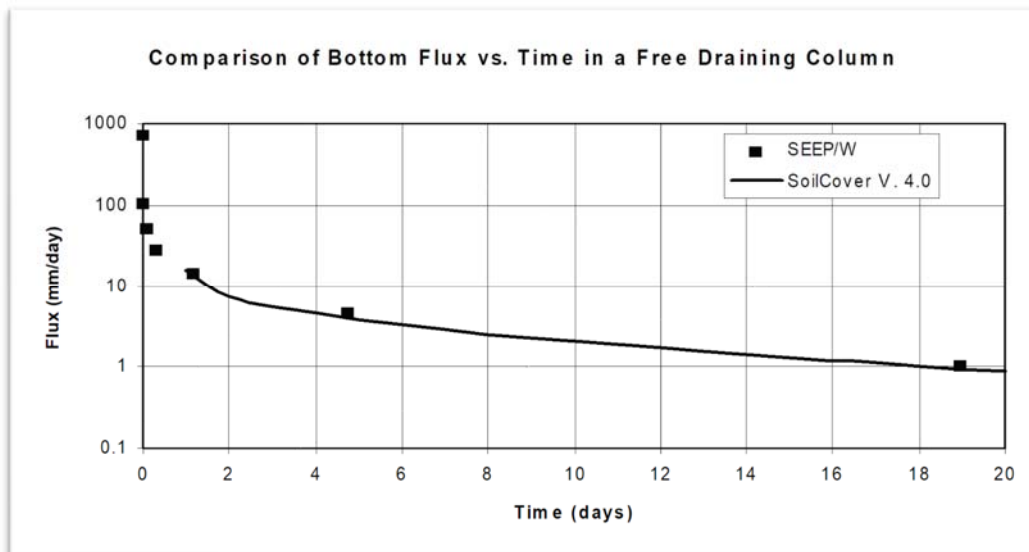


Figure 2: Verification of the Mass Transfer Analysis (Geo-Analysis 2000 Ltd. 1997)

The figure below compares SoilCover and TEMP/W results for a column of sand that is initially at a uniform temperature of 1°C. The base boundary condition was set to a temperature of 1°C and the surface temperature was set to a constant temperature of 3°C. The moisture transfer component of the SoilCover program was “turned off” by

setting the surface pressure to zero and the base pressure to hydrostatic. Evaporation was shut down by setting the pan evaporation option to 0 mm/day.

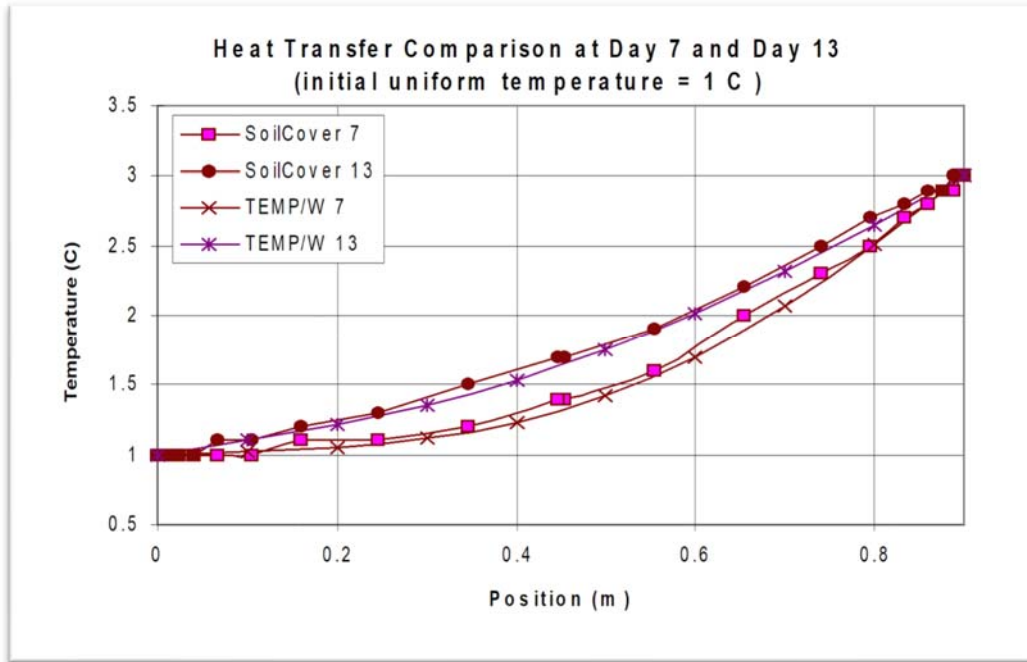


Figure 3: Verification of Heat Transfer (Geo-Analysis 2000 Ltd., 1997)

2.2 Atmospheric Coupling

Atmospheric coupling is achieved by calculating the soil evaporative flux. Soil evaporative flux is a function of the vapour pressure gradient between the cover surface and the atmosphere. A modified Penman formulation proposed by Wilson (1990) is used and is written as follows:

$$E = \frac{\Gamma Q + v E_a}{\Gamma + A_v} \quad (2.4)$$

where:

- | | | |
|----------|---|--|
| E | = | Vertical evaporative flux (mm/day), |
| Γ | = | Slope of the saturation vapour pressure versus temperature curve at the mean temperature of the air, |
| Q | = | Net radiant energy available at the surface (mm/day), |
| v | = | Psychrometric constant, |
| E_a | = | $f(u)P_a(B - A)$ |
| $f(u)$ | = | Function dependent on wind speed, surface roughness, and eddy diffusion |
| | = | $0.35(1 + 0.15U_a)$ |

U_a	=	Wind speed (km/hr)
P_a	=	Vapour pressure in the air above the evaporating surface
B	=	Inverse of the relative humidity of the air = $1/h_A$
A	=	Inverse of the relative humidity at the soil surface = $1/h_r$.

The modified Penman formulation accounts for net radiation, wind speed, and the relative humidity of both the air and soil surface while calculating the evaporation from an unsaturated soil surface. A saturated surface will have a relative humidity equal to 100% and "**A**" in the equation 2.4 will equal unity. The modified Penman formulation reduces to the conventional Penman method (Penman, 1948) when the surface is saturated. The relative humidity of the soil surface is evaluated by simultaneously solving the moisture flow equation and the modified Penman formulation.

Daily variations in temperature, relative humidity, and net radiation are represented in SoilCover using a sinusoidal relationship. For example, peak values for air temperature and net radiation will occur at midday and low values will occur in the evening and morning. For relative humidity, peak values will occur in the evening and morning and low values will occur at midday.

Temperatures within the soil profile are required for the solution of the moisture flow equation, hence the heat flow equation must also be solved simultaneously. The surface temperature may be estimated (if the information is not available to the user) with the following relationship (Wilson, 1990):

$$T_s = T_a + \frac{1}{vf(u)}(Q - E - G) \quad (2.5)$$

where:

T_s	=	Temperature at the soil surface (°C)
T_a	=	Temperature of the air above the soil surface (°C)
G	=	Ground heat flux (mm/day of equivalent latent heat).

2.2.1 Verification of Atmospheric Coupling / Actual Evaporation

Wilson (1990) performed a series of column tests on a sandy material. Two columns of sand, initially close to saturation, were allowed to dry over a 42 day period in an environmental chamber. To determine the actual evaporation from the columns, the change in mass was monitored. The columns were 30 cm in height. The bottom was a no flow boundary and the top was exposed to the air in the environmental chamber. The

air temperature was kept at 38°C. The relative humidity of the air chamber, and the temperature and relative humidity of the soil columns were measured continually.

Measured and computed actual evaporation rates are shown in Figure 4. Good agreement between measured and computed values is seen for the 42 day period. These results were obtained using the SoilCover reduced weather data option which requires potential evaporation, temperature and RH data only. The zero flux base boundary was approximated by having a very thin, very low permeability layer beneath the sand column. The base of the low permeability layer had a zero pressure boundary condition applied.

