

A COUPLED HEAT, MOISTURE AND AIR FLOW MODEL FOR UNSATURATED SOILS

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A coupled heat, moisture and air flow model for unsaturated soils

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ABSTRACT

A theoretical model has been proposed to describe fully coupled heat, moisture and air flow in unsaturated soils. The pore-liquid water and pore-air transfer were assumed to be governed by Darcy's law and the pore-water vapour transfer was considered to occur due to two effects, first, under the molecular diffusion and, second, as part of the bulk flow of the pore-air. The pore-water vapour transfer due to the molecular diffusion was described using Fick's law. The heat transfer was formulated to include the effects of conduction, convection and latent heat of vapourization. A three-dimensional computer program has been developed to incorporate the proposed model for analyzing the transient coupled flow heat, moisture and air in unsaturated soils. Both the fundamental mathematical formulation and the computer code have been verified by comparing the numerical results with the test measurements of a drying sand column.

INTRODUCTION

The analysis of the movement of heat, moisture and air in the the ground is of interest in a number of engineering applications. Typically these applications range from nuclear waste disposal, to heat losses from buried buildings to geotechnical engineering applications of soil freezing and shrinkage. In some cases the accuracy of the thermal field prediction is of paramount importance while in others, the moisture content distributions are of greater significance. In the low saturation case, the movement of moisture content is governed by pore-vapour transfer. The pore-vapour transfer is considered to occur due to two effects: molecular diffusion and as part of the bulk flow of the pore-air. In all cases, however, the three are related and therefore a fully coupled analysis is required.

The purpose of this paper is to establish a mathematical model for describing the transient coupled flows of heat, moisture and air in unsaturated soils. A three-dimensional finite element computer program has been developed to incorporate the proposed model for analyzing the coupled heat, moisture and air transfer in unsaturated soils. An example problem is presented to examine the reliability and capability of the model.

BASIC EQUATIONS

In a non-isothermal unsaturated soil, solid, liquid and air are the three basic phases. The solid phase in this paper is assumed to be a continuous medium. The liquid phase is

considered to be a continuous pore-water containing dissolved 'dry' air. The air phase is composed of two continuous sub-phases: vapour phase and 'dry' air phase. The so-called 'dry' air is the air that does not contain water vapour. Based on the two universal laws of nature: the law of mass conservation and the law of heat conservation, the governing partial differential equations for the problems in unsaturated soil can be derived.

Governing Equations for the Pore Moisture

The pore-moisture is composed of the pore-liquid water and the pore-water vapour. The mass flux of non-isothermal pore-liquid water can be defined by a generalized form of Darcy's law

$$\vec{q}_w = - \frac{k_w}{g} \nabla(u_w + \rho_w gz) \quad (1)$$

where: \vec{q}_w is the mass flux vector of the pore-liquid water; k_w is the unsaturated permeability matrix of the liquid water phase; g is gravitational constant; u_w is the pore-water pressure; z is the vertical space coordinate (positive is upward); ρ_w is the density of water. The k_w is a function of the porosity, the liquid water content or the suction of the soil and also of the temperature for non-isothermal problems. The unsaturated permeability can be formulated as

$$\underline{k}_w(t^0, u_a - u_w, n) = \frac{\mu_w(T_r)}{\mu_w(t^0 + 273.16)} \underline{k}_{ws}^r(n) k_{rw}^r(u_a - u_w) \quad (2)$$

where: $(u_a - u_w)$ is the matric suction of the soil; n is the porosity of the soil; μ_w is the dynamic viscosity of water (Nsm^{-2}); T_r is the absolute room temperature (K); t^0 is the temperature ($^{\circ}\text{C}$); \underline{k}_{ws}^r is the saturated permeability matrix related to the porosity of the soil at room temperature; k_{rw}^r is the relative unsaturated permeability associated with the suction of the soil at room temperature.

