Proceedings of the The 4th International Conference on Unsaturated Soils, Arizona, April 2-6, Vol.1, pp. 658-669. 2006

# Numerical Modelling of Soil-Atmosphere Interaction for Unsaturated Surfaces

G. Gitirana Jr.[1], M.D. Fredlund[2], and D.G. Fredlund[3]

[1]School of Civil Engineering, University of Goiás, Goiânia, Brazil. Praça Universitária, s/n, Setor Universitário, Goiânia, GO, Brazil 74605-220; PH +55 (62) 3204-6099; FAX +55 (62) 3204-6099; email: gilsongj@eec.ufg.br
[2]SoilVision Systems Ltd., 2109 McKinnon Avenue S., Saskatoon, SK, Canada S7J 1N3; PH +1(306) 477-3324; FAX +1(306) 955-4575; email: murray@soilvision.com
[3]Department of Civil and Geological Engineering, University of Saskatchewan, 57 Campus Drive, Saskatoon, SK, Canada S7N 5A9; email: unsaturatedsoil@yahoo.com

## *Abstract*

The computation of soil-atmosphere water fluxes such as infiltration, evapotranspiration, and runoff is required for the analysis of numerous problems in geotechnical, geoenvironmental engineering and hydrogeology. The soil-atmosphere interaction processes can be represented by a series of partial differential equations. This paper presents a PDE formulation that was developed for soil-atmosphere analysis and presents three cases demonstrating the application of the formulation developed to laboratory and fields conditions. Comparisons against experimental data show that evaporative fluxes can be successfully reproduced by theoretical models. The PDE solutions were used for the simulation of the fluxes through two soil cover configurations to exemplify the application of theoretical models to design. The results indicate that the manner how runoff is computed strongly affects the results. The numerical solutions appear robust and can be applied to the design of soil structures such as soil-cover systems, geo-hazard hazard quantification, and other unsaturated soil problems.

## 1. INTRODUCTION

The computation of soil-atmosphere water fluxes (e.g., infiltration, evapotranspiration, and runoff) is required for the analysis of numerous problems in geotechnical, geoenvironmental engineering and hydrogeology. The design of earth covers, for instance, requires the prediction of water fluxes through the cover as a function of the soil properties and atmospheric forcing conditions.

The analysis of soil-atmosphere water fluxes problems can be undertaken within the framework of partial differential equation (PDE) solutions. This paper describes a PDE formulation that was developed for soil-atmosphere analysis and presents three cases demonstrating the application of the formulation developed to laboratory and fields conditions.

## 2. THEORETICAL FRAMEWORK

Several physical processes are involved in the flow of soil moisture. Moisture moves through soils driven by gradients of total head of each of the moisture phases (i.e., liquid water and water vapour) and other gradients, such as heat and chemical gradients. In order to obtain the equations governing moisture transfer constitutive flow laws and water volume change constitutive laws are combined with conservation equations. Appropriate equations for the soil-atmosphere flux boundary conditions are also required.

### 2.1 Partial differential equations for water and heat flow

The two-dimensional PDEs presented herein are simplifications of the general equations presented by Fredlund and Gitirana Jr. (2005). Combining the equation of conservation of mass for the water phase, Darcy's law for the flow for liquid water, Fick's law for the flow of water vapor, and Lord Kelvin's relative humidity equation, the following PDE is obtained:

$$\begin{aligned}&\frac{\partial}{\partial x}\left[k^{w}\frac{\partial}{\partial x}\left(\frac{u_w}{\gamma_w}+y\right)+\frac{k^{vd}}{\gamma_w}\frac{\partial u_w}{\partial x}-\frac{k^{vd}}{\gamma_w}\frac{u_w}{(T+273.15)}\frac{\partial T}{\partial x}\right]\\&+\frac{\partial}{\partial y}\left[k^{w}\frac{\partial}{\partial y}\left(\frac{u_w}{\gamma_w}+y\right)+\frac{k^{vd}}{\gamma_w}\frac{\partial u_w}{\partial y}-\frac{k^{vd}}{\gamma_w}\frac{u_w}{(T+273.15)}\frac{\partial T}{\partial y}\right]=m_2^{w}\frac{d(u_a-u_w)}{dt}\end{aligned} \qquad [1]$$

where $k^w$ = hydraulic conductivity function; $u_w$ = pore-water pressure; $\gamma_w$ = unit weight of water; $y$ = elevation; $k^{vd}$ = vapour diffusivity; $T$ = temperature; $m_2^w$ = slope of the soil-water characteristic curve; and $u_a$ = pore-air pressure.

