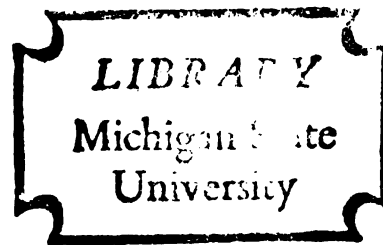


TRANSPORT PHENOMENA IN POROUS MEDIA WITH
EMPHASIS ON WATER MOVEMENT IN SOILS

Thesis for the Degree of Ph. D.
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LAWRENCE THOMAS NOVAK
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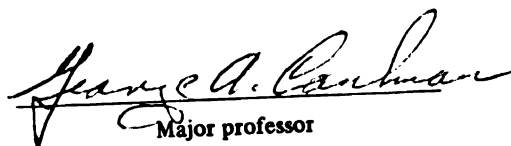
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ABSTRACT

TRANSPORT PHENOMENA IN POROUS MEDIA WITH EMPHASIS ON WATER MOVEMENT IN SOILS

By

Lawrence Thomas Novak

Unrestricted dumping of domestic and industrial waste water into the waterways will be a thing of the past in the United States. Stringent federal standards will require that waste water be treated before being returned to the waterways. One method of treating this waste water is by spray irrigation of the soil mantle.

In order to successfully design and manage a spray irrigation facility, mathematical models are required which will predict the movement of water and chemical compounds in the soil. This work addresses itself to modeling the water movement in soils.

One objective of this work is to develop a general model for water movement in soils. This model is then compared to less general models which have previously been proposed to describe water movement in soils. Another objective is to test the models by comparing the simulation results with the experimental results.

The general model was derived by making material balances on water in the liquid and vapor form, and by making an energy balance on the soil. This resulted in a set of transport equations which describe the movement of water and energy in the soils. The novel feature of this model is that the condition of interphase vapor-liquid equilibrium is not assumed. This equilibrium assumption was the basis of an earlier model for water movement in soils which was developed by Philip and DeVries.

The unsteady state numerical solution was developed for the general model, Philip and DeVries model, and the isothermal equation. An explicit finite difference technique was used in the numerical solutions. The unsteady state solution to the Philip and DeVries model has not been obtained prior to this work. With the numerical solution to the above models, soil drying simulations were run and the results were compared to experimental results.

It was found that even with dry soils the interphase vapor-liquid assumption is valid. Furthermore, the isothermal equation and Philip and DeVries model give essentially the same drying saturation profiles when identical irreducible saturations are used in the models. Good agreement was obtained between calculated and experimental drying saturation profiles.

The solution to the Philip and DeVries model developed in this work should be useful in problems involving drying of soils or porous media where a predictive capability is needed. The general model will also be useful in these types of problems to evaluate the interphase vapor-liquid equilibrium assumption upon which the Philip and DeVries model is based.

For soils which are above the irreducible saturation, the isothermal equation for water movement would be the most expedient model to use if soil temperature information was not desired. In particular, the isothermal equation would be a good base for structuring models to describe the movement of chemical compounds in soils subjected to spray irrigation with liquid wastes.

TRANSPORT PHENOMENA IN POROUS MEDIA
WITH EMPHASIS ON WATER MOVEMENT IN SOILS

By

Lawrence Thomas Novak

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DEDICATION

In memory of my father, John A. Novak

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NOMENCLATURE

A	Cross sectional area of soil column (cm^2)
a	Interfacial area per volume (cm^{-1})
$\tilde{C}$	Molar concentration of gas phase ($\text{gm.mole}/\text{cm}^3$)
$\tilde{C}_w$	Molar concentration of water vapor ($\text{gm.mole}/\text{cm}^3$)
$\tilde{C}_w^*$	Equilibrium molar concentration of water vapor ($\text{gm.mole}/\text{cm}^3$)
C	Volumetric heat capacity of soil ($\text{cal.}/\text{cm}^3\text{-}^\circ\text{K}$)
C_p	Heat capacity ($\text{cal.}/\text{gm.}-^\circ\text{K}$)
D_{aw}	Diffusion coefficient for water vapor in soil (cm^2/day)
$\mathcal{D}_{aw}$	Ordinary diffusion coefficient for water vapor in air (cm^2/day)
D_i	Inside column diameter (cm)
D_o	Outside column diameter (cm)
D_p	Particle or droplet diameter (cm)
D_w	Outside column wall diameter (cm)
D_T, D_θ	
$D_\theta, \text{ vap}$	Parameters in the equations of Philip and De Vries
E	Interphase evaporation rate ($\text{gm.}/\text{cm}^3\text{-day}$)
ΔH_{vap}	Enthalpy of vaporization for water ($\text{cal.}/\text{gm.}$)
h	Film coefficient for heat transfer ($\text{cal}/\text{cm}^2\text{-day-}^\circ\text{K}$)

h_s	Surface film coefficient for heat transfer (cal./cm ² -day-°K)
k	Thermal conductivity (cal./cm-day-°K)
k_e	Effective thermal conductivity (cal./cm-day-°K)
k_m	Film coefficient for mass transfer (cm/day)
$k_{m,s}$	Surface film coefficient for mass transfer (cm/day)
K	Hydraulic conductivity (cm ² /day)
K_o	Over all interphase mass transfer coefficient (cm/day)
L	Column length (cm)
M_w	Molecular weight of water (gm./gm.mole)
$\tilde{N}_w$	Molar flux of water vapor with respect to fixed coordinates (gm.mole/cm ² -day)
$\tilde{N}_{w,c}$	Convective molar flux of water vapor at the soil-atmosphere interface (gm.mole/cm ² -day)
p_w	Partial pressure of water in the gas phase (atm.)
P	Total pressure (atm.)
P	Total gas phase pressure (atm.)
P_c	Capillary pressure (cm)
P_{vap}	Vapor pressure of liquid water (atm.)
q	Total energy flux (cal./cm ² -day)
q_c	Convective energy flux (cal./cm ² -day)
q_r	Radiative energy flux (cal./cm ² -day)
Q	Volumetric flow rate (cm ³ /day)
r	Radius of capillary (cm)
R	Gas law constant (atm.cm ³ /gm.mole-°K)
S	Saturation = volume of liquid water per volume of gas and liquid in soil (dimensionless)

$\bar{S}$	Saturation = volume of water per volume of gas and liquid in soil (dim.)
t	Time variable (day)
T	Temperature ($^{\circ}\text{K}$)
T_A	Ambient temperature ($^{\circ}\text{K}$)
U	Internal energy (cal./gm.)
U_o	Over all column wall heat transfer coefficient (cal./cm ² -day- $^{\circ}\text{K}$)
$\bar{V}$	Molar volume (cm ³ /gm.mole)
V^o	Volumetric flux of liquid water (cm/day)
$\bar{V}^o$	Volumetric flux of water (cm/day)
V^*	Molar average velocity (cm/day)
V_i	Velocity of component i with respect to fixed coordinates (cm/day)
W	Width of soil column (cm)
$\bar{x}_w$	Mole fraction of water in the gas phase (dim.)
$\bar{x}_w^*$	Equilibrium mole fraction of water in the gas phase (dim.)
$\bar{x}_{w,A}$	Ambient mole fraction of water in the gas phase (dim.)
z	Spatial variable (cm)

<u>Dimensionless Number</u>	
$Nu = \frac{hD_p}{k}$	Particle Nusselt number
$Nu = \frac{h_s W}{k}$	Nusselt number
$Pr = \frac{C_p \mu}{k}$	Prandtl number
$Re_p = \frac{V D_p \rho}{\mu}$	Particle Reynolds number

$$Re = \frac{V_g W \rho}{\mu} \quad \text{Reynolds number}$$

$$Sc = \frac{\mu}{\rho D_{aw}} \quad \text{Schmidt number}$$

$$Sh = \frac{k_m D_p}{D_{aw}} \quad \text{Particle Sherwood number}$$

$$Sh = \frac{k_{m,s} W}{D_{aw}} \quad \text{Sherwood number}$$

Greek Symbols

ϵ	Porosity or void fraction (dim.)
Φ	Total potential (cm)
Ψ	Capillary potential (cm)
θ	Water content = liquid water volume per volume of soil (dim.)
$\bar{\theta}$	Water content = water volume per volume of soil (dim.)
ϕ_i	Concentration of component i (gm. mole/cm ³)
μ	Viscosity (gm./cm-day)
ρ	Density (gm./cm ³)
λ	Effective conductivity and part of the distillation effect--see the equations of Philip and De Vries
σ	Surface tension (or free energy) (dyne/cm)
ϕ_s	Shape factor (dim.)
ζ	Channeling factor (dim.)
γ	Conversion factor (1.01324 x 10 ⁶ dyne/cm ² -atm.)