The mass flux of the pore-water vapour can be considered to occur due to two effects, first, under the molecular diffusion and, second, as part of the bulk flow of the pore-air. The mass flux of the pore-water vapour due to the molecular diffusion can be described using Fick's Law (de Vries, 1975). The total mass flux of the pore-water vapour can be expressed as

$$\vec{q}_v = - D_{\text{atm}} \alpha \beta \nabla \rho_v + \frac{\rho_v}{\rho_a} \vec{q}_a \quad (3)$$

where: D_{atm} is the molecular diffusivity of the pore-water vapour in air (i.e., $2.29 \times 10^{-5} (1 + t^0/273.16)^{1.75} (\text{m}^2/\text{s})$) (Kimball et al., 1976); α is the tortuosity factor for soil (i.e., $\beta^{2/3}$) (Lai et al., 1976); β is the cross sectional area of the soil that is available for vapour flow (i.e., $(1-S)n$); \vec{q}_a is the mass flux of the pore-air due to the air pressure gradient; ρ_v and ρ_a are the densities of the pore-water vapour (i.e., $\rho_v^0 h_r$) and the pore-air (i.e., $\rho_{\text{ad}} + \rho_v$), respectively. Assuming that the pore-liquid water is in equilibrium with the pore-water vapour, and both

the pore-‘dry’ air and the pore-water vapour are ideal gases, the following density equations can be written as,

$$\rho_v = \frac{M_w u_v}{R(t^0 + 273.16)} \quad (4)$$

$$\rho_{ad} = \frac{M_{ad} (u_{atm} + u_{ad})}{R(t^0 + 273.16)} \quad (5)$$

$$\rho_a = \frac{M_a (u_{atm} + u_a)}{R(t^0 + 273.16)} \quad (6)$$

where: R is the universal gas constant (J/mol.K); u_{atm} is the standard atmospheric pressure (kPa); The pore-air pressure u_a is equal to u_{ad} plus u_v ; u_{ad} and u_v are the pore-‘dry’ air pressure and the partial pressure of the pore-water vapour (i.e., $u_v^0 h_r$), respectively; u_v^0 is the partial pressure of saturation water vapour (i.e., $1.36075 \times 10^5 \exp(-5239.7 / (t^0 + 273.16))$ (MPa)); h_r is the relative humidity (i.e., $\exp(-(u_a - u_w)M_w / \rho_w R(t^0 + 273.16))$); M_{ad} is the molecular weight of the ‘dry’ air (0.02895 kg/mol); M_w is the molecular weight of water (0.018 kg/mol); M_a is the molecular weight of air (i.e., $[M_{ad}(u_{atm} + u_{ad}) + M_w u_v^0] / (u_{atm} + u_{ad} + u_v)$ (kg/mol)); ρ_v^0 is the density of saturation water vapour (i.e., $M_w u_v^0 / R(t^0 + 273.16)$ (kg/m³)); The mass flux of the pore-air due to the air pressure gradient \vec{q}_a is computed by applying the generalized form of Darcy’s law for multiphase flow (Barden, 1965). Therefore, ignoring gravitational effects, the mass flux is given as,

$$\vec{q}_a = -\underline{k}_a \frac{\rho_a \nabla u_a}{\rho_w g} \quad (7)$$

where: \underline{k}_a is the unsaturated permeability matrix of the air phase that is defined as

$$\underline{k}_a = \frac{\mu_a(T_r)}{\mu_a(t^0 + 273.16)} \underline{k}_{as}^r(n) k_{ra}^r(u_a - u_w) \quad (8)$$

where: μ_a is the dynamic viscosity of the pore-air (Nsm⁻²); \underline{k}_{as}^r is the permeability matrix for the air phase related to the porosity of the soil at dry and room temperature; k_{ra}^r is the relative unsaturated permeability associated with the matric suction of the soil at room temperature. Substituting Eqs. (4) and (7) into Eq. (3) gives,