A PDE governing heat flow must be solved along with Eq. 1 for the variables $u_w$ and $T$. In order to obtain the heat flow PDE, the equation of conservation of heat must be combined with the heat flow laws (conduction and latent heat), and Lord Kelvin's equation. Furthermore, the total amount of heat within the R.E.V. must be written as a function of the volumetric specific heat of the soil. The following equation results:

$$\begin{aligned}&\frac{\partial}{\partial x}\left[\left(\lambda-L_v k^{vd}\frac{\rho_w}{\gamma_w}\frac{u_w}{T+273.15}\right)\frac{\partial T}{\partial x}+L_v k^{vd}\frac{\rho_w}{\gamma_w}\frac{\partial u_w}{\partial x}\right]\\&+\frac{\partial}{\partial y}\left[\left(\lambda-L_v k^{vd}\frac{\rho_w}{\gamma_w}\frac{u_w}{T+273.15}\right)\frac{\partial T}{\partial y}+L_v k^{vd}\frac{\rho_w}{\gamma_w}\frac{\partial u_w}{\partial y}\right]=\zeta\frac{\partial T}{\partial t}\end{aligned} \qquad [2]$$

where $\lambda$ = thermal conductivity of the soil; $L_v$ = latent heat of vaporization; $\rho_w$ = specific mass of water; and $\zeta$ = volumetric specific heat of the soil.

Equations 1 and 2 present five non-linear unsaturated soil property functions (i.e., $k^w$, $k^{vd}$, $m_2^w$, $\lambda$, and $\zeta$) that render the equations non-linear. Equation 1 may be simplified by neglecting temperature gradients and neglecting Eq. 2. This simplification will be employed in one of the computer codes presented in the next sections.

## 2.2 Soil-atmosphere coupling

The net soil-atmosphere moisture flux is a function of some of the key components of the hydrology cycle; namely, precipitation, actual evaporation, and run-off. The net soil-atmosphere flux may result in either infiltration (positive flux) or exfiltration (negative flux) as indicated by the following water balance equation:

$$NF = P\cos\alpha - AE - R \qquad [3]$$

where $NF$ = the net moisture flux; $P$ = precipitation; $\alpha$ = ground surface slope; $AE$ = actual evaporation; $R$ = runoff.

The terms in Eq. 3 are illustrated in Fig. 1. The net moisture flux, $NF$, corresponds to a natural (i.e., flux) boundary condition. The amount of precipitation, $P$, is a "known" input. The term $\cos\alpha$ is based on the assumption that precipitation falls in a vertical trajectory and is typically measured on a horizontal surface. The terms $AE$ and $R$ are a function of weather and the soil suction at the soil-atmosphere boundary.

Actual evaporation can be computed based on the potential evaporation and a limiting function (Wilson et al., 1997). Runoff must be computed in an interactive manner. If the embankment being analysed has an efficient drainage system, any runoff water will be removed from the ground surface. In this case, the amount of net moisture flux, $NF$, should not produce pore-water pressures higher than zero at ground surface. The following equations can be used to represent this condition (Gitirana Jr., 2005):

$$NF = \begin{cases} P\cos\alpha - AE & : \text{if } P\cos\alpha - AE > 0 \text{ and } u_{ws} < 0 \\ EF(0 - u_{ws}) & : \text{if } P\cos\alpha - AE > 0 \text{ and } u_{ws} \geq 0 \\ P\cos\alpha - AE & : \text{if } P\cos\alpha - AE \leq 0 \end{cases} \qquad [4]$$

where $u_{ws}$ = pore-water pressure at the surface; $EF$ = a large number.

If the multiplier $EF$ tends to infinity, the area flux boundary condition $NF = EF(0 - u_{ws})$ becomes mathematically equivalent to an essential (i.e., node value) boundary condition, $u_w = 0$. Therefore, the boundary condition from Eq. 4 is an alternative to switching to an essential boundary condition when the pore-water pressure at the soil surface becomes positive.

The approach based on switching boundary conditions often results in numerical oscillations due to instantaneous changes on node values. These instantaneous $u_w$ value changes do not represent real-world conditions. Instantaneous changes in node values require mesh refinements that should theoretically be infinitesimal (Gitirana Jr., 2005, Nelson, 2004). Equation 4 appears to impose a more realistic condition.