Subscript

VL	Vapor-liquid
L	liquid
aw	air-water
g	gas

CHAPTER I

INTRODUCTION

There is a growing desire today to achieve a cleaner aquatic environment by cleaning up domestic and industrial waste water. One method of treating waste water is by spray irrigation of the soil mantle. This method is gaining popularity in areas where inexpensive land is available.

The soil mantle can act as a living filter. As waste water trickles down through the soil, some chemical compounds are adsorbed onto soil particles. Others are absorbed by the roots of surface vegetation. Also, microbial life in the soil feed on suspended solids and soluble chemical compounds in the water and convert them into microbial biomass and other chemical compounds which are excreted. Chemical compounds which are not accumulated into the biomass of surface vegetation or soil organisms, will accumulate in the soil. As this accumulation continues, the soil becomes saturated and these chemical compounds eventually wash downward into the water table. A management goal of a spray irrigation facility would be to minimize the amount of chemical compounds entering the water table.

It can be seen from the above discussion, that the water acts as a carrier of chemical compounds in the soil. In order to successfully design and manage a soil mantle spray irrigation facility, one would like to be able to predict the outcome of various spraying policies. To do this a model is required which could accurately predict water movement in soils over a range of operating conditions. The water model would be the foundation upon which other models could be built. For example, a model to describe phosphorous movement in soils would recognize that soluble phosphorous compounds move with the soil water and are adsorbed or desorbed from the soil particles and also taken up by the roots of terrestrial vegetation.

The objectives of this work are to develop a general model for water movement in soils and to compare this model to less general models which have been proposed to describe water movement in soils. Another objective is to test the models by comparing the simulation results with experimental results.

The first model to describe water movement in soils was proposed by Darcy in 1856. Darcy studied the flow of water through the sand filters of Dijon, France and concluded that the volumetric flow rate of water could be predicted by the following empirical equation [1].

$$(1.1) \quad Q = V^0 A = - KA \left(\frac{\Delta P}{L} \right)$$

Equation (1.1) is called Darcy's law and states that the volumetric flow rate of water is proportional to the pressure drop (ΔP) across a sand column of length L . The proportionality constant is the product of the hydraulic conductivity (K) and the column cross sectional area (A). Hydraulic conductivity is a function of the water viscosity, the particle sizes, and the particle size distribution of the porous media. Darcy's law has been found valid for low flow rates in porous media.

$$(1.2) \quad Re_p = \frac{\rho Q D_p}{A \mu} < 1$$

This is because at low flow rates, the frictional forces outweigh the inertial forces [2].

The type of flow problem studied by Darcy is described by the terms saturated, isothermal, and steady state flow. A saturated porous media or soil consists of two phases: liquid and solid. When the volumetric flux (V^0) of water through a constant temperature soil does not change with time, the flow is said to be steady state and isothermal.

Water flow in soils also occurs when a gas phase is present in the soil. This type of flow is called unsaturated. Collis-George experimentally verified that Darcy's law holds for unsaturated flow if the driving force is changed from a pressure gradient to a potential gradient [3].

$$(1.3) \quad v^0 = -K \nabla \phi$$

where,

$$(1.4) \quad \phi = \psi - z$$

The potential (ϕ) includes a capillary potential (ψ) and a gravitational potential ($-z$). The capillary potential is equivalent to the other literature terms soil potential, suction, and tension. The potential (ϕ) has been shown to be the free energy per weight of water of the soil water at a given depth z [4]. Appendix A illustrates the dependence of capillary potential on saturation, temperature, history, and composition.

A practical problem of interest is the distribution of water in the soil during and following irrigation [5,6]. The water flow in this type of problem is called unsteady state. That is, the volumetric flux of water (v^0) changes with time. To handle this type of problem, Gardner proposed the following model [7].

$$(1.5) \quad \frac{\partial \bar{\theta}}{\partial t} = - \frac{\partial \bar{V}^0}{\partial z}$$

where,

$$(1.6) \quad \bar{\theta} = \bar{S}\epsilon$$

$$(1.7) \quad 0 \leq \bar{S} \leq 1.0$$

Gardner's equation for isothermal water movement in soils is a material balance on water in the soil. Equation (1.5) states that the rate of accumulation of water (volume) per bulk volume of soil is equal to the rate of gain of water (volume) per bulk volume of soil due to convective flow. The amount of water per bulk volume of soil is called the water content ($\bar{\theta}$) and is defined in Equation (1.6) as the product of saturation ($\bar{S}$) and porosity (ϵ).

A phenomenon which is more difficult to model is the drying of a soil or other porous media. The water flow in soils during drying is unsaturated, non-isothermal, and unsteady state. Water movement can occur in the gas phase by water vapor diffusion and in the liquid phase by capillary movement.

The first attempts to handle the drying phenomenon were by engineers. Their main concern was to develop models which would predict the drying rates of porous media. They did not concern themselves with models based on the detailed

mechanisms of water movement in porous media during drying. As a result, their models were a blend of theory and empiricism. The engineering drying literature has been reviewed in references 8 and 9. To describe the saturation profiles in a drying porous media, a diffusion equation was used with a constant diffusivity [10]. This approach did not fit the experimental data. In Appendix B, it is shown that Gardner's equation and Darcy's law can be combined to yield a diffusion equation with a variable diffusivity.

A new model to describe the drying phenomenon was proposed by Philip and De Vries [11]. They assumed that the water vapor was in equilibrium with soil water. In this situation, the soil air is saturated with water vapor. The main point is that for the first time a model was proposed which mathematically described water movement occurring in two phases: gas and liquid.

The model of Philip and De Vries is given below. A reader interested in a detailed derivation is referred to Reference 11.

$$(1.8) \quad \frac{\partial \bar{\theta}}{\partial t} = \nabla \cdot (D_T \nabla T) + \nabla \cdot (D_{\theta} \nabla \bar{\theta}) + \frac{\partial K}{\partial z}$$

$$(1.9) \quad C \frac{\partial T}{\partial t} = \nabla \cdot (\lambda \nabla T) - H_{\text{vap}} \nabla \cdot (D_{\theta_{\text{vap}}} \nabla \bar{\theta})$$

Equations (1.8) and (1.9) neglect the effect of soil water composition on the capillary potential and hence no composition variable appears in these equations. The energy balance (1.9) contains a conductivity (λ) which includes the thermal distillation effect [11].

At a later date, Taylor and Cary used the thermodynamics of irreversible processes to develop a model for unsaturated, nonisothermal, and unsteady state flow [12]. Their model also assumes vapor-liquid equilibrium and the equations are of the same form as the equations of Philip and De Vries.

To solve practical problems using models for water movement in soils, the model equations must be solved. For unsteady state problems, the equations are nonlinear partial differential equations.

Gardner's equation has been solved numerically for infiltration, redistribution, and some drying problems. A literature survey on numerical solutions to these unsteady state problems has been given in Reference 13.

The drying of soils like many porous media consists of a constant drying rate and falling drying rate period. Covey studied the constant drying rate period using Gardner's equation. The model parameters were varied and saturation profiles were calculated [14]. Later, Klute et al. studied the falling rate period using Gardner's equation [15]. Neither of these studies compared the numerical results with experimental results.

A study by Fritton et al. used Gardner's equation to simulate the drying of soil and compared computed results with experimental results [16]. Gardner's equation fits the cumulative evaporation versus time data but did not fit the saturation profiles. The experimental saturation profiles had an inflection point whereas the numerical results did not.

The equations of Philip and De Vries have not previously been used to simulate unsteady state water movement in soils or other porous media. Their usage has been in calculating the water vapor, liquid, and energy fluxes from experimental saturation and temperature profiles at some instant of time.

CHAPTER II

THEORY

This chapter will be concerned with the development of a general model for water movement in soils. Although developed specifically for soils, it is general enough to apply to other porous media such as crystalline catalysts, wood, fibers, and paper. Before developing this theory, some important concepts and terminology will be discussed.

The general model for water movement in soils will be a set of equations which describe the transport of fluids and energy through the soil. One fluid will be the liquid phase and the other fluid will be the gas phase. Both phases are fluid mixtures because the fluids contain more than one component.

A theory of fluids is conveniently divided into equilibrium and nonequilibrium properties of fluids. The equilibrium properties are the thermal equation of state ($P = P(T, V_1, \dots, V_n)$) and caloric equation of state ($U = U(T, V_1, \dots, V_n)$). These equations relate the local pressure and internal energy of the fluid to the local temperature and volume occupied by the components of the fluid. The equations of state along with the equations

of change and appropriate boundary conditions describe the transport phenomena of the fluid. Transport phenomena is concerned with the fluxes of mass, momentum, and energy which occur in fluids not at equilibrium.