$$\vec{q}_v = D_{atm} \tilde{\alpha} \tilde{\beta} \frac{M_w u_v^0}{R(t^0 + 273.16) \rho_w} \nabla(u_a - u_w) - D_{atm} \tilde{\alpha} \tilde{\beta} \tilde{\xi} \left(h \frac{d\rho_v^0}{dT} + \frac{M_w (u_a - u_w) u_v^0}{R(t^0 + 273.16)^2 \rho_w} \right) \nabla T - \underline{k}_a \frac{\rho_v}{\rho_w g} \nabla u_a \quad (9)$$

where: ξ is the ratio of microscopic temperature gradient in the pore space to the macroscopic temperature gradient, $(\nabla T)_a / \nabla T$ and assumed to be 1.0. Applying the principle of mass conservation to the pore-moisture phase yields

$$\frac{\partial}{\partial t} (\rho_w n S + \rho_v n (1 - S)) = -\nabla \cdot (\vec{q}_w + \vec{q}_v) + f^w \quad (10)$$

where: n is the porosity of soil; f^w is evapotranspiration mass rate per unit of soil volume due to the uptake of water by the evaporation and transpiration or external supply rate of the moisture mass per unit volume of soil.

Governing Equations for the Pore-‘Dry’ Air

The pore-‘dry’ air is composed of the ‘dry’ air within the pore-air and the ‘dry’ air dissolved in the pore-liquid water. The transfer of the pore-‘dry’ air is assumed to take place due to two effects: first, as part of the bulk flow of the pore-air under the air pressure gradient and, second, within the pore-liquid water under the influence of the pore-water pressure gradient. The volumetric mass of dissolved ‘dry’ air contained within the pore-liquid water can be obtained by the use of Henry’s volumetric coefficient of solubility. The application of the law of conservation of mass for the pore-‘dry’ air phase therefore yields

$$\frac{\partial}{\partial t} ((1 - S)n\rho_{ad} + \bar{H}Sn\rho_{ad}^*) = -\nabla \cdot (\vec{q}_a^{ad} + \vec{q}_w^{ad}) + f^{ad} \quad (11)$$

where: f^{ad} is external supply rate of the pore-‘dry’ air mass per unit volume of soil and the density of the dissolved ‘dry’ air, ρ_{ad}^* can be assumed to be the density of the pore-‘dry’ air (i.e., ρ_{ad}) for simplicity. The Henry’s volumetric coefficient of solubility, \bar{H} is equal to 0.02 under one standard atmospheric pressure (kPa) and room temperature of 20 °C. The ‘dry’ air mass flux in the pore-air phase, \vec{q}_a^{ad} and the ‘dry’ air mass flux in the pore-liquid water phase, \vec{q}_w^{ad} can be given as

$$\vec{q}_a^{ad} = -\underline{k}_a \frac{\rho_{ad}}{\rho_w g} \nabla u_a \quad (12)$$

$$\vec{q}_w^{ad} = -\bar{H}\underline{k}_w \frac{\rho_{ad}^*}{\rho_w g} \nabla (u_w + \rho_w g z) \quad (13)$$

Governing Equations for Heat

In general, the heat transfer in unsaturated soils is governed by the thermal conduction in accordance with Fourier’s law. The factors that affect the heat transfer are the convection of sensible heat in the pore-moisture phase and in the pore-‘dry’ air phase, and the latent heat flow in the pore-water vapour. The energy flux of heat can therefore be given as,

$$\vec{Q} = -\lambda \nabla T + C_{pw}(T - T_0)\vec{q}_w + C_{pv}(T - T_0)\vec{q}_v + C_{p,ad}(T - T_0)\left(\vec{q}_a^{ad} + \vec{q}_w^{ad}\right) + L_v \vec{q}_v$$