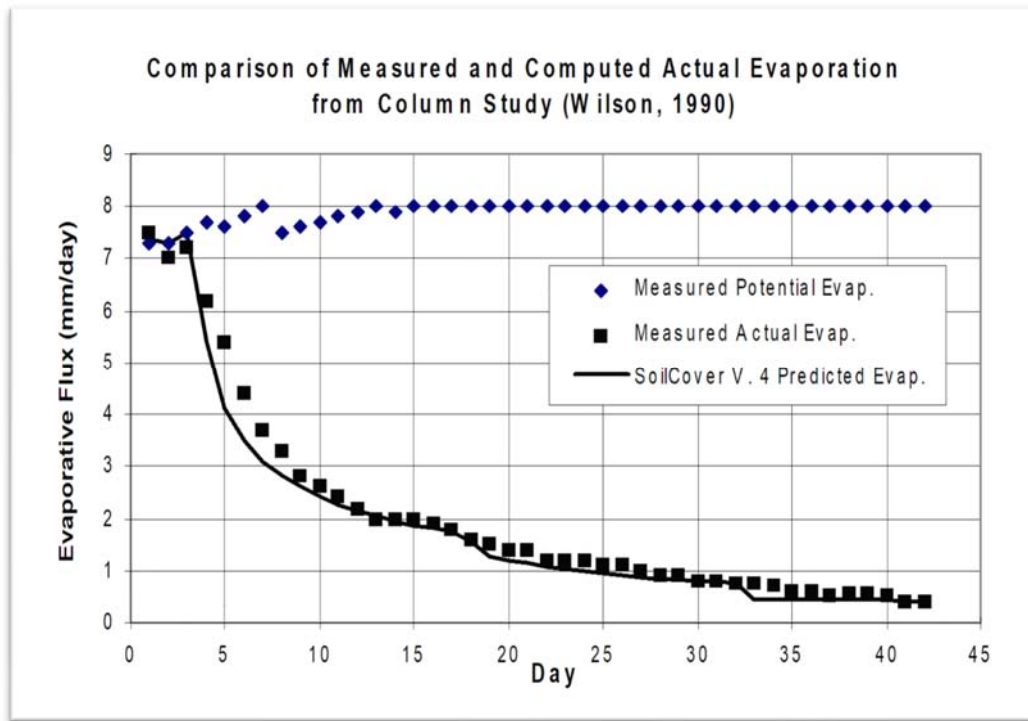


Figure 4: Verification of Actual Evaporation Calculations (Geo-Analysis

2.3 Heat And Mass Transfer Theory For Freezing Soils

The heat and mass transfer equations presented above represent the transient thermal and water pressure stress states in a soil for non-freezing conditions. To illustrate how these are modified for freezing conditions, it is advantageous to begin with the water phase continuity equation for a partially frozen soil (Newman, 1995).

$$\theta_w = \theta_u + \frac{\rho_i}{\rho_u} \theta_i \quad (2.6)$$

where:

- θ_w = total volumetric moisture content in the soil (m^3/m^3),
- θ_u = total volumetric liquid water content in the soil (m^3/m^3),
- θ_i = total volumetric ice content in the soil (m^3/m^3), and
- ρ_i = density of ice (kg/m^3).

2.3.1 Coupling the Heat and Mass Transfer Equations

Harlan (1973) provided a typical mass transfer equation for freezing in unsaturated soils. A form of the equation proposed by Harlan (1973) is as follows:

$$\frac{\partial \theta_u}{\partial t} = \frac{\partial}{\partial z} \left(k \frac{\partial}{\partial z} \left(\frac{\psi}{\rho_u g} + z \right) \right) + \frac{\rho_i}{\rho_u} \frac{\partial \theta_i}{\partial t} \quad (2.7)$$

where, θ_u is the unfrozen volumetric water content (m^3/m^3), t is time (s), z is vertical position (m), k is the coefficient of permeability (m/s), ρ_u is the density of liquid water (kg/m^3), g is the acceleration due to gravity (m/s^2), ψ is matric suction (kPa), and ρ_i is the density of ice (kg/m^3). The corresponding heat transfer equation given by Harlan (1973) is as follows:

$$\rho_c \frac{\partial T}{\partial t} = \frac{\partial}{\partial z} \left(\lambda \frac{\partial T}{\partial z} \right) - L_f \rho_i \frac{\partial \theta_i}{\partial t} \quad (2.8)$$

where, λ is the thermal conductivity of the soil ($\text{W}/\text{m} \text{ } ^\circ\text{C}$), T is temperature ($^\circ\text{C}$), ρ_c is the volumetric heat capacity of the soil ($\text{kJ}/\text{kg} \text{ } ^\circ\text{C}$), and L_f is the latent heat of fusion of water (kJ/kg).

2.3.2 Verification of Soil Freezing Theory

Newman (1995) verified the unique soil freezing equation in a modified SoilCover by simulating results of 72 hour freezing tests carried out using silica flour (similar to fine silt). The results for the test carried out on a sample initially at 10% gravimetric water content (30% saturated) are given in Figure 5 and Figure 6.

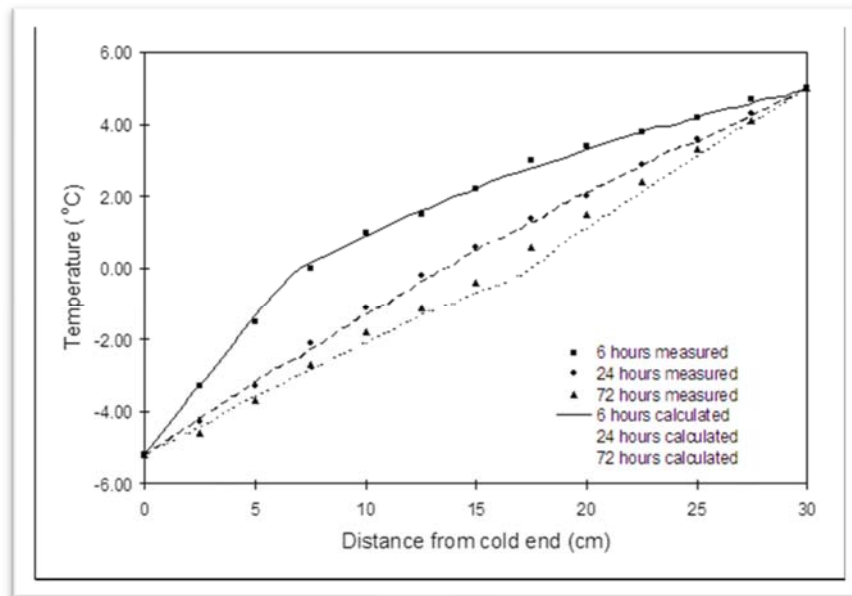


Figure 5: Temperature Profiles over Time for Silica Flour Freezing Tests

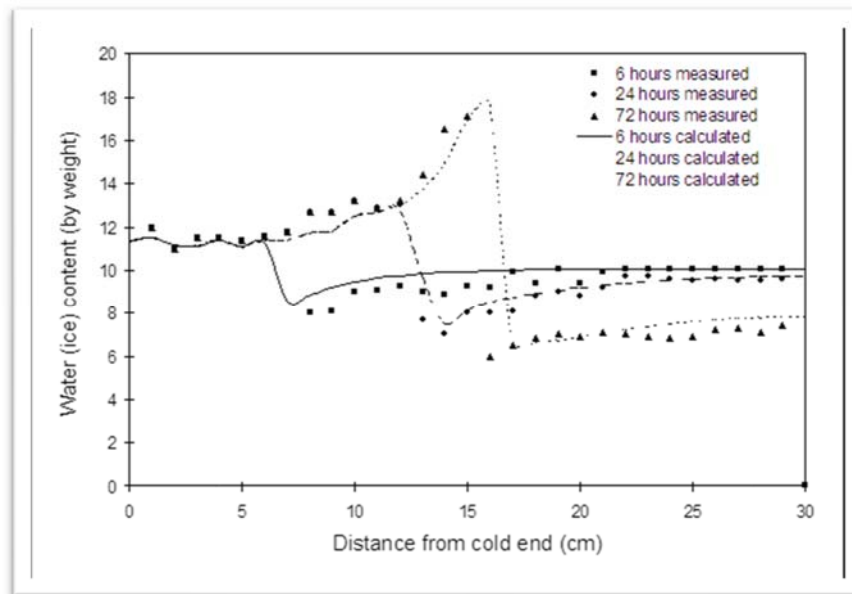


Figure 6: Water / Ice Content Profiles over Time for Silica Flour Freezing Tests (Newman, 1995)

Note in Figure 6 the buildup of ice on the left side (i.e., cold side) and the reduction in water content on the right side as the test proceeded. This figure illustrates the importance of including mass transfer in the analysis of freezing unsaturated soils.

2.4 Vegetation Effects

Vegetation plays a significant and dynamic role in the evapo-transpiration process (Saxton, 1982). SoilCover can account for vegetation effects in a manner that is dependent on the input specified by the user. A vegetative uptake source term method is combined with a shade, or cover factor term. The method used by SoilCover accounts for the effects of canopy cover, root depth and density, and water stress.