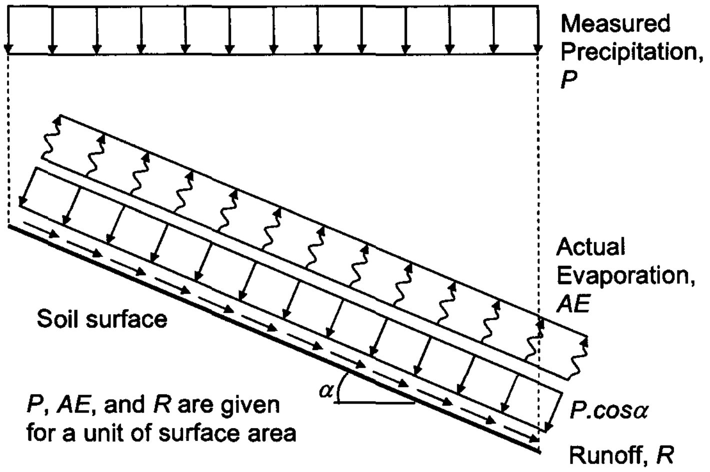

Figure 1 Soil-atmosphere moisture flux components.

## 3. METHODOLOGY

Two software packages were used in this study; namely, SVFlux and Vadose/W. SVFlux (SoilVision Ltd., 2005) is a seepage analysis package capable of solving 1D, 2D, and 3D seepage problems under steady-state and transient conditions. SVFlux uses FlexPDE (PDE Solutions Inc., 2005) as a PDE solver engine. Liquid water and water vapour flow are considered in the PDEs adopted, according to the formulation presented in Gitirana Jr. (2005). Soil-atmosphere interaction is reproduced using Eq. 4. SVFlux makes use of an automatic adaptive mesh technique. The adaptive mesh refinement algorithm is tuned to be sensitive to high gradients in pore-water pressure, hydraulic conductivity, or any other variable that needs to be solved with a given desired accuracy.

Vadose/W (Geo-Slope International, 2005) is capable of solving seepage problems where soil-atmosphere interaction is of interest. Vadose/W is primarily a 2D package but can be used for 1D problems through the use of appropriate geometries and boundary conditions. Vadose/W has a special feature that allows the accumulation of runoff in surface depressions and subsequent infiltration. The mesh construction in Vadose/W is manual and the mesh remains fixed throughout the analysis.

Vadose/W uses a technique for computing infiltration and runoff were "natural" and "essential" boundary conditions are switched based on the soil conditions at the ground surface. The ground surface is treated as a "potential seepage surface". The instantaneous application of "essential" boundary conditions that are not continuous may result in numerical oscillations. However, small time steps are expected to minimize such oscillations.

Three problems were investigated as part of this study. First, the data from a laboratory evaporation test was reproduced. Significantly high gradients were expected in this problem, resulting in demanding computations. Next, two problems are analyzed that involved alternating weather conditions. The fluxes past soil covers associated with the reclamation of mine sites are presented.

## 4. ANALYSIS OF EVAPORATION FROM A SOIL COLUMN LABORATORY TEST

This verification example demonstrates the coupling between moisture and heat and the importance of the water vapour flow component during evaporation. The results of a sand column drying experiment performed by Wilson (1990) were selected. Both experimental and simulation results are available for comparison. The drying test was performed in the laboratory, under controlled temperature and relative humidity conditions. Measurements of actual evaporation and the distributions of temperature along the column depth were obtained, providing several measures that can be used for the verification of the theoretical and numerical model. Wilson (1990) presented also a one-dimensional finite difference numerical model called "Flux" for the simulation of the drying test. Reasonable results were obtained from the comparison of measured data and results computed using the Flux program. Both the measured and computed results from Wilson (1990) are compared against the result obtained using the numerical model presented herein.

Figure 2 presents the geometry of the drying column experiment and the initial and boundary conditions. Due to the problem geometry and boundary conditions, the flow is essentially one-dimensional. Therefore, the three-dimensional axisymmetric geometry was reduced to a one-dimensional problem. Boundary conditions forcing zero water and heat flow were applied at the bottom and lateral boundaries.

More complex boundary conditions were applied to the upper boundary, which is in contact with the atmosphere. The temperature boundary condition applied to the upper end of the column was the experimentally measured surface temperatures. The moisture flow boundary condition applied was Eq. 4 along with the actual evaporation equation proposed by Wilson et al. (1997). The values of potential evaporation required by the equation proposed by Wilson et al. (1997) were obtained during the drying column test; from measured values of evaporation from a water pan. Wilson (1990) presents additional variables required by the soil-atmosphere coupling boundary condition; namely, the relative humidity and the air temperature.