(14) where: C_{pw} is specific heat capacity of the pore-liquid water ($\text{Jkg}^{-1}\text{K}^{-1}$); C_{pv} is specific heat capacity of the pore-water vapour ($\text{JKg}^{-1}\text{K}^{-1}$); $C_{p,ad}$ is specific heat capacity of the pore-‘dry’ air (i.e., $1000 (\text{Jkg}^{-1}\text{K}^{-1})$); L_v is latent heat of vapourization of the pore-liquid water ($\text{Jkg}^{-1}\text{K}^{-1}$); T_0 is absolute reference temperature (K); C_{ps} is specific heat capacity of the soil solids and is dependent on the types and characteristics of the soil solids. The thermal conductivity of an unsaturated soil, λ can be determined using the method described by de Vries (1963). Applying the law of energy conservation yields

$$\frac{\partial}{\partial t} \Phi = -\nabla \cdot \vec{Q} + f^\Phi \quad (15)$$

where: f^Φ is internal and/or external energy supply rate per unit volume of soil; The total internal energy of heat in the soil, Φ can be expressed in the following equation by assuming that the differential heat of wetting of the soil is negligible

$$\Phi = C_{ps}\rho_s(1-n)(T - T_0) + C_{pw}\rho_w S n(T - T_0) + C_{p,ad}(\rho_{ad}(1-S)n + \bar{H}\rho_{ad}^* S n)(T - T_0) + C_{pv}\rho_v(1-S)n(T - T_0) + L_v\rho_v(1-S)n \quad (16)$$

The heat energy of the soil, Φ consists of two terms, one represents the storage of latent heat due to the accumulation of the pore-water vapour and the other represents the local capacity for heat comprising the capacity of the soil solids, the pore-liquid water, the pore-‘dry’ air and the pore-water vapour.

A general mathematical model for solving coupled heat, moisture and ‘dry’ air flow in unsaturated soils can be formulated by combining Eqs. (10), (11) and (15) and applying the necessary initial and boundary conditions (i.e., either Dirichlet or Neumann type). This model contains three independent variables that are pore-water pressure, u_w , pore-air pressure, u_a and absolute temperature, T (i.e., $t^0 + 273.16$), as the essential unknown variables.

Material Parameters

The saturated permeability matrix for the pore-liquid water phase at room temperature $\underline{k}_{ws}^r(n)$, the unsaturated relative permeability for the pore-liquid water phase at room temperature $k_{rw}^r(u_a - u_w)$ or $k_{rw}^r(S)$, the permeability matrix for the pore-air phase under dry and room temperature conditions $\underline{k}_{as}^r(n)$ and the unsaturated relative permeability for the pore-air phase $k_{ra}^r(u_a - u_w)$ or $k_{ra}^r(S)$ can be obtained from laboratory tests. $\underline{k}_{ws}^r(n)$ can be assumed to be constant in many cases. Many empirical expressions of $k_{rw}^r(u_a - u_w)$ or $k_{rw}^r(S)$ are available (Alonso et al., 1987). To date, only a few empirical expressions for $\underline{k}_{as}^r(n)$ and $k_{ra}^r(u_a - u_w)$ or $k_{ra}^r(S)$ have been proposed (Yoshimi & Osterberg, 1963; Brun, 1989 and Alonso et al., 1988). Based on the definition in Eq. (12) and the empirical expressions proposed by Alonso et al. (1988), \underline{k}_a can be redefined in Eq. (13) as

$$\underline{k}_a = \frac{\mu_a(T_r)}{\mu_a(t^0 + 273.16)} \underline{k}_a^r(e, S) \quad (17)$$

where: $\underline{k}_a^r(c, S)$ is equal to $\underline{B}_a \rho_{wg} [e(1-S)]^{\beta_a} / \mu_a(T_r)$; β_a is a constant and \underline{B}_a is a constant matrix. If the soil is isotropic, \underline{B}_a can be reduced to a constant. The values of \underline{B}_a and β_a can be determined from curve-fitting techniques applied to the experimentally determined data. If there is no available experimental data, \underline{k}_a can be obtained theoretically as,

$$\underline{k}_a = \frac{\mu_a(T_r)}{\mu_a(t^0 + 273.16)} \underline{k}_{as}^r(n, u_a - u_w) \quad (18)$$

$$\underline{k}_{as}^r(n, s) = \frac{\mu_w(T_r)}{\mu_a(T_r)} \underline{k}_{ws}^r(n) k_{ra}^r(u_a - u_w) \quad (19)$$