The equations of change are the equation of continuity, the equation of motion, and the equation of energy. In their most general form, they are written in terms of fluxes of mass, momentum, and energy. These equations have been derived for transport phenomena in fluids by Bird et al. [17].

The equations of continuity and energy are mathematical statements of the conservation laws of science applied to a fluid: conservation of mass and conservation of energy. An early statement of the conservation of mass principle was given by the Roman poet Lucretius (ca. 96-55 BC), contemporary of Julius Caesar: "Things cannot be born from nothing, cannot when begotten be brought back to nothing" [18]. The conservation of mass principle was modified much later by Albert Einstein in his theory of relativity. For systems in which the velocity of mass approaches the speed of light, the conservation of mass principle is obeyed if relativistic mass is used. The principle of conservation of energy says that energy may be transformed from one kind to another, but it cannot be destroyed. This principle and the principle of conservation of mass are generalizations of man's experience, so far not contradicted by observation of nature.

The equation of motion is a statement of Newton's second law of motion applied to a local fluid element. Newton's second law says the unbalanced force acting on a body is equal to the time rate of change of motion (or momentum) of the body.

There are three levels of analysis which can be applied to develop the theory of transport phenomena in soils: molecular, microscopic, and macroscopic. The molecular level of analysis develops theories of transport based on the movement of molecules [19]. The movement of molecules is caused by intermolecular forces. On this level of analysis even a fluid is discontinuous as there are voids between molecules. This difficulty is overcome by using statistical distribution functions, and the equations of change derived by molecular considerations are partial differential equations with continuous functions [19].

The microscopic level views a fluid as a continuum and is not concerned with the individual movement of molecules. It is concerned with the microscopic properties of fluids such as local temperature, pressure, and velocity. Transport in soils is then described by applying the microscopic equations of change to the regions of the soil where fluids are present such as the macropores and micropores. The difficulty of this approach is the complexity of the boundary conditions between the phases present.

This difficulty is circumvented in the macroscopic analysis as the complex microscopic boundary conditions are incorporated into the macroscopic equations of change. Furthermore, the macroscopic approach is concerned with macroscopic properties of soils which are directly measurable such as temperature and saturation.

The general model for water movement in soils will be the macroscopic equations of change. The macroscopic equations of change for soils can be derived by two methods. The first method involves volume averaging the microscopic equations of change over a small macroscopic volume of soil. Bird et al. have used this method to develop the macroscopic equations of change for a general nondistributive flow system [20]. The second method involves definition of macroscopic quantities and derivation of the macroscopic equations of change in terms of these quantities.

The following derivation of the macroscopic equations of change will utilize the second method since it is more simple and straightforward. The nomenclature is defined on pages ix-xii and Appendix C contains the three dimensional form of the macroscopic equations of change.

Derivation of the Macroscopic Equation of
Continuity for Liquid Phase Water in the Soil

A mass balance on liquid phase water in a differential element of soil (see Figure 1) yields the macroscopic equation of continuity for liquid water. Liquid water enters the differential element at position z with a volumetric flux V^0 and leaves the element at position $z + dz$ with a volumetric flux V^0 . Liquid water may evaporate or water vapor may condense in the element also. The mass rate of water evaporation per bulk volume of soil will be represented by the letter E .

The rate of accumulation of liquid water mass in the differential element is equal to the rate of gain of liquid water mass by convective flow plus the rate of gain of liquid water mass by condensation of water vapor. That is,

$$(2.1) \quad \rho_w V^0 A|_z - \rho_w V^0 A|_{z+dz} - EAdz = \frac{\partial \rho_w \theta Adz}{\partial t} .$$

where, ρ_w = mass density of liquid phase water

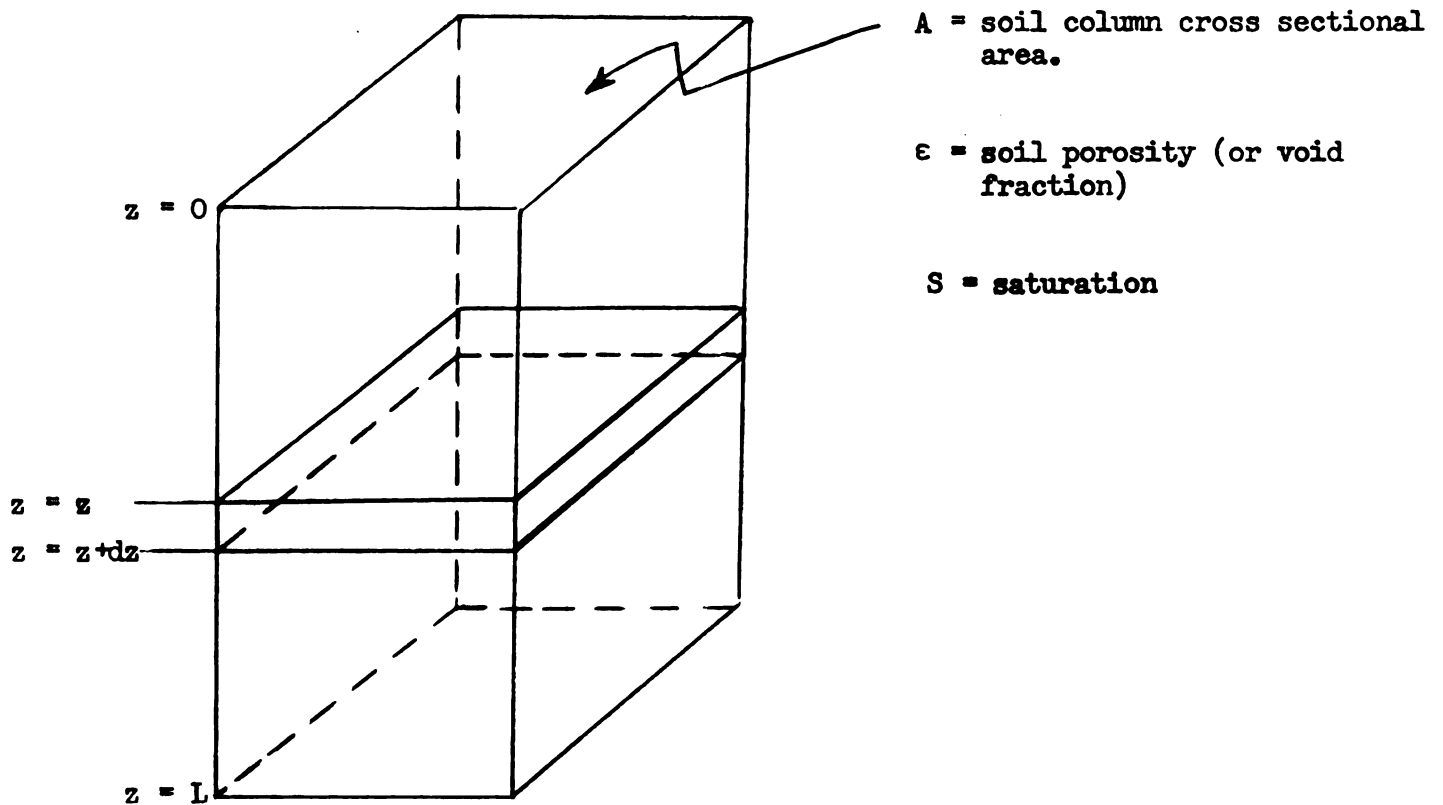
θ = liquid water content

S = saturation (liquid water volume per volume of voids)

and, $\theta = S\varepsilon$

Since the cross sectional area is a constant, we can divide by Adz and then take the limit as dz approaches zero.

Equation (2.1) becomes



volume of soil particles in the differential element $= (1 - \epsilon) A dz$

volume of liquid water in the differential element $= S \epsilon A dz$

volume of soil air in the differential element $= (1 - S) \epsilon A dz$

Figure 1.--Differential element in a soil column.

$$(2.2) \quad - \frac{\partial \rho_w V^O}{\partial z} - E = \frac{\partial \rho_w \theta}{\partial t}$$

Macroscopic Equation of Continuity for Liquid Phase Water

The rate of evaporation (E) will be defined mathematically later in this chapter.

Derivation of the Macroscopic Equation of Continuity for Water Vapor in the Soil

A molar balance on water vapor in a differential element of soil (Figure 1) results in the macroscopic equation of continuity for water vapor. Water vapor enters the differential element at z with a molar flux $\tilde{N}_w$ and leaves the element at $z + dz$ with a molar flux $\tilde{N}_w$. The flux $\tilde{N}_w$ is with respect to a fixed coordinate system and contains convective and diffusional flow contributions. Water vapor may also enter or leave the vapor state by liquid evaporation or vapor condensation.