The soil selected by Wilson (1990) for the analyses was the Beaver Creek sand. Figure 3 presents the hydraulic soil properties of the soil used. The soil-water characteristic curve was obtained by Wilson (1990) using Tempe cell tests and desiccators. The hydraulic conductivity function was obtained from the saturated hydraulic conductivity obtained in the laboratory and using the Brooks and Corey equation. The moisture conductivity corresponding to the vapour diffusion coefficient is also presented in Fig. 3. A comparison of the functions $k^w$ and $k^{vd}$ provides an estimation of the range of soil suction and water content for which liquid water flow or water vapour flow dominate. For the Beaver Creek sand, vapour diffusion takes over for values of soil suction higher than 20 kPa and degree of saturation lower than approximately 20%. The highly steep hydraulic conductivity function shown in Fig. 3 poses a considerable challenge for the numerical model.

Figure 4 presents the thermal property functions of the Beaver Creek sand. These functions were obtained using the formulations presented by de Vries (1963). According to the prediction equations, the thermal conductivity and the volumetric specific heat are function of the characteristics of the individual phases and are functions of the amount of water stored in the soil. The effect of the amount of water stored in the soil pores is shown by the decrease in thermal conductivity and volumetric specific heat, as soil suction increases.

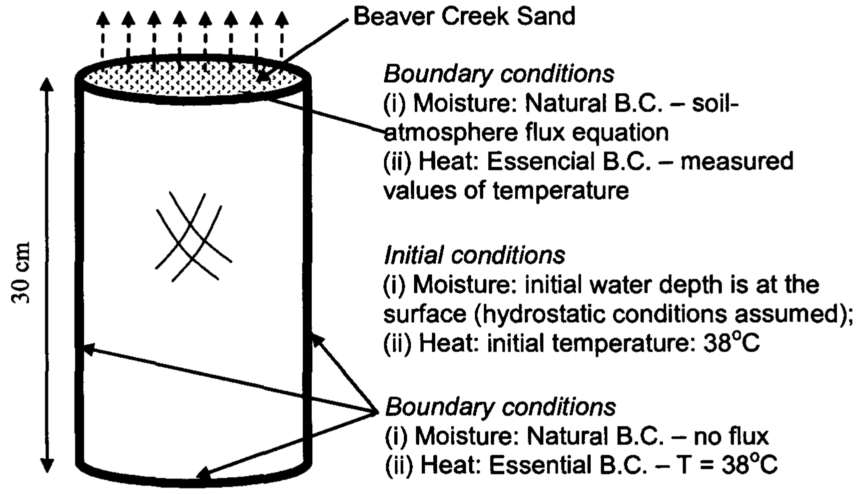

Figure 2 Numerical simulation of the drying column test – initial and boundary conditions (Wilson, 1990).

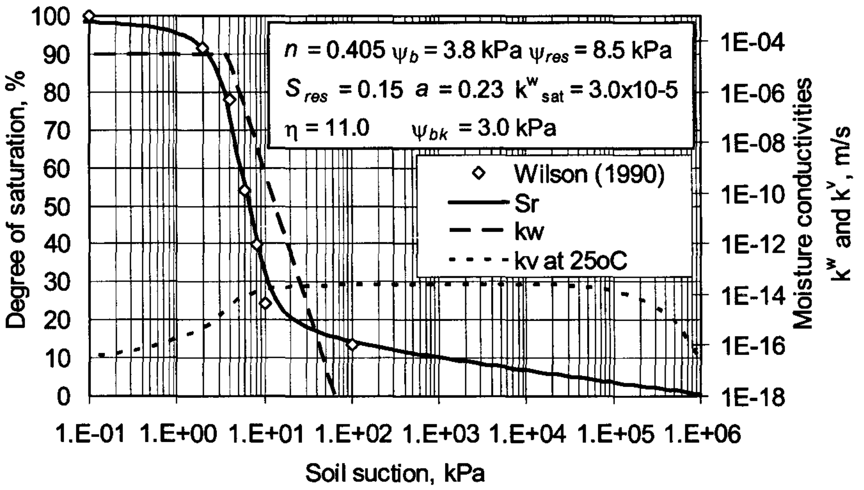

Figure 3 Hydraulic properties for the Beaver Creek sand.