Besides the permeabilities for the pore-liquid water phase and the pore-air phase, the degree of saturation is another important soil parameter. The degree of saturation is related to matric suction. The state surface with respect to the degree of saturation can be determined from experimental tests. Recently the following general form of relationship between volumetric water content and matric suction has been proposed by Fredlund & Xing(1994):

$$\theta_w = C(u_a - u_w) \frac{\theta_{ws}}{\{\ln[e + [(u_a - u_w)/a]^n]\}^m} \quad (20)$$

where: $C(u_a - u_w) = 1 - \ln[1 + (u_a - u_w) / (u_a - u_w)_r] / \ln[1 + 1000000 / (u_a - u_w)_r]$ is a correction function; $(u_a - u_w)_r$ (kPa) is the matric suction corresponding to the residual volumetric water content θ_r ; a , n and m are three material parameters; θ_w and θ_{ws} are volumetric water content (i.e., S_n) and saturated volumetric water content (i.e., n), respectively.

NUMERICAL METHOD

In this paper, the Galerkin finite element method is used to discretise Eqs.(10), (11), and (15), and the formulation $\int_{t_k}^{t_k + \Delta t} () dt = \Delta t [(1 - \alpha)()_{t_k} + \alpha()_{t_k + \Delta t}]$ is applied to discretise the time domain, where: Δt is the time step; $()_{t_k}$ and $()_{t_k + \Delta t}$ are the values of the function at time t_k and $t_k + \Delta t$, respectively; α is an integral parameter. If the increments of the pore-water pressure Δu_w , the pore-air pressure Δu_a and the temperature ΔT are accepted as the independent variables, the finite element formulae for solving coupled heat, moisture and air flow in unsaturated soils can be expressed as

$$\sum_{j=1}^N [k_{ij}]^{t_k + 0.5\Delta t} \{\Delta V_j\} = \{\Delta F_i\} \quad (i = 1, 2, 3, \dots, N) \quad (21)$$

where: $\{\Delta V_j\} = [\Delta u_{wj}, \Delta u_{aj}, \Delta T_j]^T$ is column matrix of the increments of the node variables at node j within time interval Δt ; $\{\Delta F_i\} = [\Delta f_i^1, \Delta f_i^2, \Delta f_i^3]^T$ is column matrix of the increments of the generalized equivalent nodal moisture mass, air mass and heat energy at

node i within time interval Δt ; the elements of the sub-matrix $k_{ij}, k_{ij}^{11}, k_{ij}^{12}, \dots, k_{ij}^{33}$, can be derived using the finite element technique; N is the total number of nodes; $()^{t_k + 0.5\Delta t}$ is the values of the function at time $t_k + \Delta t / 2$. Based on the formulae described above, a three-dimensional finite element program for analyses of coupled heat, moisture and air transfer in unsaturated soils has been developed. Two kinds of spatial isoparametric elements, i.e. eight-noded and six-noded spatial isoparametric elements are incorporated in this program. Within this program, solution of the resulting set of global matrices is achieved using a nonsymmetric solution algorithm. An iterative technique is used to solve the nonlinear equations established above and convergence of solution is assumed to have been achieved when the difference between successive iterations falls within a specified tolerance.

MODEL VERIFICATIONS AND APPLICATIONS

In this section, an example problem will be presented to illustrate the ability and reliability of the new model. Comparisons are made between the experimental data reported in the literature (Wilson, 1990) and those calculated using the model developed.