The molar rate of accumulation of water vapor in the differential element is equal to the molar rate of gain of water vapor by convective flow and diffusion plus the molar rate of gain of water vapor due to liquid water evaporation. That is,

$$(2.3) \quad \tilde{N}_w A|_z - \tilde{N}_w A|_{z+dz} + \frac{E A dz}{M_w} = \frac{\partial (\tilde{C}_w \epsilon (1-S) A dz)}{\partial t}$$

where, M_w = molecular weight of water

and

$$(2.4) \quad \tilde{C}_w = \frac{p_w}{RT} = \frac{p\tilde{X}_w}{RT}$$

Dividing by Adz and taking the limit as dz approaches zero, Equation (2.3) becomes

$$(2.5) \quad -\frac{\partial \tilde{N}_w}{\partial z} + \frac{E}{M_w} = \frac{\partial (\tilde{C}_w \epsilon (1-S))}{\partial t}$$

Macroscopic Equation of Continuity for Water Vapor

In Equation (2.4), the molar concentration of water vapor is given by the ideal gas law. The partial pressure of water, the total gas pressure, and the mole fraction of water vapor present in the gas phase has been represented by the symbols, p_w , p , and $\tilde{X}_w$ respectively.

Derivation of the Macroscopic Equation of Energy for the Soil

By making an energy balance on the differential element of soil (see Figure 1) we obtain the macroscopic equation of energy for the soil column. Energy enters the differential element at z with a conductive energy flux q and leaves the element at $z + dz$ with a conductive energy flux q . Sensible heat transferred by the fluxes of liquid water and water vapor also contribute to an energy flux. This flux has been assumed negligible compared to the conductive energy flux and will be justified by the

simulation calculations later in this work. A cooling or heating effect is also present in the element due to evaporation or condensation of water.

The rate of accumulation of enthalpy in the differential element is equal to the rate of gain of conductive energy plus the rate of gain of enthalpy due to condensation of water vapor.

That is,

$$(2.6) \quad qA|_z - qA|_{z+dz} - \Delta H_{\text{vap}} E A dz = \left(\frac{C \partial T}{\partial t} \right) A dz$$

where, C = volumetric heat capacity of the soil

ΔH_{vap} = enthalpy of vaporization of water

Dividing by $A dz$ and taking the limit as dz approaches zero, Equation (2.6) becomes

$$(2.7) \quad - \frac{\partial q}{\partial z} - \Delta H_{\text{vap}} E = C \frac{\partial T}{\partial t}$$

Macroscopic Equation of Energy for the Soil

Thus far we have derived the macroscopic equations of change in one dimensional form. An implicit assumption in these derivations has been that fluxes, concentrations, and temperature are constant over the cross sectional column area (A).

The macroscopic equation of motion has been derived by Raats for a soil. He has shown that if inertia is negligible, the equation of motion yields Darcy's law [21]. Darcy's law can be used to describe the volumetric flux of liquid water in the soil (see Equations (1.3) and (1.4)). Darcy's law is written in terms of a potential driving force (ϕ). Appendix A indicates the dependence of capillary potential (Ψ) on saturation, temperature, history, and composition.

The expression for the flux of water vapor in soils is dependent on the number of components diffusing and the convective flux of the gas phase. In general,

$$(2.8) \quad \tilde{N}_w = - \tilde{C} D_{aw} \epsilon (1-S) \frac{d\tilde{x}_w}{dz} + \tilde{x}_w \sum_i \tilde{N}_i$$

where,

$$(2.9) \quad \tilde{C} V^* = \sum_i \tilde{C}_i V_i = \sum_i \tilde{N}_i$$

$$(2.10) \quad \tilde{C} = \sum_i \tilde{C}_i = \frac{P}{RT}$$

and,

V^* = molar average velocity with respect to fixed coordinates

V_i = average velocity of molecules i with respect to fixed coordinates

D_{aw} = diffusion coefficient of water in soil air

When water is the only component moving and it is moving by diffusion, Equation (2.8) reduces to

$$(2.11) \quad \tilde{N}_w = - \tilde{C}_{D_{aw}} \frac{\epsilon(1-S) d\tilde{X}_w}{(1-\tilde{X}_w) dz}$$

The energy flux is written in terms of an effective conductivity.

$$(2.12) \quad q = - k_e \frac{dT}{dz}$$

Model Parameters

Rate of Evaporation (E): Interphase Mass Transfer

Evaporation and condensation of water in soils involves the transfer of water molecules across the gas-liquid interface present in the soil. This phenomenon is referred to as interphase mass transfer. The theory of interphase mass transfer is developed in a textbook by Treybal [22]. In summary, the rate of water mass transfer per unit area of gas-liquid interface is equal to the product of an over-all mass transfer coefficient (K_O) and a concentration driving force ($\tilde{C}_w^* - \tilde{C}_w$).

The evaporation rate (E) can now be written as

$$(2.13) \quad E = K_O a (\tilde{C}_w^* - \tilde{C}_w) M_w$$

where,

$$(2.14) \quad \tilde{C}_w^* = \frac{P_{\text{vap}}}{RT} = \frac{P \tilde{X}_w^*}{RT}$$

and a = gas-liquid interfacial area per bulk volume of soil (Adz).

P_{vap} = water vapor pressure

It should be noted that the water vapor pressure (P_{vap}) is dependent on saturation, temperature, and water phase composition. This mathematical dependence is indicated in Appendix D.

When the liquid phase contains only trace amounts of components other than water, the main resistance to water mass transfer is in the gas phase. An exception to this statement would be if a trace component is a surface active agent which creates a small film of resistance at the interface. When the gas phase is the main resistance,

$$(2.15) \quad K_O \approx k_m$$

where,

k_m = gas phase film coefficient for mass transfer

$\frac{1}{k_m}$ = gas phase resistance to mass transfer

For concentrated water solutions, the liquid phase resistance may become significant and must be included in calculating the over all mass transfer coefficient (see Treybal Reference 22).

To allow mass transfer calculations using Equation (2.13), the mass transfer coefficient and interfacial area need to be quantified. The gas-liquid operations such as humidification, absorption, and stripping also require knowledge of the volumetric mass transfer coefficient ($K_o a$). This coefficient is determined experimentally. Since no one has previously considered a general water movement in soils model of the form presented here, the volumetric mass transfer coefficient has not been measured.

The model presented here could be used to determine the volumetric mass transfer coefficient from a drying experiment. In addition to the model physical parameters, the data required are the saturation (S), temperature (T), and the gas phase water mole fraction ($\tilde{X}_w$). No one has measured all of these quantities together. As a result, this work will theoretically estimate the volumetric mass transfer coefficient.

Soils (porous media) are packed beds of small particles, so earlier work on heat and mass transfer in packed beds will be useful for determining the film mass transfer coefficient (k_m). Since packed beds are composed of particles, some early investigations of mass transfer from single particles are pertinent. Frössling studied evaporation from liquid drops and proposed the following dimensionless correlation [23].

$$(2.16) \quad Sh = 2.0 + 0.55 Re_p^{1/2} Sc^{1/3}$$

where,

$$(2.17) \quad Sh = \frac{k_m D_p}{D_{aw_i}}$$

$$(2.18) \quad Re_p = \frac{D_p V_g \rho}{\mu}$$

$$(2.19) \quad Sc = \frac{\mu}{\rho D_{aw_i}}$$

and, Sh = Sherwood number
 Re_p = Particle Reynolds number
 Sc = Schmidt number
 k_m = gas phase film coefficient for mass transfer
 D_p = liquid droplet diameter
 D_{aw_i} = ordinary diffusion coefficient of component
 w_i in air
 μ = air viscosity
 ρ = air density
 V_g = air velocity

Later, Ranz and Marshall also studied evaporation from liquid drops and proposed the following correlation [24].

$$(2.20) \quad Sh = 2.0 + 0.60 Re_p^{1/2} Sc^{1/3}$$

It can be seen that Equations (2.16) and (2.20) predict Sherwood numbers of 2.0 when the air is stagnant. This number is a theoretical value for a sphere in an infinite stagnant medium. However, a recent mass transfer study using the collapsing bubble method verified the theoretical value of the Sherwood number ($Sh = 2.0$) for an oxygen bubble in stagnant water ($Re_p = 0.0$) [25].