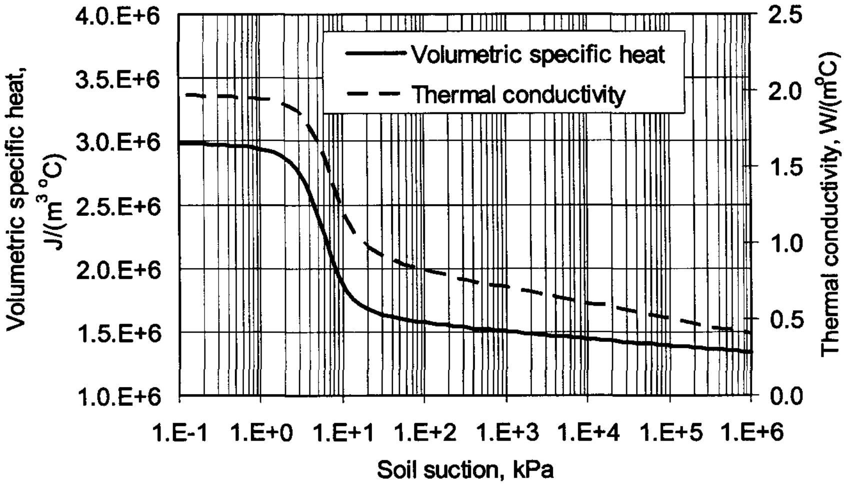

Figure 4 Thermal properties for the Beaver Creek sand.

The experiment and the numerical analyses were carried out for a period of 40 days. Figure 5 presents the actual evaporation values obtained experimentally, using the numerical model proposed by Wilson (1990), using a fully coupled solution presented by Gitirana Jr. (2005) and using a isothermal solution provided by SVFlux. Close agreement was observed between the all the results. The hydraulic property functions of the sand are extremely steep, and pose a numerical challenge. The automatic mesh and time refinement procedures were able to track the nonlinearities and ameliorate the numerical difficulties in solving the nonlinear system. The computing time required was approximately 20 hours on a Pentium 3 600MHz.

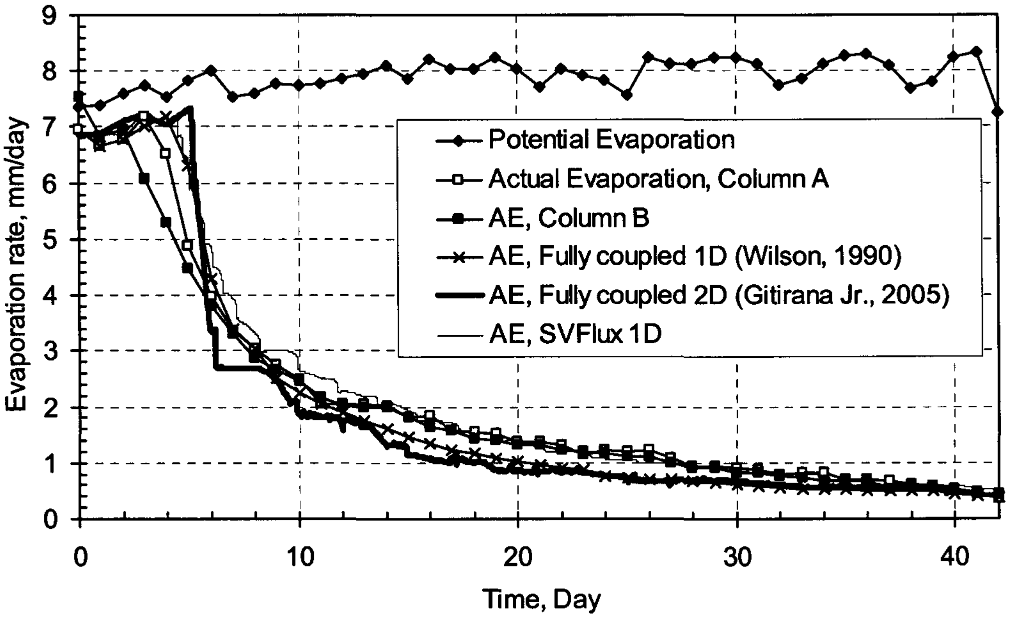

Figure 5 Verification of the coupled heat and moisture flow model: evaporation rates.

Figure 6 presents the pore-water pressure profiles for $t = 29$ days. Close agreement is observed between the experimental measurements, the results obtained using the numerical codes. A sharp drying front is observed. The pore-water pressure near the ground surface corresponds to a considerably dry condition, and approaches 1,000,000 kPa as time advances. The difficulty in computing extremely low hydraulic conductivities at the drying front were considered the cause of the small differences between computed and measured values.

Figure 7 presents the temperature profiles for $t = 1$ day, 6 days, and 12 days. Close agreement is once again observed between the experimental measurements and the computer code results. As the soil begins drying, the surface starts to cool, because of the latent heat of vaporization (see profile for day 1 in Fig. 7). The profiles for day 6 and 12 show that the cooling front follows the drying front, as expected.