Wilson (1990) performed a column drying test to measure the actual rates of evaporation from a soil. The test column was filled with a saturated Beaver Creek sand and was allowed to drain to hydrostatic condition. The column was then sealed at the base and the upper surface was allowed to evaporate for a period of 42 days. The details of the apparatus used to conduct the column drying test can be found in Wilson (1990). The test set-up is showed in Fig. 1. The soil-water characteristic curve for the Beaver Creek sand can be expressed in the empirical form of Eq. (20). The parameters a , n and m can be obtained using a curve fitting-technique from the test data as 4.482 kPa, 13.98 and 0.61, respectively. The coefficients of permeability for the pore-water and the pore-air can be written in the following forms (Wilson, 1990):

$$k_w = \begin{cases} k_{ws} [(u_a - u_w)_b / (u_a - u_w)]^n & \text{for } (u_a - u_w) > (u_a - u_w)_b \\ k_{ws} & \text{for } (u_a - u_w) \leq (u_a - u_w)_b \end{cases} \quad (22)$$

$$k_a = k_{as} [(1 - S) / (1 - S_r)]^{D_2} \quad (23)$$

where: $\eta = 2 + 3L$, L is the pore-size distribution index (i.e., 3); $(u_a - u_w)_b$ is the bubbling suction or air entry suction (i.e., 3.8 kPa); k_{ws} is the saturated permeability for the water phase (i.e., 3.0×10^{-5} m/s); k_{as} is the permeability for the air phase at dry (i.e., 3.1369×10^{-3} m/s); S_r is the residual degree of saturation (i.e., 0.0); D_2 is a constant (i.e., 2.47).

The empirical relationship for the thermal conductivity versus water content for the Beaver Creek Sand (Wilson, 1990) is given as

$$\lambda = \lambda(\theta_w) = 0.4414 + 8.1903 \theta_w - 14.1358 \theta_w^2 + 10.6851 \theta_w^3 \quad (\text{W / m}^0 \text{C}) \quad (24)$$

The theoretical equation for the evaporation rate used in this paper is that suggested by Wilson (1990):