2.4.1 Moisture Limiting Point/Moisture Wilting Point

Lack of available plant water and/or high evaporative demands will cause most plants to biologically react by closing stoma, reducing transpiration, and reducing metabolic reactions (Saxton, 1982). Under continued and increasing stress the plant will reach its wilting point. The wilting point results in leaf drop and tissue death (Saxton, 1982). Between 100 kPa and 1500 kPa the plant limiting factor is reduced linearly as a function of the log of matric suction. The actual plant transpiration reaches zero at a value of suction equal to 1500 kPa. Figure 7 illustrates a typical relationship used by SoilCover to calculate the plant limiting factor. In SoilCover, the user is required to specify the moisture limiting point and the wilting point.

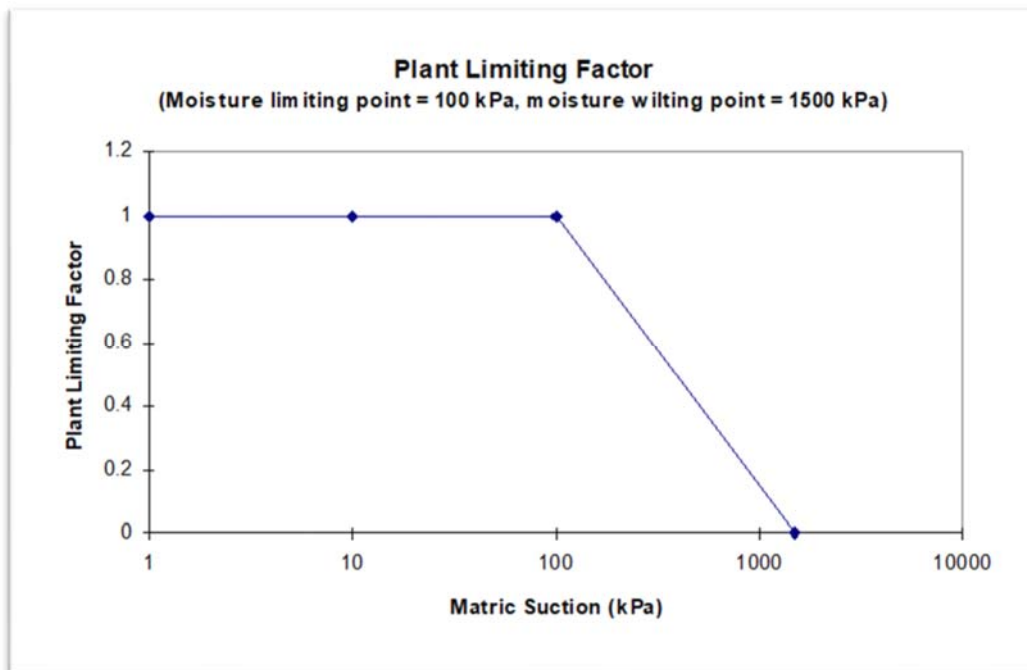


Figure 7: Plant Transpiration Reduction Versus Log Suction at the Root Centroid Node.

2.4.2 Leaf Area Index Functions

SoilCover will automatically generate a leaf area index (LAI) function for the duration of your growing season. You must enter the first day of the growing season, number of days in the growing season, and the type of grass quality expected at the site. Figure 8 illustrates the different values for the LAI. The leaf area index is used by SoilCover to reduce the amount of net radiation intercepting the soil surface, which in turn reduces the computed actual evaporation.

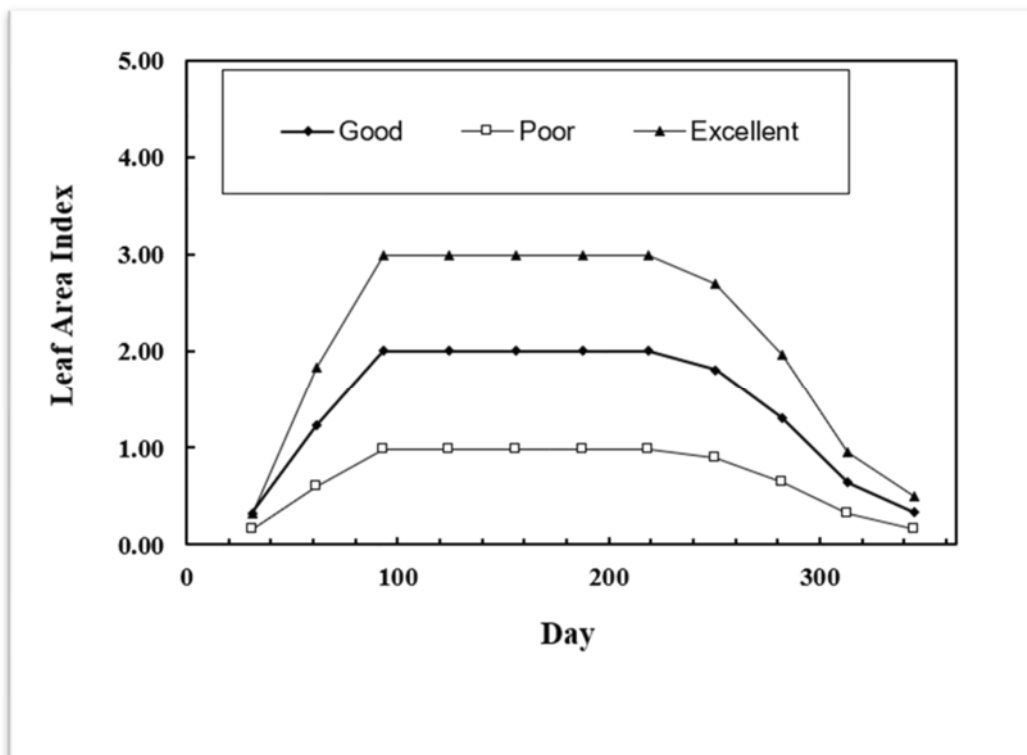


Figure 8: Leaf Area Index Function

2.4.3 Daily Root Zone Information

You are required to enter the anticipated depth to the top and bottom of the roots for every day in the analysis. This specifies a depth at which the vegetative cover will extract water from the soil profile. SoilCover treats the depth to water extraction as a nodal flux during simulations. This depth, which is user specified, should be based on the location of the centroid of the root system. This is dependent on the type and quality of vegetative cover present. Figure 9 is an example of a root system for a generic vegetative cover.

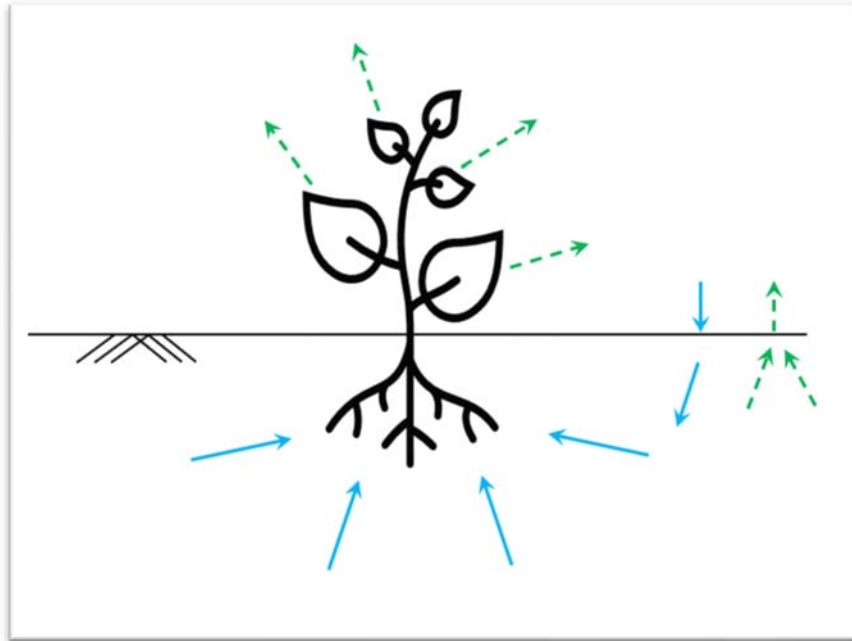


Figure 9: Root Centroid Depth, Note: Solid arrows represent liquid flow and dashed arrows represent vapour flow (after van Haveron and Brown, 1971)