## 5. ANALYSIS OF TWO SOIL COVER CONFIGURATIONS

Analysis of infiltration past soil covers is a common type of analysis used in the long-term reclamation of mine sites. 1D or 2D finite element seepage software packages are typically used for this type of analysis. The final proposed design is often based on the results of the finite element analysis of the system. Calculation of actual evaporation rates and runoff becomes significant in the long-term fluxes through cover systems. Two soil column problems were used to illustrate the impact of varying methods of calculating runoff, infiltration, and evaporation on calculations performed over the course of one year. In the examples presented here the input data was kept as much the same as possible between the various computer codes.

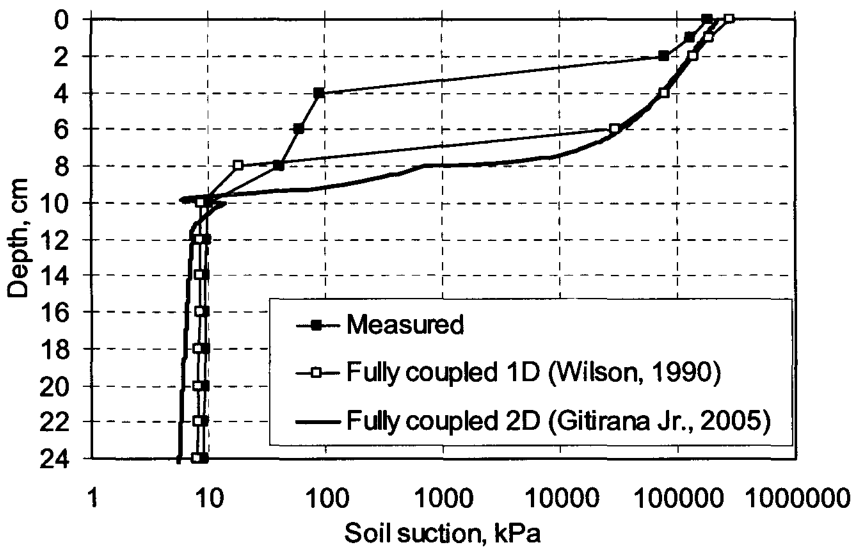

Figure 6 Verification of the coupled heat and moisture flow model: pore-water pressure distributions for $t = 29$ days.

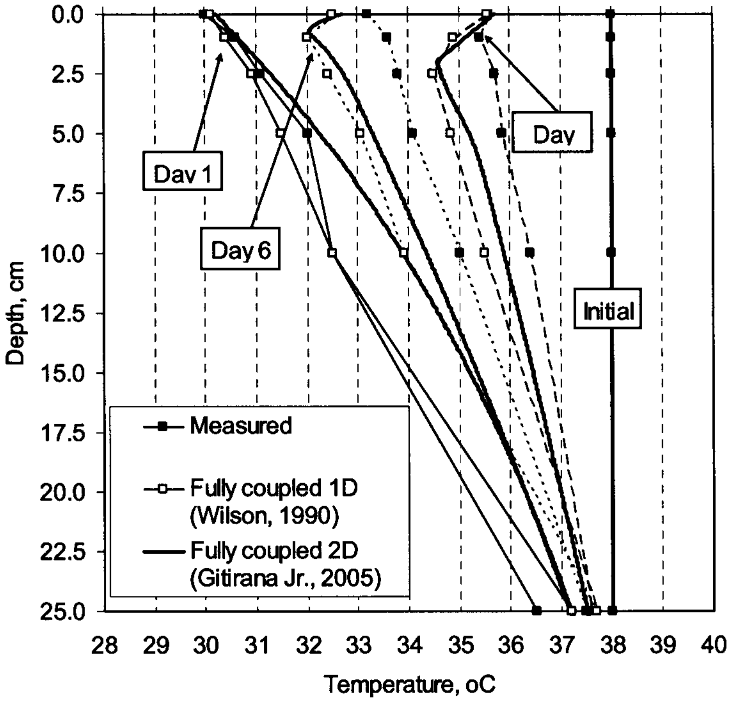

Figure 7 Verification of the coupled heat and moisture flow model: temperature distributions for several time steps.

Applied precipitation levels in the first 14 days of analysis are abnormally high due to the occurrence of snowmelt during this time. The daily precipitation values were assumed to be concentrated at a period of eight hours. The first soil column is comprised of a Till cover 1 m thick with $k^{w}_{sat} = 9\times10^{-2}$ m/day. The van Genuchten and Mualem representation of the unsaturated hydraulic conductivity curve was used for all soils. Beneath the cover there were two layers of tailings each 2.5 m thick with varying hydraulic parameters of $9\times10^{-1}$ m/day and $9\times10^{-2}$ m/day respectively.