$$ET = f(u) [u_{vs}(T_s)h_{rs} - u_{vs}(T_a)h_{ra}] \quad (25)$$

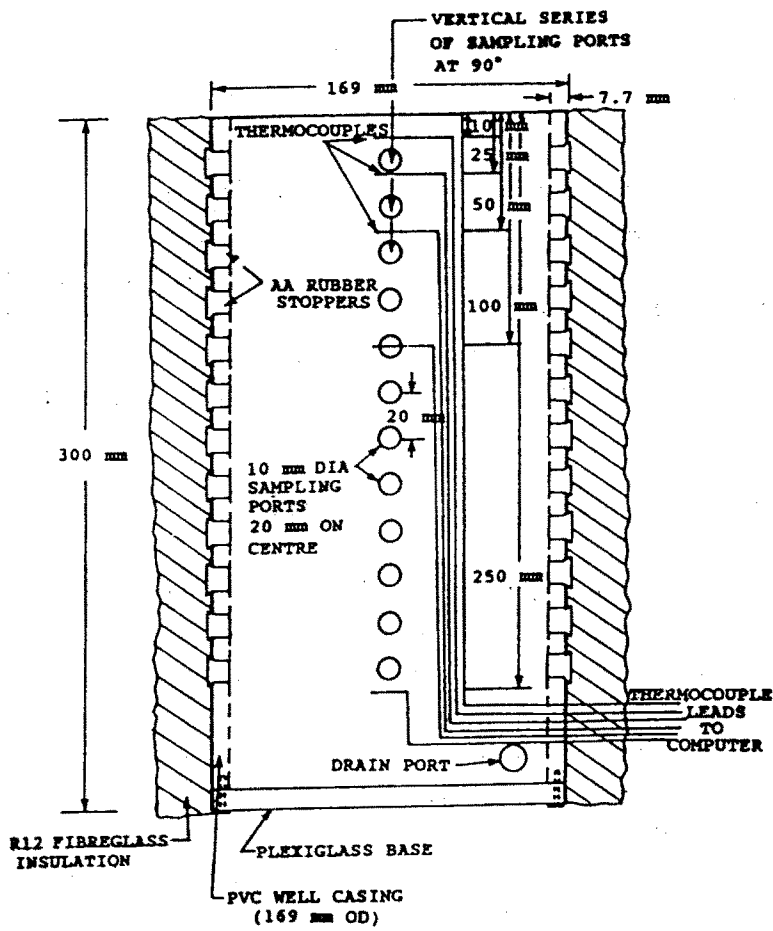
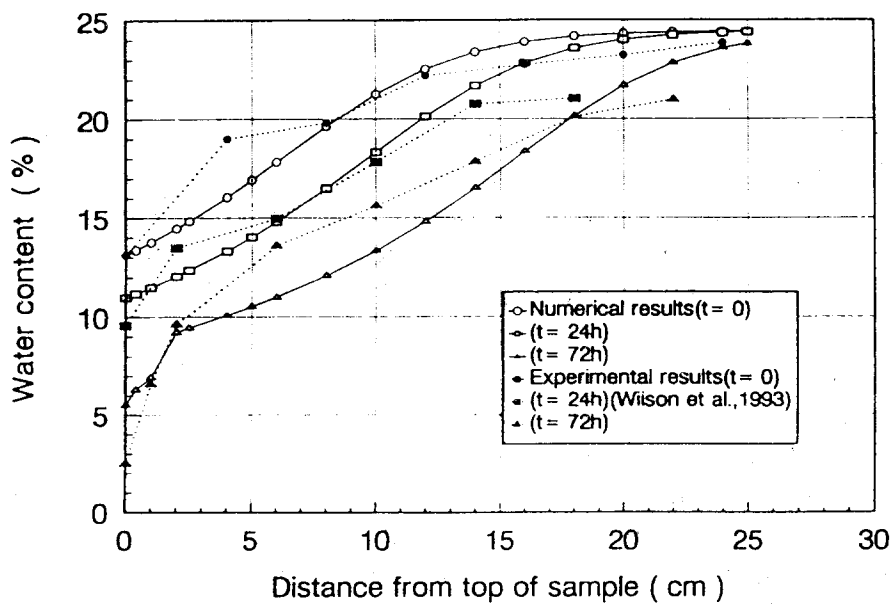


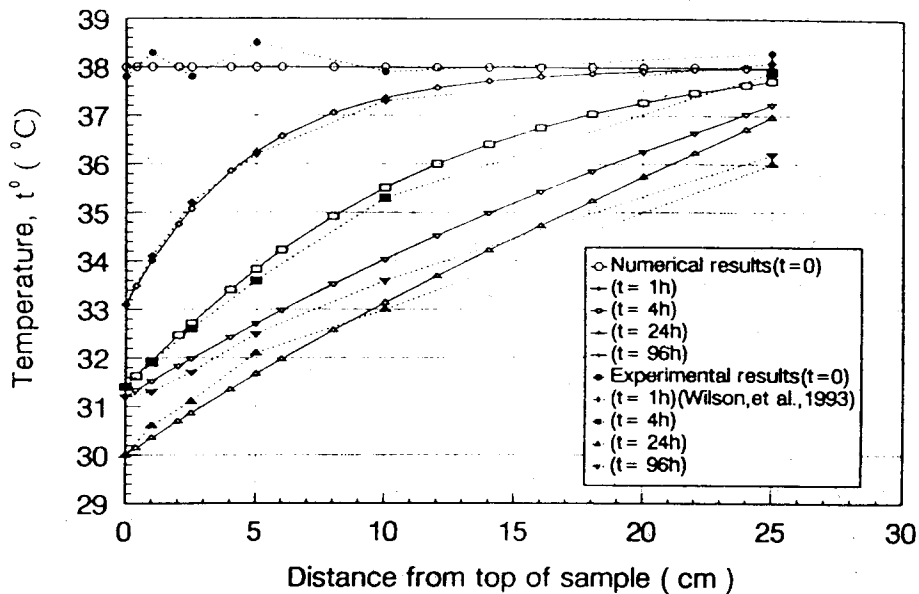
Figure 1. Detailed set-up of a drying column test (Wilson, 1990).