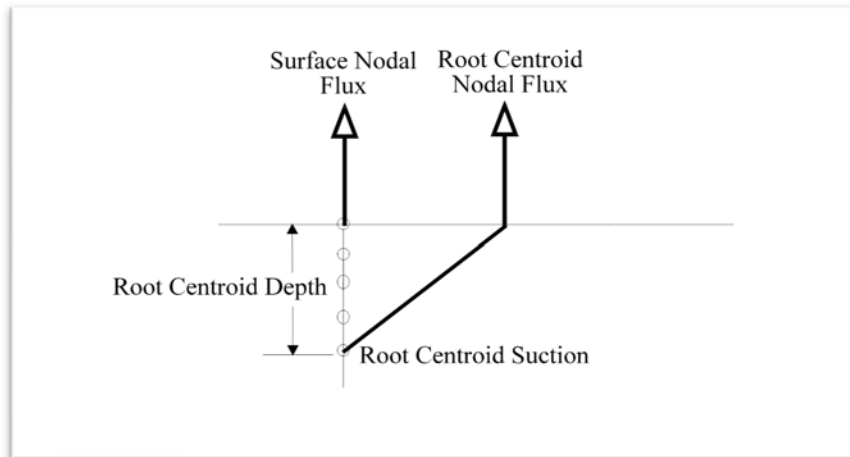


Figure 10: Surface and Root Centroid Flux Boundary Conditions

2.4.4 Verification of the Vegetation Algorithm

Tratch (1995) verified the SoilCover vegetation algorithm by modelling an evapo-transpiration experiment that was carried out in a carefully controlled environmental

chamber. The experiment was similar to the Wilson (1990) column study except, in this case, plants were allowed to grow and the leaf area index and root depth were monitored. The results of the Tratch (1995) study are given below in Figure 11. In the figure it can be seen how the growth of plants slowly shuts down the actual evaporation component, how the sum of the transpiration and actual evaporation equal the potential evaporation, and how the plant transpiration begins to shut down once the soil suction values exceed the moisture limiting point.

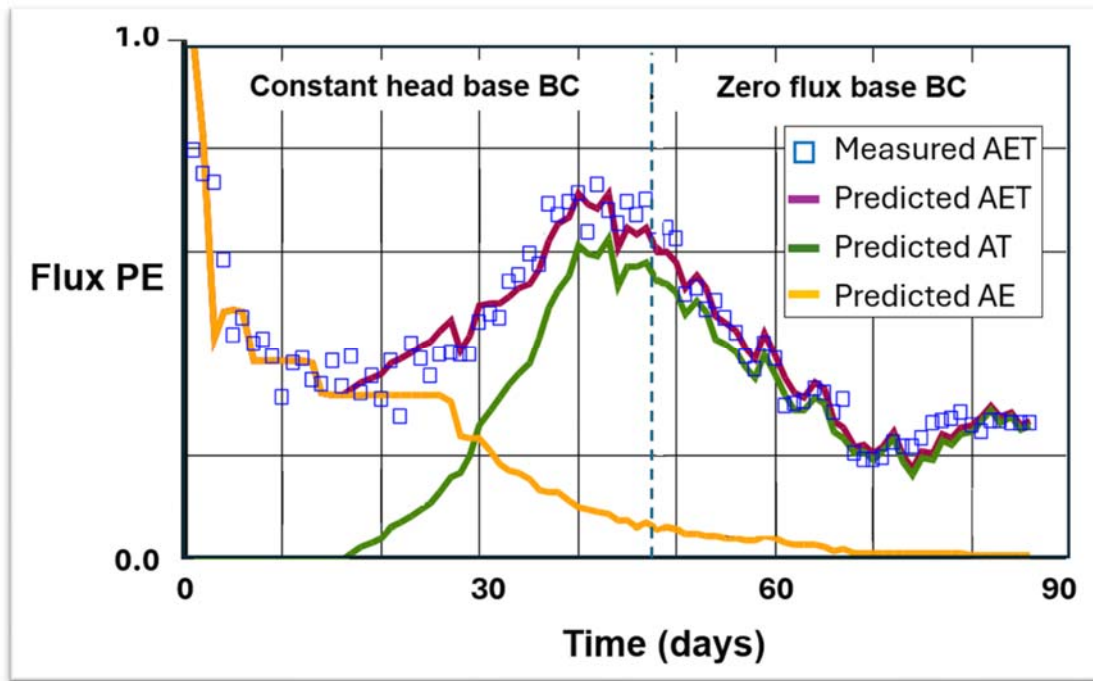


Figure 11: Verification of Vegetation Algorithm (Tratch, 1995)

2.5 Oxygen Flux Monitoring

Oxygen flux monitoring uses Fick's law for diffusion of oxygen through a user specified section of the soil. This equation is:

$$q = D_o \frac{dC_o}{dy} \quad (2.12)$$

where:

- q = the oxygen flux (g/s),
- D_o = the diffusion coefficient as a function of soil saturation (m^2/s),
- C_o = the oxygen concentration (g/m^3), and
- y = the elevation (m).

The oxygen concentration at the surface is assumed constant at 280g/m³ and the user is required to specify a concentration at one other point (mesh node number) in the cover. For example, if you are modelling a cover over waste rock you may assume that the oxidation in the waste rock consumes 90% of the oxygen. In this case, you would specify an oxygen concentration of 28g/m³ at the node which corresponds with the bottom of the cover.

In SoilCover, you are required to select a method for computing the diffusion coefficient. You can choose the method of Millington and Shearer (1971) or Nicholson (1989). If you choose the Millington and Shearer method then you do not need to have experimental curve fit parameters. If you choose the Nicholson method, then you are required to enter the 'A' and 'B' parameters. If you do not specify that you are going to monitor oxygen fluxes and concentrations, then you should not rely on the oxygen data generated by SoilCover as the program will compute fluxes for whatever default data is in the input file. This default data is necessary to make the program execute, but it may not represent your situation.

2.6 Finite Element Formulation

The finite element formulation of the SoilCover model is based on the Galerkin weighted residual approach and was developed by Joshi (1993). The finite element formulation requires replacement of vapour pressure terms in the heat flow and moisture flow equations with equivalent water pressures. The result is two equations with two dependent variables (i.e., pressure and temperature).

The global equation for moisture flow is as follows:

$$[K_W]\{\Psi_N\} + [K_{WH}]\{T_N\} + [C_1]\{\dot{\Psi}_N\} = \{F_W\} \quad (2.13)$$

where:

$[K_W]$	=	Global stiffness matrix associated with suctions
$[K_{WH}]$	=	Global stiffness matrix associated with coupling
$[C_1]$	=	Global moisture storage mass matrix
$\{F_W\}$	=	Global moisture load vector
$\{\Psi_N\}$	=	Vector of nodal heads
$\{T_N\}$	=	Vector of nodal temperatures
$\{\dot{\Psi}_N\}$	=	Time derivative of nodal heads.

Equation 2.14 gives the global equation for heat flow (Joshi, 1993):

$$[K_H]\{T_N\} + [K_{HW}]\{\Psi_N\} + [C_2]\{\dot{T}_N\} = \{F_H\} \quad (2.14)$$

where:

$[K_H]$ = Global stiffness matrix associated with temperatures

$[K_{HW}]$ = Global stiffness matrix associated with coupling

$[C_2]$ = Global heat storage mass matrix

$\{F_H\}$ = Global heat load vector

$\{\dot{T}_N\}$ = Time derivative of nodal temperatures.

Equations 2.13 and 2.14 are then combined and written as a single system of simultaneous equations for coupled moisture and heat flow:

$$\begin{pmatrix} K_W & K_{WH} \\ K_{HW} & K_H \end{pmatrix} \begin{pmatrix} \Psi \\ T \end{pmatrix} + \begin{pmatrix} C_1 & 0 \\ 0 & C_2 \end{pmatrix} \begin{pmatrix} \dot{\Psi}_N \\ \dot{T}_N \end{pmatrix} = \begin{pmatrix} F_W \\ F_H \end{pmatrix} \quad (2.15)$$

2.6.1 Convergence Criteria

SoilCover utilizes a relative convergence scheme for the dependent variables of suction and temperature. The *relative convergence* scheme is *evaluated at every node* in the system. Two convergence parameters PUSNORM and PUTNORM are used to represent the suction and temperature convergence parameters respectively.

$$PUSNORM = \frac{\text{Suction from Current Iteration} - \text{Suction from Previous Iteration}}{\text{Suction from Previous Iteration}}$$

$$PUTNORM = \frac{\text{Temperature from Current Iteration} - \text{Temperature from Previous Iteration}}{\text{Temperature from Previous Iteration}}$$

If the calculated values of PUSNORM and PUTNORM are equal to or less than the specified convergence parameters, then convergence is achieved.

The values of PUSNORM and PUTNORM are entered by the user as maximum allowable change in suction and temperature respectively. A value in percentage form is input to describe the minimum change in nodal suctions (or temperatures) that must be

obtained in order for a solution to be considered converged before proceeding on to the next time step. A value of 1% indicates that if suctions at every node change by 1 % or less between iterations, convergence will be achieved with respect to suction. If both the suction and temperature convergence criteria are satisfied at every node the solution will be allowed to proceed to the next time step.