At low Reynolds numbers ($Re_p < 10$), most of the experimental data in packed beds are from heat transfer studies. Kunii and Suzuki predict values of Sherwood numbers much less than 2.0 at low Reynolds numbers. Their experimental data substantiates their model [26].

$$(2.21) \quad Nu = \frac{\phi_s}{6(1-\epsilon)\zeta} (Re_p Pr)$$

$$(2.22) \quad Sh = \frac{\phi_s}{6(1-\epsilon)\zeta} (Re_p Sc)$$

where,

$$(2.23) \quad Nu = \frac{hD_p}{k}$$

$$(2.24) \quad Pr = \frac{C_p \mu}{k}$$

$$(2.25) \quad \phi_s = 1.0 \text{ (shape factor)}$$

$$\epsilon = 0.4 \text{ (porosity or void fraction)}$$

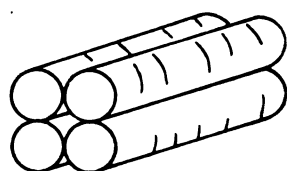
$$\zeta = 10.0 \text{ (ratio of average channeling length to particle diameter)}$$

and, Nu = Nusselt number
 Pr = Prandtl number
 h = gas phase film coefficient for heat transfer
 k = gas phase thermal conductivity
 C_p = gas phase heat capacity

Later, Littman et al. used frequency response techniques to study heat transfer from packed beds of small particles (porous media). They have claimed Kunii's method for calculating the film heat transfer coefficient from experimental data is incorrect. They have presented their own data and data of others at low Reynolds numbers to show that the Nusselt number asymptotes to a value of two [27]. The conclusions of Littman et al. will be used to calculate the film mass transfer coefficient (k_m).

In order to determine the gas-liquid interfacial area per volume of soil (a), the model illustrated in Figure 2 was used. The soil is viewed as a packed bed of cylindrical rods arranged in simple cubic packing. This model predicts a porosity of 0.22 and a drainage saturation of 0.37.

To calculate interfacial area per volume of soil (a) from the model, something must be said about the manner in which the water distributes itself at a given saturation. In this model, the water interface is assumed to have a constant radius of curvature. Also, for saturations up to



simple cubic packing of rods

porosity = 0.22

drainage saturation = 0.37

front view

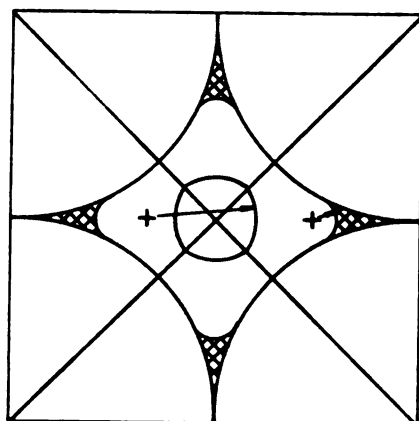


Figure 2.--Interfacial area model.

the drainage point the interface is tangent to the rod at the point of intersection. When surface tension measurements are made with capillary tubes, it is also common to assume that the gas-liquid interface is tangent to the tube surface at the point of contact.

The drainage point is reached during wetting when adjacent interfaces first touch one another. This occurs where the square diagonals intersect the rods (see front view, Figure 2). The saturation at the drainage point is calculated to be 0.37.

Beyond the drainage point, it is assumed that drainage is slow enough so that the water will distribute itself as shown in the front view of Figure 2. The radius of curvature beyond drainage is taken to be the radius of curvature of a capillary tube which has the same capillary potential as experimental capillary potential data on a soil.

The mathematical development and computer program for this model are given in Appendix E. Figure 3 contains the calculated relationship between interfacial area and saturation. At the irreducible saturation of the soil, the interfacial area must be zero. In Figure 3 the irreducible saturation is zero.

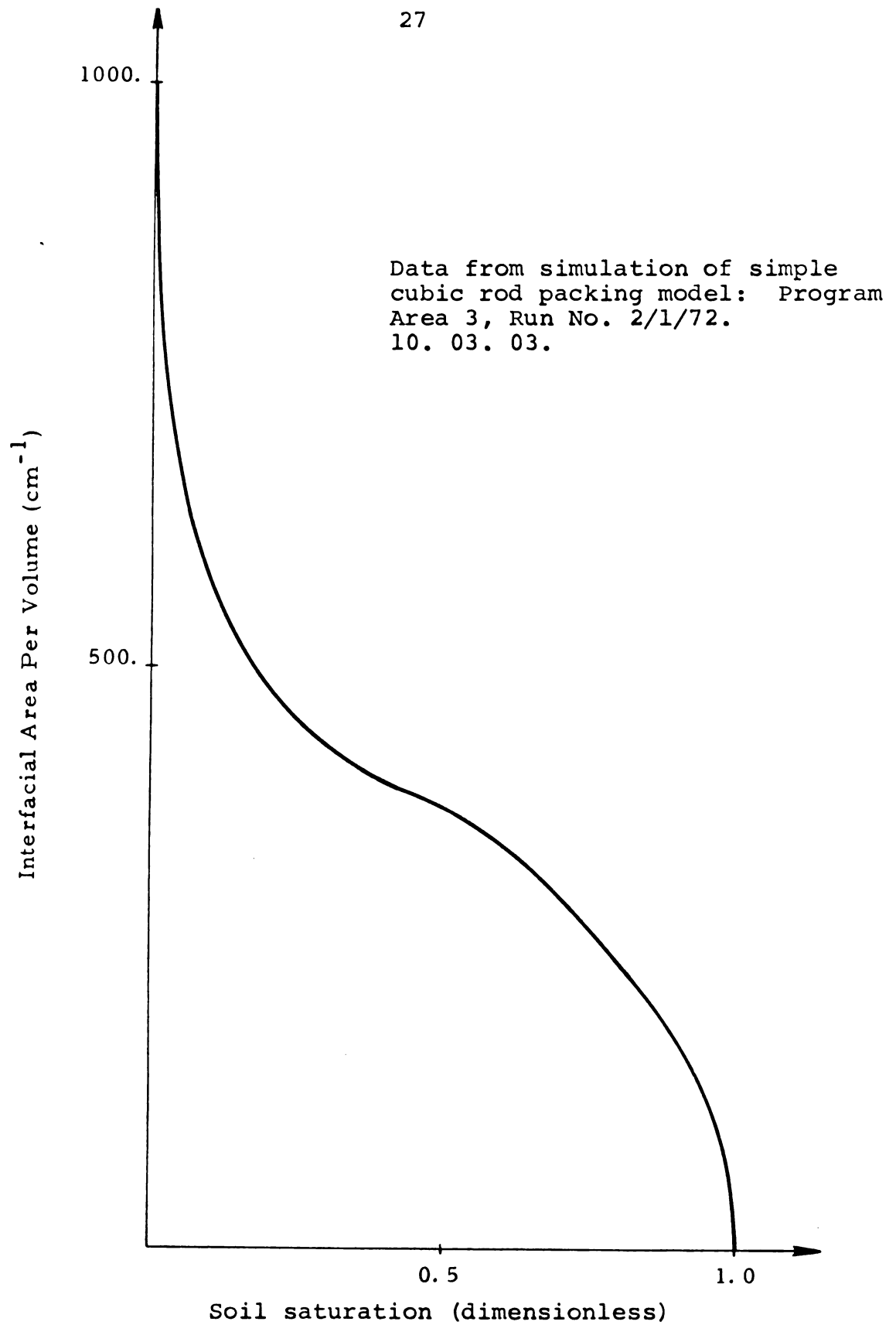


Figure 3.--Interfacial area per volume versus soil saturation.

Other models for interfacial area were considered. A model consisting of a simple cubic packing of spheres arrangement resulted in a porosity of 0.48 and a drainage saturation of 0.18. With a body centered packing of spheres arrangement, the porosity is 0.32. At a saturation of 0.12, the body centered packing of spheres was near drainage. Both of these models predict drainage saturations much lower than actually occur for sandy soils. For example, a sandy soil on the south campus swine waste disposal site had a drainage saturation of 0.35. For this reason and the computational difficulties involved with the sphere models, the simple cubic packing of rods model was chosen for this work.

The over all mass transfer coefficient and interfacial area are two physical parameters which have just been discussed. Other physical parameters in the general soil water model are hydraulic conductivity, capillary potential, water vapor diffusion coefficient, liquid water vapor pressure, liquid water enthalpy of vaporization, effective thermal conductivity, and volumetric heat capacity.

Hydraulic Conductivity

Experimental data on hydraulic conductivity on Uplands sand is given in Figures 4-6. For high saturations, hydraulic conductivity is determined by steady flow experiments and Darcy's law. For lower saturations, hydraulic conductivity is determined from unsteady state flow

Data reference: W.J. Staple, Soil Sci. Proc.,
33 (840) 1969.