Results of the analysis of column 1 are presented in Figure 8. From these results it can be seen that this scenario accentuates the differences in runoff calculation. Vadose/W overestimates runoff values. As a result, less water entered the system than what was predicted using SVFlux. The reduced amount of water entering the system results in higher soil suctions, thereby producing lower evaporation rates.

In the second column the same soil geometry was used but the conductivity of the top layer was decreased to $9\times10^{-3}$ m/day. This should have the effect of increasing the total runoff calculation. The results for the second column may be seen in Figure 9. Significantly greater quantities of runoff were predicted using both software packages. It can also be seen that Vadose/W again presents higher runoff rates with the resulting decrease in actual evaporation.

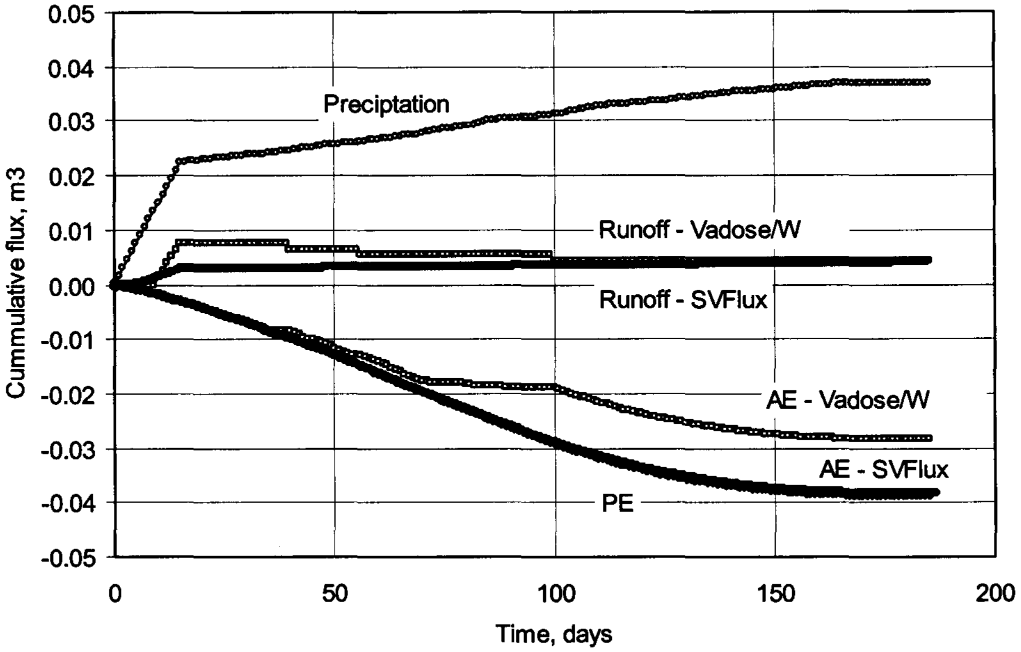

Figure 8 Runoff and AE predictions for column 1.