It should be noted that since the relative convergence is applied at every node in the system very tight control is maintained. The least accurate node will be out by the specified tolerance (i.e. PUSNORM) whereas 99% of the nodes may have converged by orders of magnitude.

2.6.2 Maximum Number of Iterations Allowed to Converge During a Time Step

The maximum number of iterations required to reach convergence will vary depending on the situation. Typical values can range anywhere from 50 to 100 iterations. If a solution has not converged by 100 iterations it will likely never converge. An error message will be printed to both the screen and the output file if convergence is not achieved. The error message written to the output file will summarize the total time in seconds that convergence was not achieved for a given day.

2.6.3 Time Step Control

An adaptive time stepping scheme is used by SoilCover to automatically calculate the size of the time step during each day. The first time step of each day is specified by the user. The time step is controlled by specifying timestep tolerances. The time step tolerances refer to the maximum percentage difference allowed in nodal suction and temperature for a time step. SoilCover uses the specified tolerances to calculate a time step control parameter used to adjust the magnitude of the time step. The magnitude of the time step is calculated by dividing the previous time step by the larger of the two time step control parameters. This procedure is used to calculate an initial guess for the time step. The suctions and temperatures calculated after the first iteration of a time step are then used to calculate what the time step should have been. To control the extreme sizes of the time step the user simply specifies a minimum and a maximum time step.

TOLS and TOLT are time step control parameters used to control the size of the time steps used throughout each day. TOLS and TOLT refer to the maximum allowable percentage difference in nodal suctions and temperatures respectively that are allowed

for a particular time step. Two ratios are calculated, one is the maximum percentage change in suction over TOLS; and the other is the maximum percentage change in temperature divided by TOLT. The magnitude of the next time step guess is then determined by dividing the previous time step by the larger of the two ratios. These values should not be less than the specified convergence parameters (i.e., PUSNORM and PUTNORM). The time step is then used for the first iteration. The suctions and temperatures calculated after the first iteration are then used to back calculate what the change in time should have been in the Crank Nicholson marching-forward-in-time method used in the finite element formulation.

The minimum time step specified will be the first time step used at the start of every day. This minimum time step helps to reduce the shock imposed on the system through new boundary conditions that can be specified for each day. The maximum and minimum time steps will control the maximum and minimum size of the time step during each day. The maximum time step allowed is 86400 seconds (1 day) but to accurately simulate the diurnal variations in climate conditions a time step no larger than 1000 seconds should be used.

2.7 Calculation of Runoff

SoilCover assumes that any precipitation that cannot infiltrate will run off. This is handled within the finite element program on every iteration and for every time step as follows:

1. If the surface is not saturated the user specified **precipitation** minus any internally calculated **actual evaporation** will be applied at the top node as a liquid flux boundary condition. For small precipitation with high evaporation, this boundary flux can be negative, or leaving the soil.
2. If the surface has a zero pore pressure (i.e., saturated), then the finite element routine applies a pressure equals 0 kPa boundary condition and **runoff** equals **precipitation** minus **actual evaporation** minus **darcy flux** infiltration across the first two gauss points between the top and second node in the mesh.
3. If runoff is calculated as a negative number, then, according to the mass balance equation in step 2, the top node is passing enough darcy liquid flux to de-saturate the surface. When this occurs, the top boundary condition is applied as in step 1, above.

Note: this method has some small inherent error because in step 2 the runoff depends on the darcy flux between two points just **below** the soil surface, not **at** the surface. It is possible, to have a small water balance error when there is a very steep hydraulic gradient between the first and second nodes in the mesh. This happens, for example, when the surface is very, very dry and a rainfall event occurs. The first node wets up faster than the darcy flux below the surface can respond. The result is a low suction at the top node and a very high suction at the second node. The darcy flux used in step 2 above, is based on average material properties in the region between the top two nodes and this approximation loses accuracy when the gradient is so steep. The user is cautioned to watch the water balance values on these days and to make adjustments to input values to minimize error where possible.

2.8 Calculation of Cumulative Water Balance

SoilCover cumulates the water balance error from the first time step of the first run day, through to the end of the run. This is done as follows:

$$\% WB = \% WB + \frac{\sum \text{volume changes} - \sum \text{boundary fluxes}}{\text{initial volume}}$$

$$\sum \text{volume changes} = \text{current volume} - \text{initial volume}$$

$$\sum \text{fluxes} = \sum \text{fluxes} + \left(\begin{array}{l} \text{rain} - \text{actual evaporation} - \text{actual transpiration} \\ - \text{runoff} + \text{internal source / sink flux} - \text{bottom flux} \end{array} \right)$$

The water balance is the most important value to help you determine the reliability of your results. If the water balance error exceeds 5% to 7% by the end of your run, you should check why this happened. You can check the daily water balance values in the FLUX_SUM page once you have imported all your run data into the project workbook.

If the water balance error accumulates about the same amount each day then there is likely some error in the relationship between your M_v value, K_{sat} , or steepness of the soil water characteristic curve. If the water balance error jumps up on one day, then the error is likely due to one time step where a precipitation event occurred on a dry soil and the darcy flux (as explained in the previous section) did not respond fast enough to the rain event.

Good modelling judgment is required to assess the reliability of your results.

3.0 SOIL PROPERTIES

- SoilCover requires the following soil property information.
- Specific gravity and porosity,
- Soil water characteristic curve data,
- Saturated hydraulic conductivity,
- User defined or SoilCover generated conductivity versus suction function,
- User defined or SoilCover generated thermal conductivity versus water content function, and
- User defined or SoilCover generated specific heat versus water content function.

3.1 Soil Water Characteristic Curves (Storage Function)

The storage function describes the relationship between soil suction (negative pore-water pressure) and volumetric water content. It is fundamental to unsaturated soil mechanics. The ability of the soil to store water is a function of both the soil suction and the physical characteristics of the soil (i.e., grain size distribution, porosity, structure, etc.). Figure 3.1 shows a typical storage function with its slope function superimposed on top and referenced to the right vertical axis. The soil water characteristic curve is used to determine water contents for various suctions. These water contents are required to determine degree of saturation as well as soil thermal properties.

The volumetric water content at zero pore-water pressure is equivalent to the soil porosity. The negative pore water pressure that corresponds to the point where the curve realizes a sharp drop in water content is referred to as the air entry value (AEV). The air entry value indicates the negative pore-water pressure at which the soil will begin to de-saturate and, depending on the soil type, may or may not be well defined. Fine grained soils tend to have flat functions with high air entry values, whereas coarse grained soils tend to have steep functions with low air entry values.

The slope of the storage function in the negative pore- water pressure range is referred to as m_{2w} and the slope in the positive pore water pressure region is referred to as M_v . The M_v term is the coefficient of volume change as measured in a normal consolidation test. The slope defines the volume of water taken on or released by a change in pore-

water pressure. This function controls the transient nature of soil moisture movement. As such, it is crucial that the slope function be smooth, continuous function from zero pore pressure to 1 million kPa suction. The slope function should approach the user M_v values near saturation, then increase towards the air entry value of the soil, and then decrease towards 1 million kPa suction as shown in Figure 12.

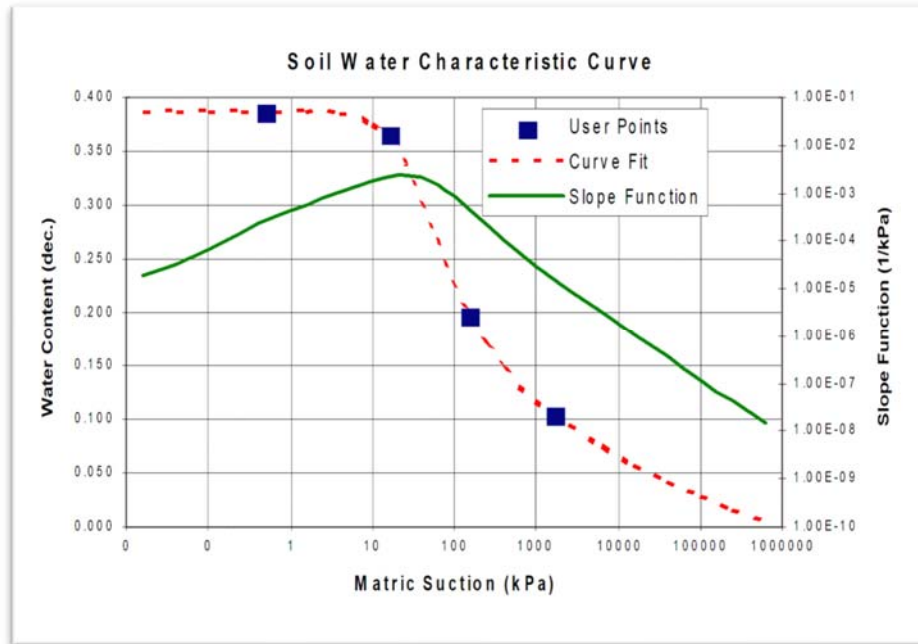


Figure 12: Volumetric Water Content Versus Suction Relationship

SoilCover analysis is somewhat sensitive to the M_v value and the saturated coefficient of permeability. The user will notice that the cumulative water balance value that appears on the screen during the simulation may, from time to time, diverge from the ideal zero percent error. When this happens, the error may be caused by assuming M_v and K_{sat} values that do not “make sense” together. The user is advised to adjust these parameters very slightly until the water balance shows minimum error. Additional causes for water balance error are slope functions that are too steep near the air entry value, or too shallow at very high suctions. Careful scrutiny of the effects of small changes to slope functions is advised. In addition, node spacings that are too large can cause error.