Uplands sand (78% 30-100 mesh)

- Experimental data points
- Least squares data points

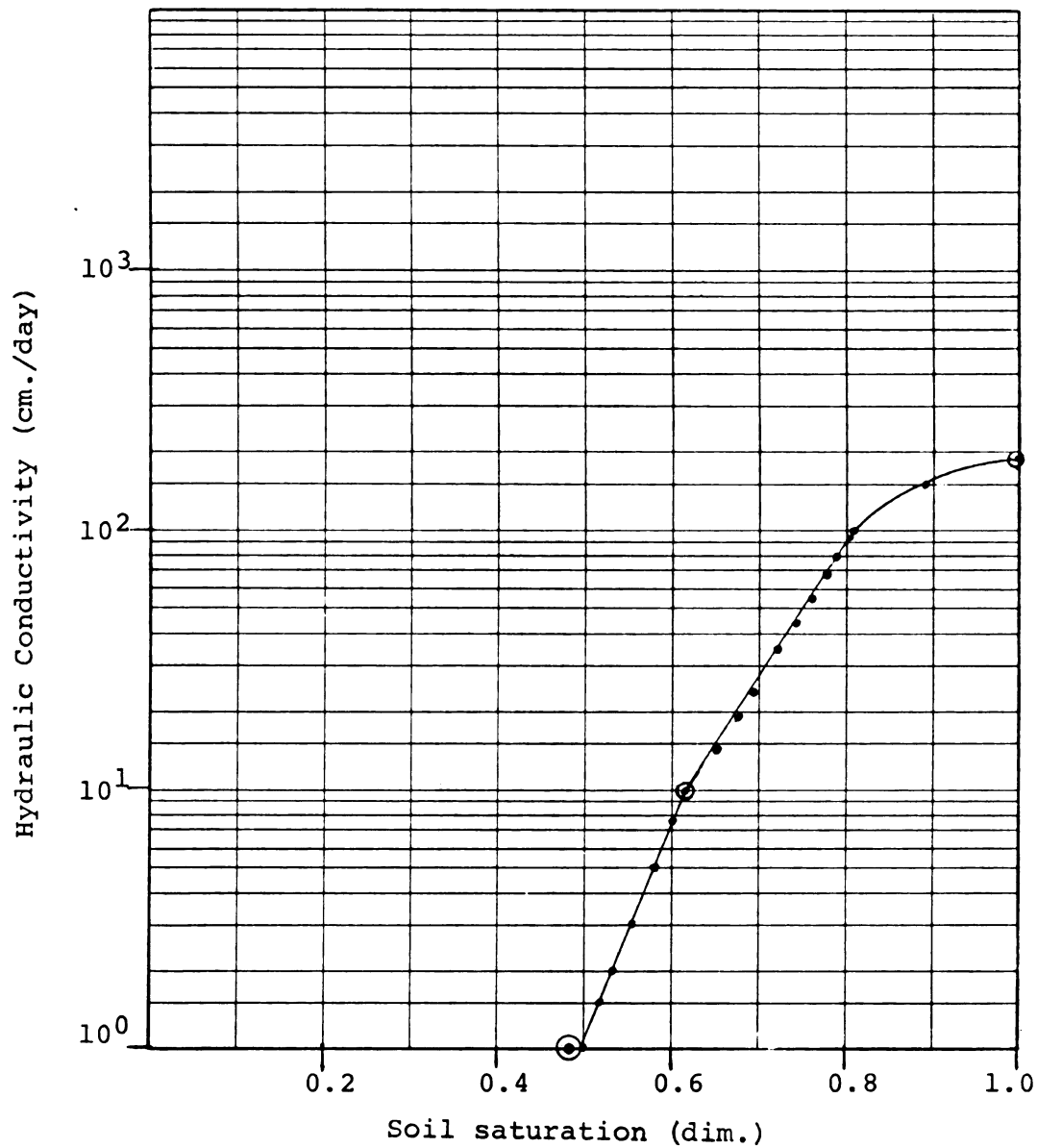


Figure 4.--Hydraulic conductivity versus soil saturation.

Data reference: W.J. Staple, Soil Sci. Proc.,
33 (840) 1969.

Uplands sand (78% 30-100 mesh)

- ⊙ Experimental data points
- Least squares data points

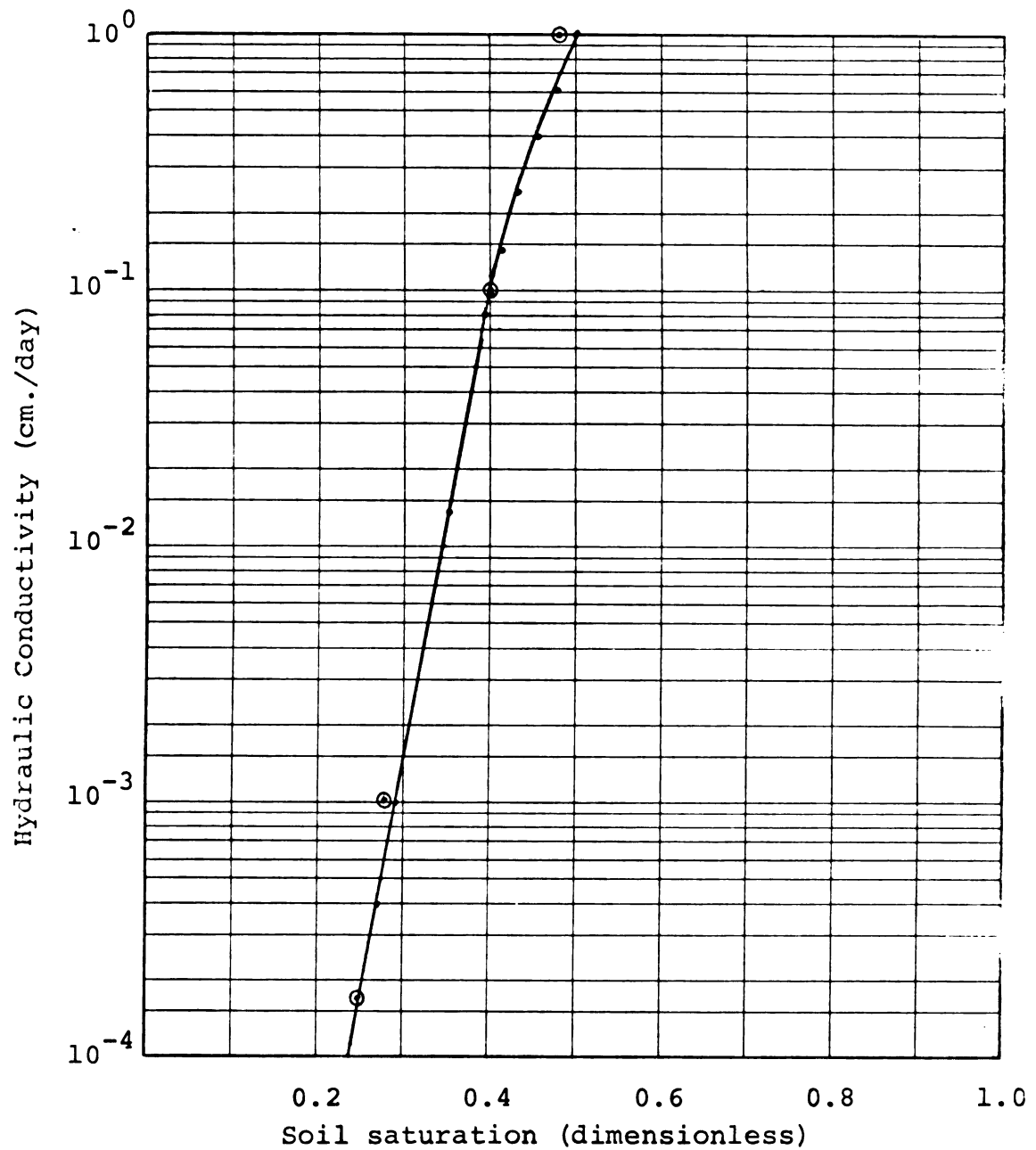


Figure 5.--Hydraulic conductivity versus soil saturation.

Data reference: W.J. Staple, Soil Sci. Proc.,
33 (840) 1969.