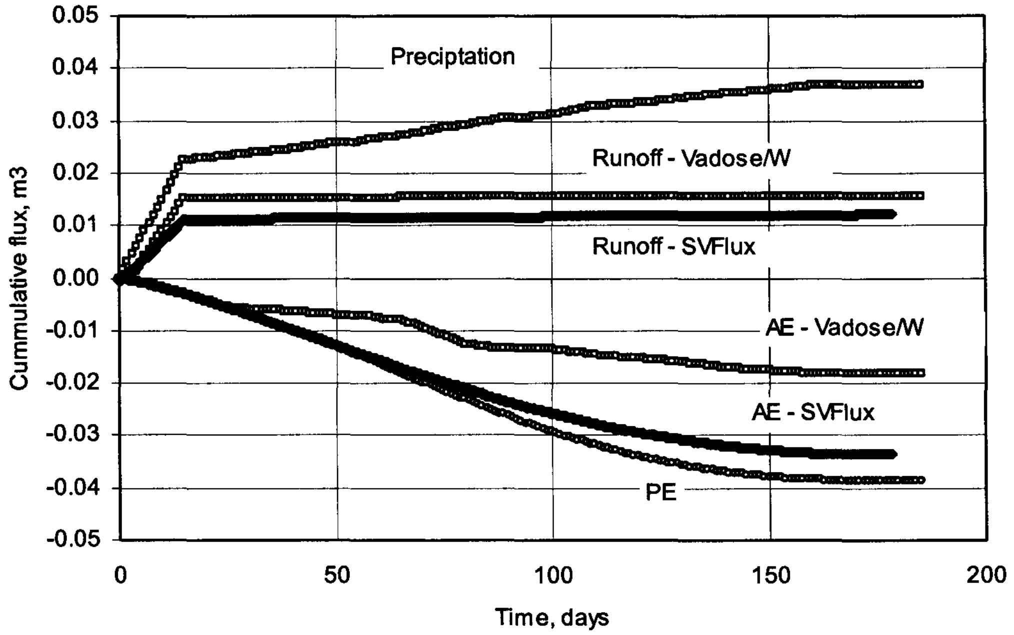

Figure 9 Runoff and AE predictions for column 2.

Mass balance checking was performed on all SVFlux runs and all scenarios solved with a total mass balance error of less than 5%. Figures 10 and 11 present a closer look at infiltration and runoff predictions using Vadose/W and SVFlux. The manner how precipitation is represented by each package is somewhat different. Vadose/W uses a sinusoid whose total area is equal to the amount of daily precipitation. SVFlux uses a step-function that also corresponds to the daily amount of precipitation. As precipitation progresses, both packages predict high rates of infiltration, close to the total amount of precipitation. However, the amount of precipitation predicted by Vadose/W is slightly lower. The lower values of infiltration predicted by Vadose/W are in agreement with the observation from Example 1. Runoff progressively increases until a peak value is achieved.

## 6. CONCLUDING REMARKS

This paper presented a PDE formulation that was developed for soil-atmosphere analysis and presented three cases demonstrating the application of the formulation developed to laboratory and fields conditions. Comparisons against experimental data showed that evaporative fluxes can be successfully reproduced by theoretical models. The PDE solutions were used for the simulation of the fluxes through two soil cover configurations. The results indicate that the manner how runoff is computed strongly affects the results. The numerical solutions appear robust and can be applied to the design of soil structures such as soil-cover systems.

## ACKNOWLEDGEMENTS

The authors would like to thank the "Conselho Nacional de Desenvolvimento Científico e Tecnológico – CNPq", Brazil, NSERC, Canadian Pacific Railway, and Saskatchewan Highways, for financial support.

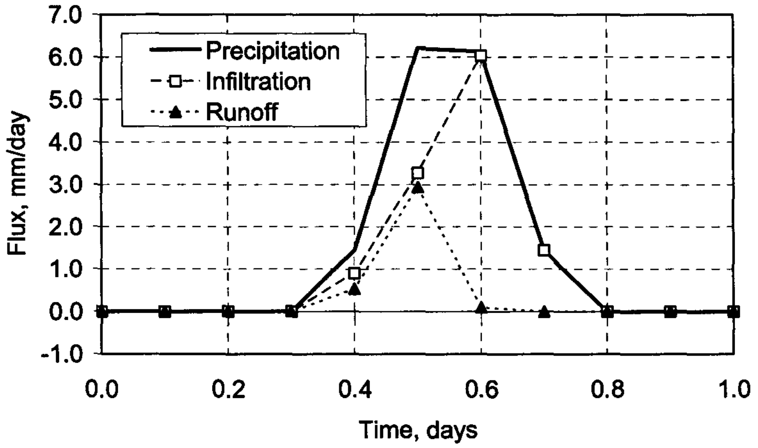

Figure 10 Vadose/W predictions for column 1, day 1.

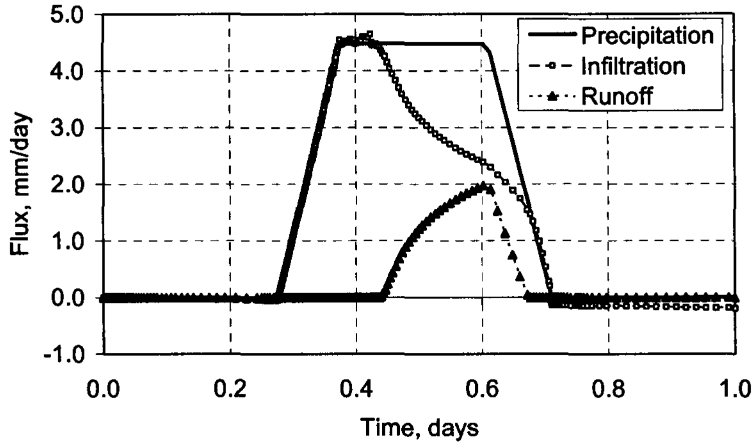

Figure 11 SVFlux predictions for column 1, day 1.

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