3.1.1 Curve Fit Features

SoilCover does not use splined functions for the soil water characteristic curve during the numerical solution. The splined functions in earlier versions were often hard to fit and convergence problems were common when the numerical solution tried to compute the slope. SoilCover uses an equation for the soil water characteristic curve developed by Fredlund and Xing (1994) and then takes the derivative of the equation to get the slope. Curve fit parameters are also used to generate a permeability function.

After you have entered your measured data points for the first time you must generate a curve fit so the curve fit parameters will be available in the program. You can generate the curve fit by pressing the button above the soil water characteristic curve showing your measured data points. The first time you generated a curve fit, the program will use a first guess for **a**, **n**, and **m** of 10, 2, 2 respectively. The curve fit subroutine will then take several seconds to generate a best-fit curve. The generated actual values of **a**, **n** and **m** will be written into the cells allocated for these values. If the curve fit you see in the graph is not to your liking, you can alter the values for **a**, **n** and **m** and run the curve fit subroutine again. This time, it will use your values of **a**, **n**, and **m** as a first guess in the solver.

It is very important to get a nice curve fit as the generated values of **a**, **n** and **m** will be used in the numerical solution for water content look-ups and slope computations. It will take a while to learn what changing **a**, **n** and **m** will do to the shape of your curve fit. In general, the '**a**' parameter controls the air entry position of the curve break, the '**n**' parameter controls the linear slope portion, and the '**m**' parameter controls the radius of curve at the residual water content. Be patient and you will eventually get a decent curve fit for all types of soils. If you have problems getting a curve fit, it sometimes helps to reduce the number of data points entered.

Figure 13 shows some example curve fit soil-water characteristic curves for three materials showing the variation in saturated porosity (volumetric water content), air entry value and the function being defined out to 1,000,000 kPa.

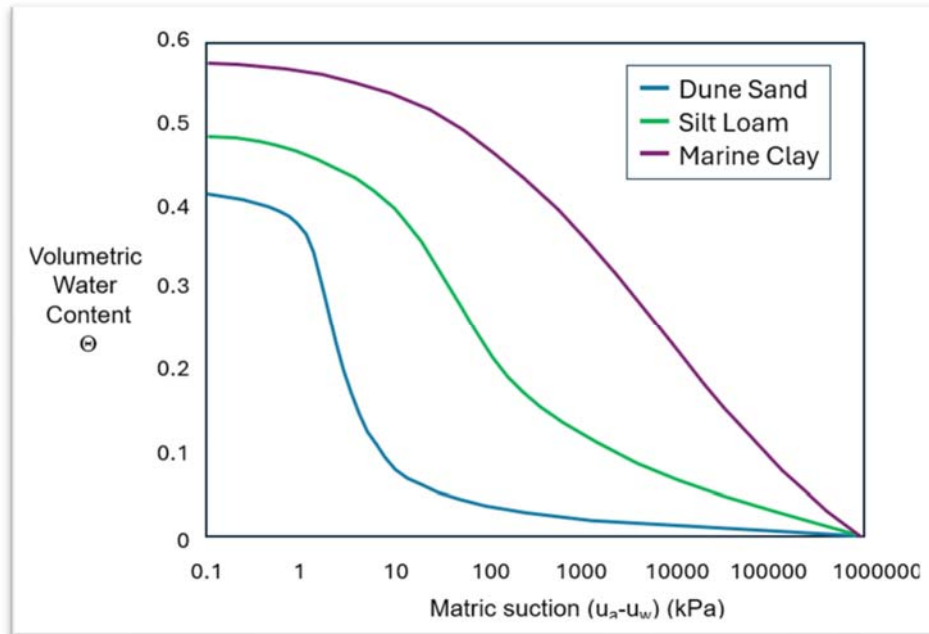


Figure 13: Soil Water Characteristic Curves (storage function) for Different Soil Types

3.2 Hydraulic Conductivity Functions

The hydraulic conductivity reflects the ability of the soil to transmit water. Water in soils flows through a series of water filled conduits as shown in Figure 14. Under saturated conditions, all the pores are available for flow and the hydraulic conductivity is at its highest (i.e., K_{sat}). As matric suctions increase, some of the interstitial pores become air-filled and the water content decreases. As the water content decreases, the pathway for liquid water flow becomes more tortuous, and as a result, the hydraulic conductivity of the soil decreases.

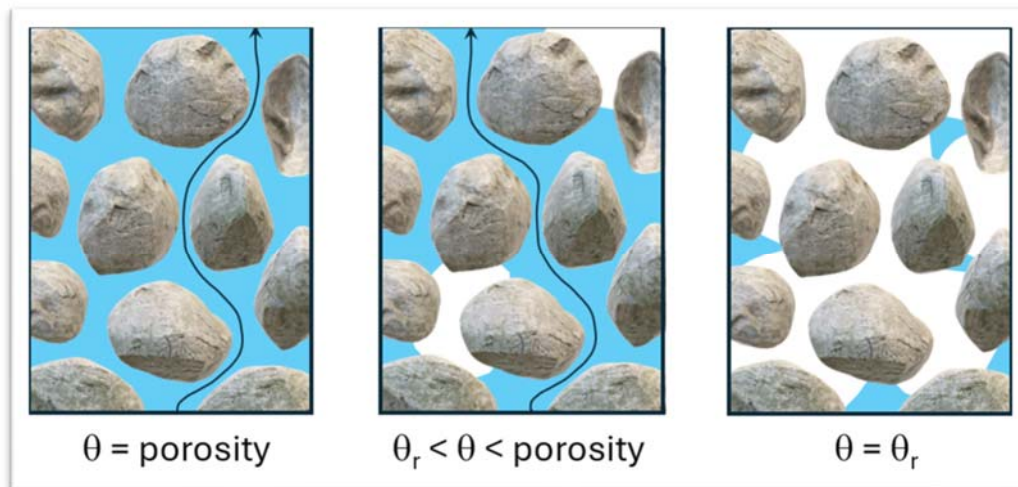


Figure 14: Schematic of Saturated and Unsaturated Soil Pores

Determination of the hydraulic conductivity function is somewhat more involved than the determination of the SWCC (storage function). Direct measurements of unsaturated hydraulic conductivity in the lab or in the field are very difficult. As a result, predictive methods have been developed which use the volumetric water content versus suction relationship. SoilCover can predict a conductivity function based on the generated curve fit SWCC. The method used by SoilCover was recently developed by Fredlund et. al. (1994) and gives excellent predictions of conductivity functions for fine-grained soil types for suctions ranging from 0 kPa to 1×10^6 kPa. It may be necessary to flatten the computed relative conductivity function for coarse grained soils at suctions well above residual. User experience is required to make these manual adjustments.

SoilCover uses *RELATIVE* conductivity functions. This means that the actual conductivity for any given suction is the relative hydraulic conductivity multiplied by the saturated hydraulic conductivity (K_{sat}). This allows the user to make slight changes to K_{sat} without having to generate a new function every time. If you do not want to use the SoilCover generated function, then you can specify your own data points.

An example of a SoilCover generated conductivity function for a SWCC is shown in Figure 15. In this figure, the SWCC is also shown to illustrate how the shape of the conductivity function begins to decrease as soon as the soil starts to de-saturate (i.e., the air-entry value of the soil is exceeded). If the user does not like the generated conductivity function, they have the option of manually adjusting any of the data points to get the desired function.