Uplands sand (78% 30-100 mesh)

- ⊙ Experimental data points
- . Least squares data points

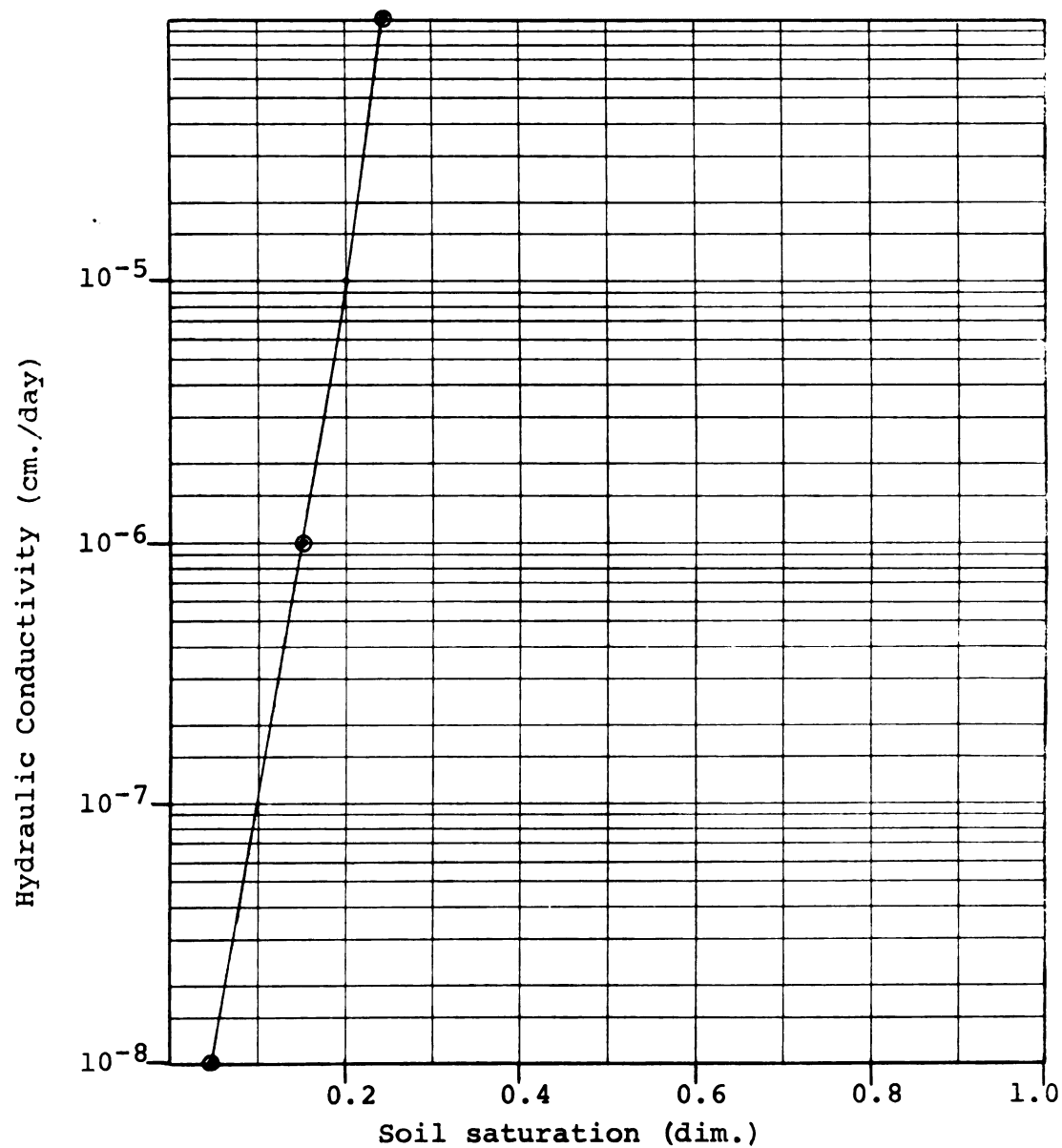


Figure 6.--Hydraulic conductivity versus soil saturation.

experiments and the equations of Gardner and Darcy (i.e., Equations (1.5) and (1.3)). The data contained in Figures 4-6 was curve fitted using a least squares technique so that the data could be used in computer calculations. Appendix F contains the documented subroutine for this data.

Capillary Potential

Figures 7-8 contain the capillary potential data on Uplands sand. At high saturations the capillary potential is determined by making measurements with a manometer. For lower saturations vapor pressure measurements are used to determine capillary potential (see Appendix A) [2] . Appendix F contains the documented subroutine which is a capillary potential curve fit modified to correct for temperature. Comparison of literature data on hydraulic conductivity and capillary potential demonstrates that these parameters are strongly dependent on particle size and particle size distribution. Figures 9-10 contain the capillary potential data for the Valentine sand used by Hanks et al.[30]. The calculation of some of the data points is explained in Appendix L. Appendix F contains the documented subroutine which is the Valentine sand capillary potential curve fit modified to correct for temperature.

Data reference: W.J. Staple, Soil Sci. Proc.,
33 (840) 1969.

- Drying curve for Uplands sand
(78% 30-100 mesh)
- x Least Square fit of the experimental points (○).

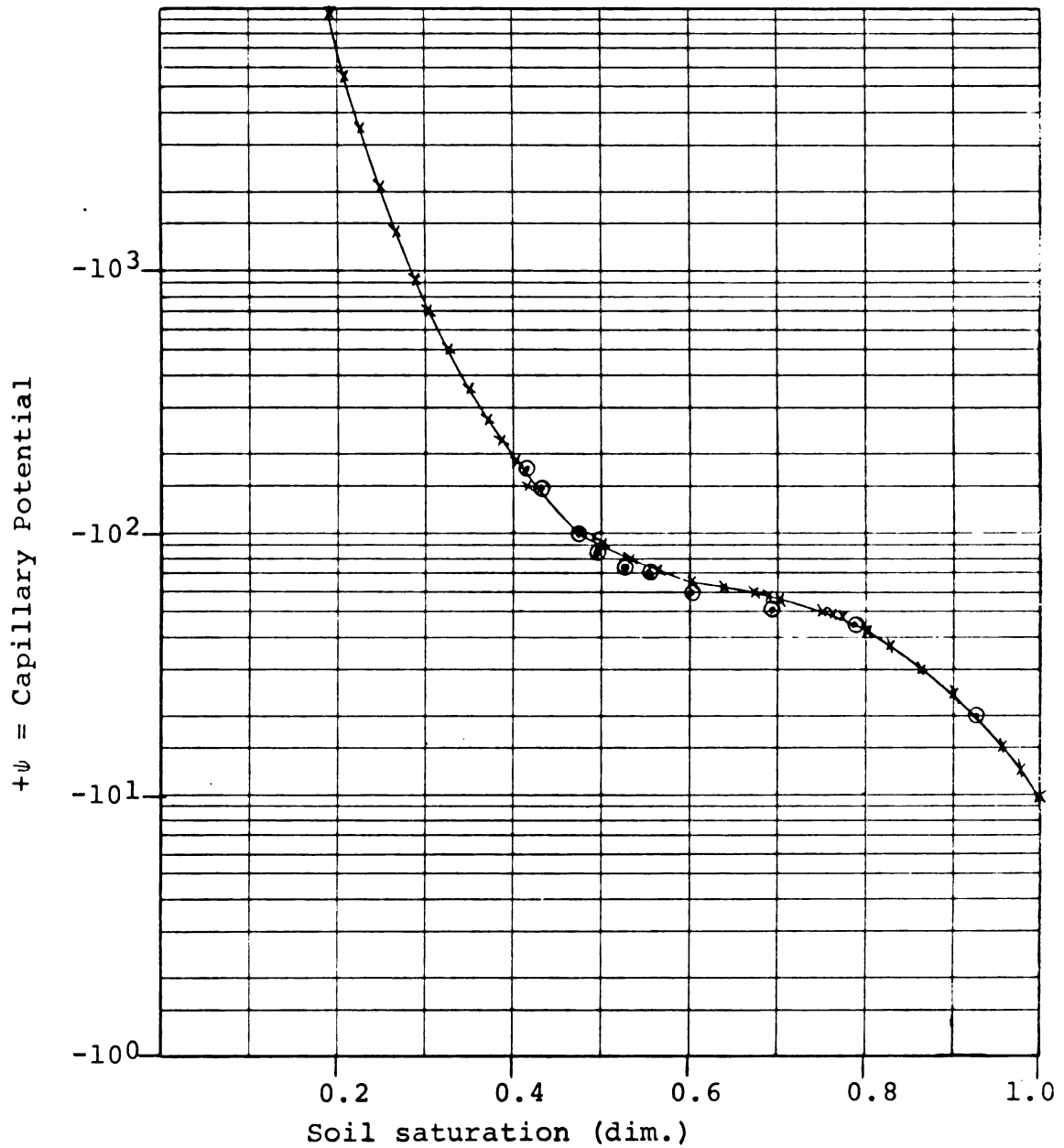


Figure 7.--Capillary potential versus soil saturation.