where: $u_{vs}(T_s)$ is the saturated vapour pressure at soil surface under surface temperature T_s ; h_{rs} is the relative humidity of the pore-air at the soil surface with surface temperature T_s ; $u_{vs}(T_a)$ is the saturated vapour pressure just above the soil surface at temperature T_a ; h_{ra} is the relative humidity of the air in the atmosphere above the soil surface at temperature T_a ; $f(u)$ is the turbulent exchange function. Eq. (25) shows that evaporation is a function of the vapour-pressure gradient between the soil surface and the overlying air. The turbulent exchange function $f(u)$ is calculated directly on the basis of the measured evaporative flux from the water-filled evaporation pan (i.e., $f(u) = PET / [u_{vs}(T_w) - u_{va}(T_a)]$), where: the vapour pressures at the water surface $u_{vs}(T_w)$ and in the atmosphere $u_{va}(T_a)$ are known and PET is the potential evaporation rate. The initial volumetric water content θ_{wi} and water content w_i on the upper surface of the test column are assumed to be 0.2119 and 0.1312 with respect to the initial matric suction, $(u_a - u_w)_i$ of 5.395 kPa, respectively.

The initial volumetric water content distribution along the height of the test column is given in Fig. 2a ($t = 0$) subject to initial hydrostatic condition. The initial temperature of the test column t_i^0 is assumed to be 38°C . The known pore-air pressure on the upper surface is given as $\tilde{u}_a(t) = \tilde{u}_{ad}(t) + \tilde{u}_v(t)$, where: $\tilde{u}_{ad}(t)$, the pore-‘dry’ air pressure on the upper surface, is assumed to be constant at the standard atmospheric pressure and the partial vapour pressure $\tilde{u}_v(t)$ is equal to $u_v^0 h_r$.



(a) Water content profiles at various times.



(b) Temperature profiles at various times.

Figure 2. Comparison of temperature and water content profiles in a drying column test.

The temperature at the base of the column is maintained at 38°C and the temperature with time on the upper surface is obtained from test measurements. The base surface is assumed to be impervious during evaporation and the flux on the upper surface is set to the evaporation rate estimated using Eq. (25). The saturated volumetric water content, θ_{ws} and the saturated water content w_s , are 0.395 and 0.2446, respectively.

Figs. 2a and 2b show the computed and measured water content and temperature profiles, respectively, at various times during the test. The good agreement between the computed and the experimental results indicates that the proposed model is capable of predicting water content and temperature profiles.

CONCLUSIONS

A theoretical model has been proposed to describe fully coupled heat, moisture and air flow in unsaturated soils. The pore-liquid water and pore-air transfers were assumed to be governed by Darcy's law and the pore-water vapour transfer was considered to occur due to two effects, first, under the molecular diffusion and, second, as part of the bulk flow of the pore air. The pore-water vapour transfer due to the molecular diffusion was described using Fick's law. The heat transfer was formulated to include the effects of conduction, convection and latent heat of vapourization. A set of fully coupled, nonlinear partial differential equations were established and solved using a Galerkin weighted residual approach in the space domain and using an implicit integrating scheme in time domain. A three-dimensional computer program has been developed to incorporate the proposed model for analyzing the transient coupled flows of heat, moisture and air in unsaturated soils. A column drying test was modelled using the program. There is good agreement between the computed and experimental results and this confirms the reliability and capability of the model. The three-dimensional computer program is quite general and suitable for the analyses of many different problems, such as isothermal or non-isothermal multiphase flow in saturated-unsaturated soils, seepage in saturated-unsaturated soils. However, more case studies are still required to further verify the proposed model in the future.

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