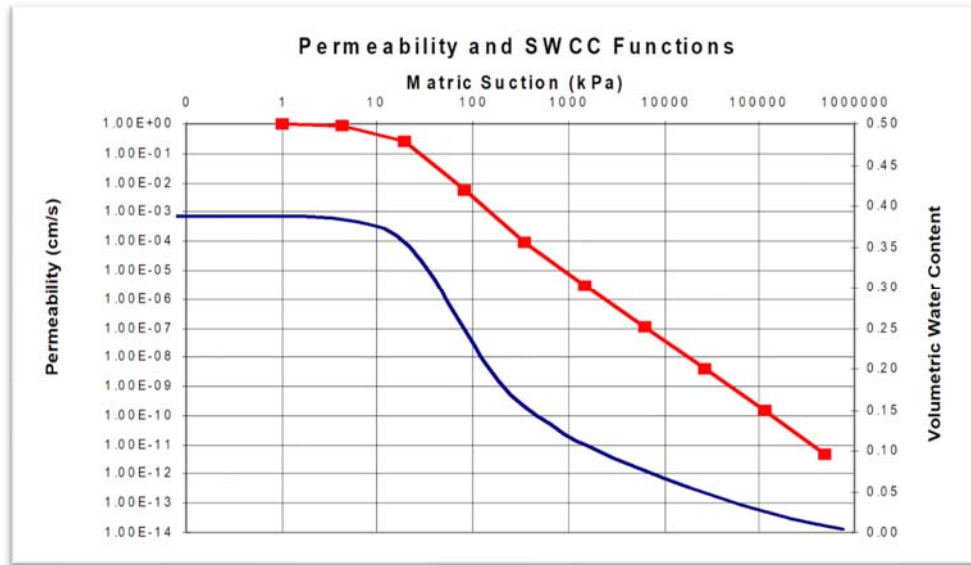


Figure 15: Unsaturated Hydraulic Conductivity vs Suction (blue – left axis) together with a Soil Water Characteristic Curve for the same soil (red – right axis)

Information about how to measure a soil water characteristic curve and saturated conductivity is provided in the Appendix.

3.3 Thermal Conductivity Function

Thermal conductivity reflects the ability of the soil to transmit heat just as the hydraulic conductivity reflects the soil's ability to transmit water. The rate at which heat is transferred depends on the temperature gradient and the thermal conductivity of the soil. The thermal conductivity of a soil can be defined as the amount of heat that flows through a unit area of soil in a unit time, under a unit gradient. The thermal conductivity relationship can be determined through experimentation or with theoretical calculations. Details regarding these methods are given in the Appendix.

As with the hydraulic conductivity function, you have the option of specifying your own data or using SoilCover to generate a function. SoilCover generates a thermal conductivity function as shown in Figure 16 using the method proposed by Johansen (1975).

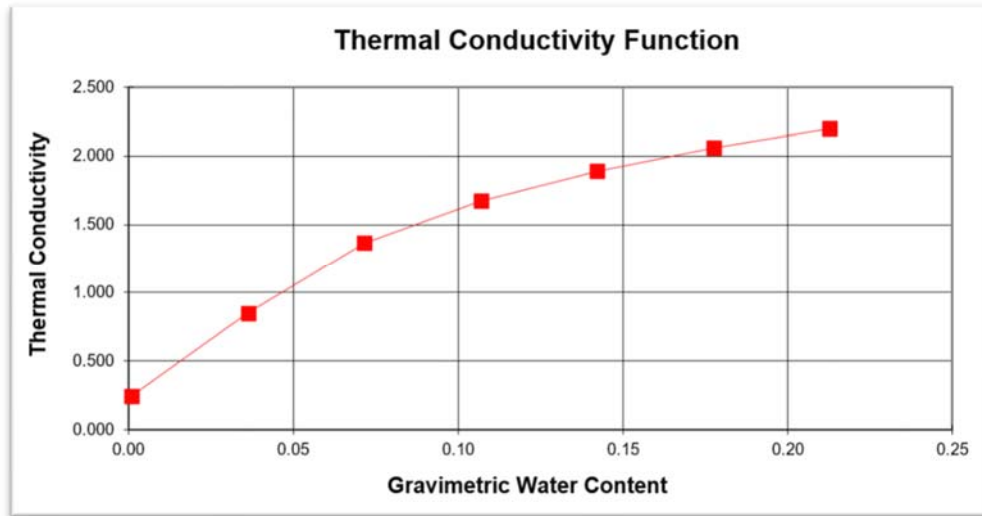


Figure 16: Thermal Conductivity Function

If you choose to have SoilCover generate the function, you must specify the overall weighted quartz percentage in the soil. This is not an easy value to determine, so typical values are given for you to try or the user can obtain a lab test that will quantify the amount of quartz in the soil sample (i.e., XRD). The typical value suggested for a clay is 0.7, that for a tailings is about 0.8, and a sand about 0.95. The user should note that the SoilCover numerical solutions have been found to be very insensitive to thermal conductivity and specific heat properties. Knowing this, you are cautioned to try and find reported thermal conductivity functions that you can match by adjusting the percent quartz value.

3.4 Volumetric Specific Heat Functions

You are required to generate a specific heat function or use the SoilCover generated function, an example of which is shown in Figure 17. The volumetric specific heat of a soil is defined as the amount of stored heat required to change the temperature of a unit volume (1 m^3) of the soil by one degree Celsius (Jumikis, 1977). The volumetric specific heat ($\text{J/m}^3\text{C}$) can be calculated from the mass specific heat as shown in Equation 3.1.

$$C_v = C_m (\rho_s) \quad (3.1)$$

where C_m is the mass specific heat ($\text{J/kg}^\circ\text{C}$) and ρ_s is the mass density of the soil (kg/m^3). Detailed methods for predicting or calculating the thermal properties required by SoilCover are also given in the Appendix.

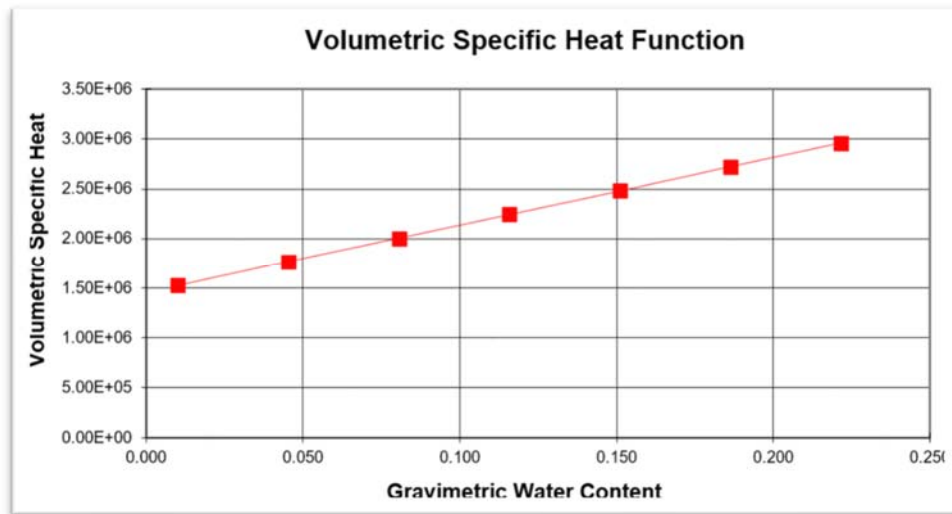


Figure 17: Volumetric Specific Heat Function

3.5 Soil Freezing Curves

A soil freezing curve is very similar in appearance to a soil water characteristic curve when plotted on a semi-log scale. The soil freezing curve serves three purposes. It can be used to determine the freezing point depression for pore-water in soils at a given water content below saturation, it can be used to determine the amount of water that remains unfrozen at any given temperature below freezing (Jame, 1972), and the slope of the curve determines how much latent heat is added to the system by the phase change during the heat and mass transfer analysis.

Typical soil freezing curves (plotted on a linear scale) are given in Figure 18 for various materials. The curves in this figure can be plotted on a semi-log scale if the user enters the necessary data points to extrapolate the curve towards the 0°C value such that it intersects 0°C at the saturated water content. The lower end of the curve on a semi-log scale can be assumed to intersect the zero unfrozen water content mark at the absolute zero temperature of -273°C .

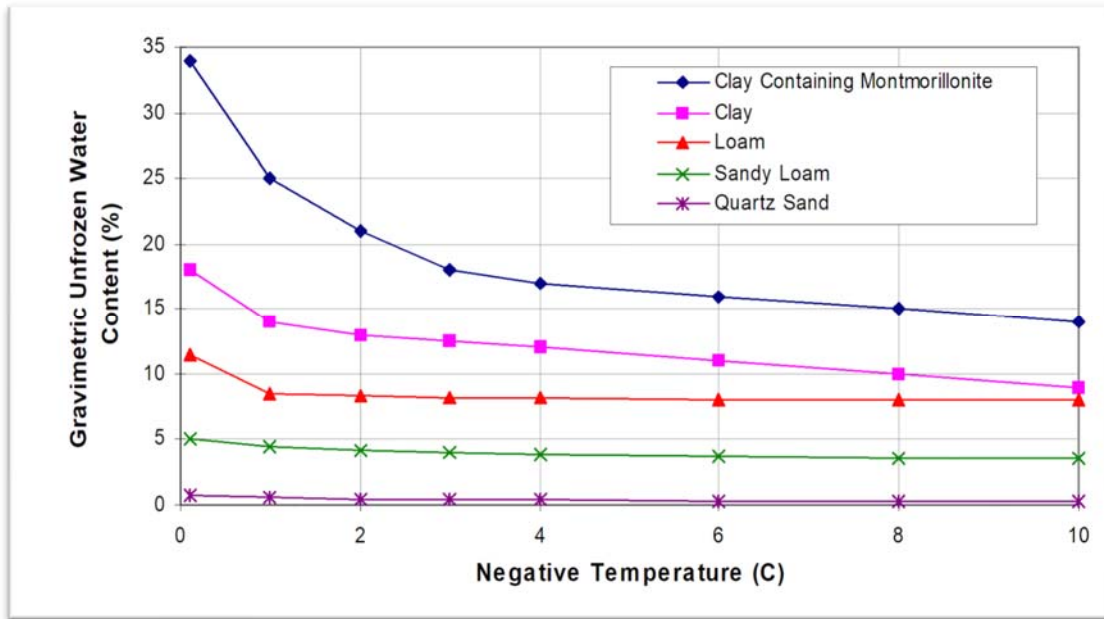


Figure 18: Soil Freezing Curves

Ideally, a soil freezing curve should be measured, but this is difficult to do. It is possible to estimate the curve using a measured soil water characteristic curve and the Clapeyron equation, which relates changes in suctions to changes in temperature based on equilibrium thermodynamics. Analysis of the Gibbs free energy for any two phases in equilibrium can be used to derive the Clapeyron equation, which relates how the equilibrium pressure changes with a change in temperature. The basic form of the Clapeyron equation is as follows:

$$\frac{dP}{dT} = \frac{\Delta h}{T\Delta V} \quad (3.2)$$

where:

- P = equilibrium pressure (kPa),
- T = temperature of the system (K),
- h = specific enthalpy difference between phases (kJ/kg), and
- V = specific volume difference between phases (m³/kg).

In the case of the phase change between water and ice, the above equation reduces to:

$$(u_a - u_w) = 1110 T^* \quad (3.3)$$

where ($u_a - u_w$) is the soil matric suction (kPa), the constant value equal to 1110 kPa/°C combines the latent heat of fusion value, specific volume, and the conversion between the freezing temperature of water in Kelvin and degrees Celsius, and the value T^* is the temperature below freezing in degrees Celsius.

The above relationship may be useful for estimating soil freezing curve data, which cannot be measured easily. There are, however, severe limitations to using this method as the Clapeyron type formulation is not ideal for soils that contain a mixture of capillary and adsorptive water forces. The freezing analysis in SoilCover uses equation 3.3 and is not intended for modelling detailed frost heave or laboratory studies. It will, however, give some indication of the tendency for moisture redistribution in freezing ground.

4.0 USING THE PROGRAM

The SoilCover user interface is all done from within Excel using custom menus and form input boxes. The exception to entering data is where the FEM mesh is created, where the soil property data is input, and where the climate data is input. In general, select the SoilCover Menu on the Excel ribbon and work from left to right.

The SoilCover menu bar within EXCEL is shown in Figure 19. There are sections to identify the project and the path / folder on your computer where it is stored. There are options to specify the application of freezing, vegetation, or evaporation. You must set up the model geometry and material properties but they are then pushed to a model page so you can visualize your model and see a summary of features you have selected. You can specify flux boundary conditions and special controls on how the climate data is used. Detailed climate data must be defined, but it can be created in another EXCEL spreadsheet and then pasted into SoilCover. There are controls on the solver convergence and automatic adaptive time stepping algorithms. The Solve button will call the Fortran solver. When complete, the results can be viewed, formatted and manipulated using the power of EXCEL.

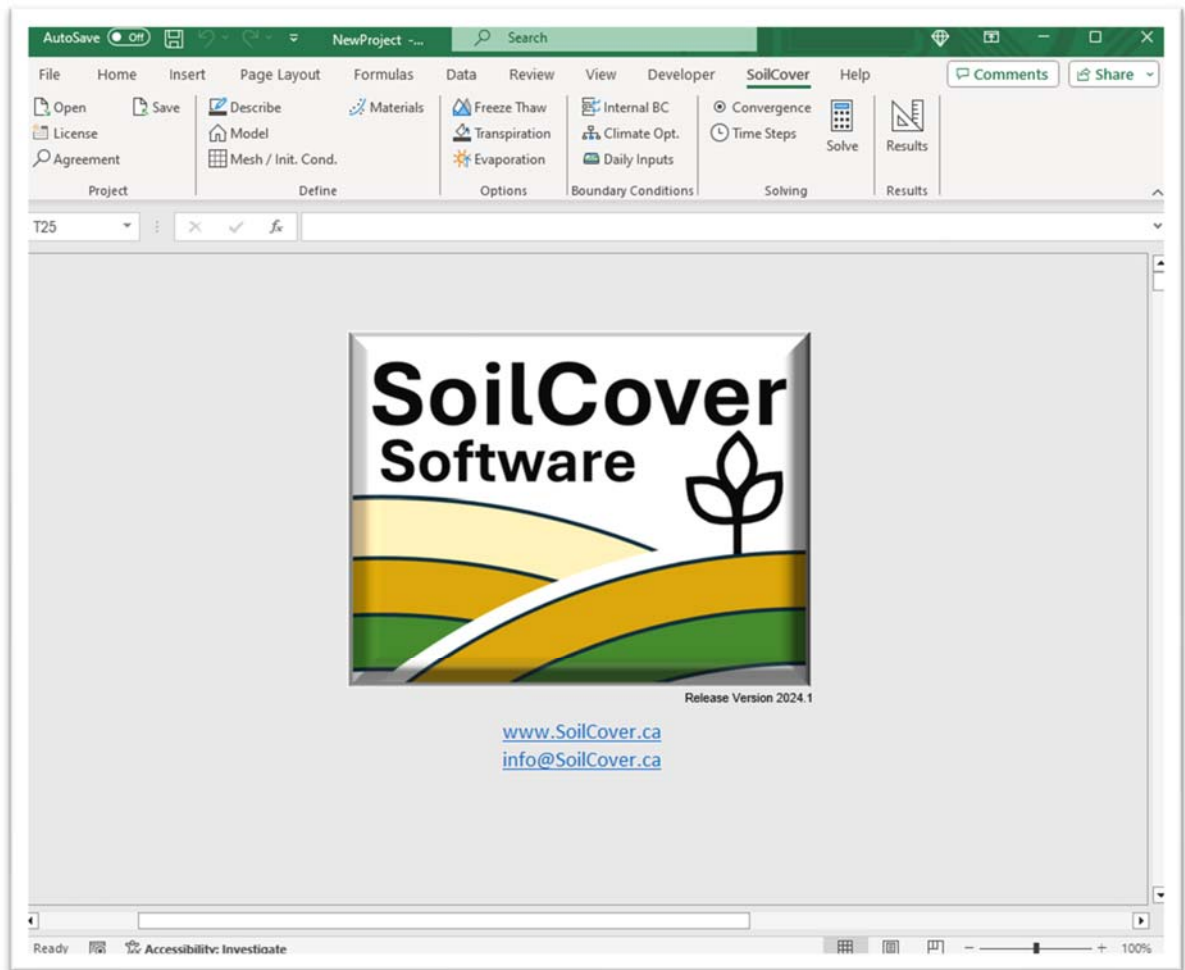


Figure 19: SoilCover Menu in EXCEL ribbon showing SoilCover specific menu items

As a rule, do not add or delete worksheet tabs manually. Use the command options in the Results menu item to do this. If you generate a graph of output data, use the Excel built in Filter button to add or hide series of data. You can also click the graph to add titles, change the axis range etc.

You can open existing project files using the main Excel File Open command and you can save it this way too. However, it is best to use the SoilCover Save option on the menu bar as it will track the project name and file path to make sure all files are in the right place.

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