Data reference: W.J. Staple, Soil Sci. Proc.,
33 (840) 1969.

- ⊙ Drying curve for uplands sand
(78% 30-100 mesh) -- Experimental
- x Least squares fit of the experimental
points (⊙).

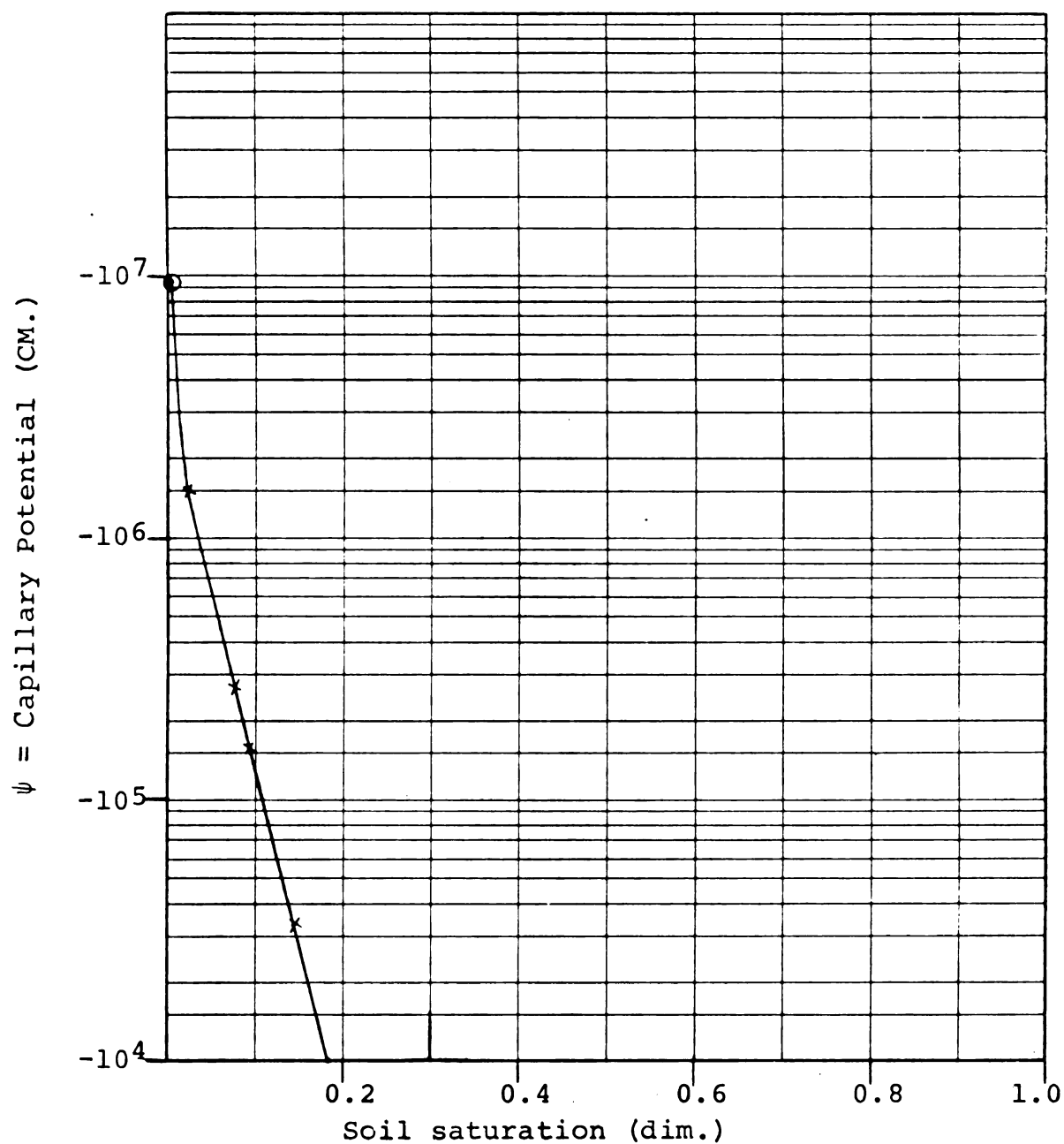


Figure 8.--Capillary potential versus soil saturation.

Data reference: R.J. Hanks, et.al., Soil Sci. Proc.,
31 (594) 1967

- ⊙ Drying curve for Valentine sand
(experimental values)
- ⊗ Drying curve for Valentine sand
(calculated from saturation profile at the start
of Hanks drying experiment--see appendix L)
- Least squares computer curve fit

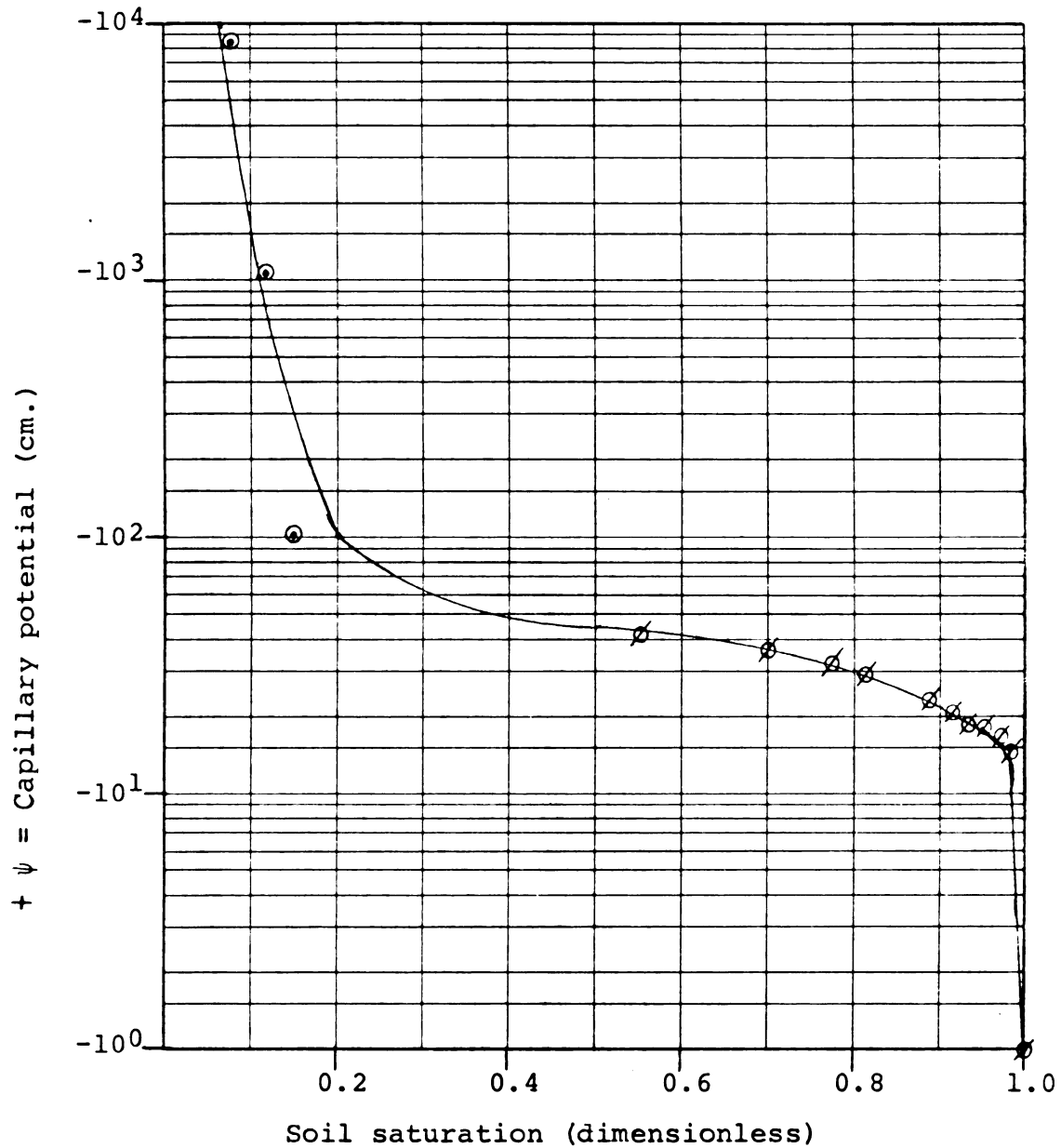


Figure 9.--Capillary potential versus soil saturation.

Data reference: R.J. Hanks, et.al., Soil Sci. Proc.,
31 (594) 1967

⊙ Drying curve for Valentine sand
(experimental values)

— Least squares computer curve fit

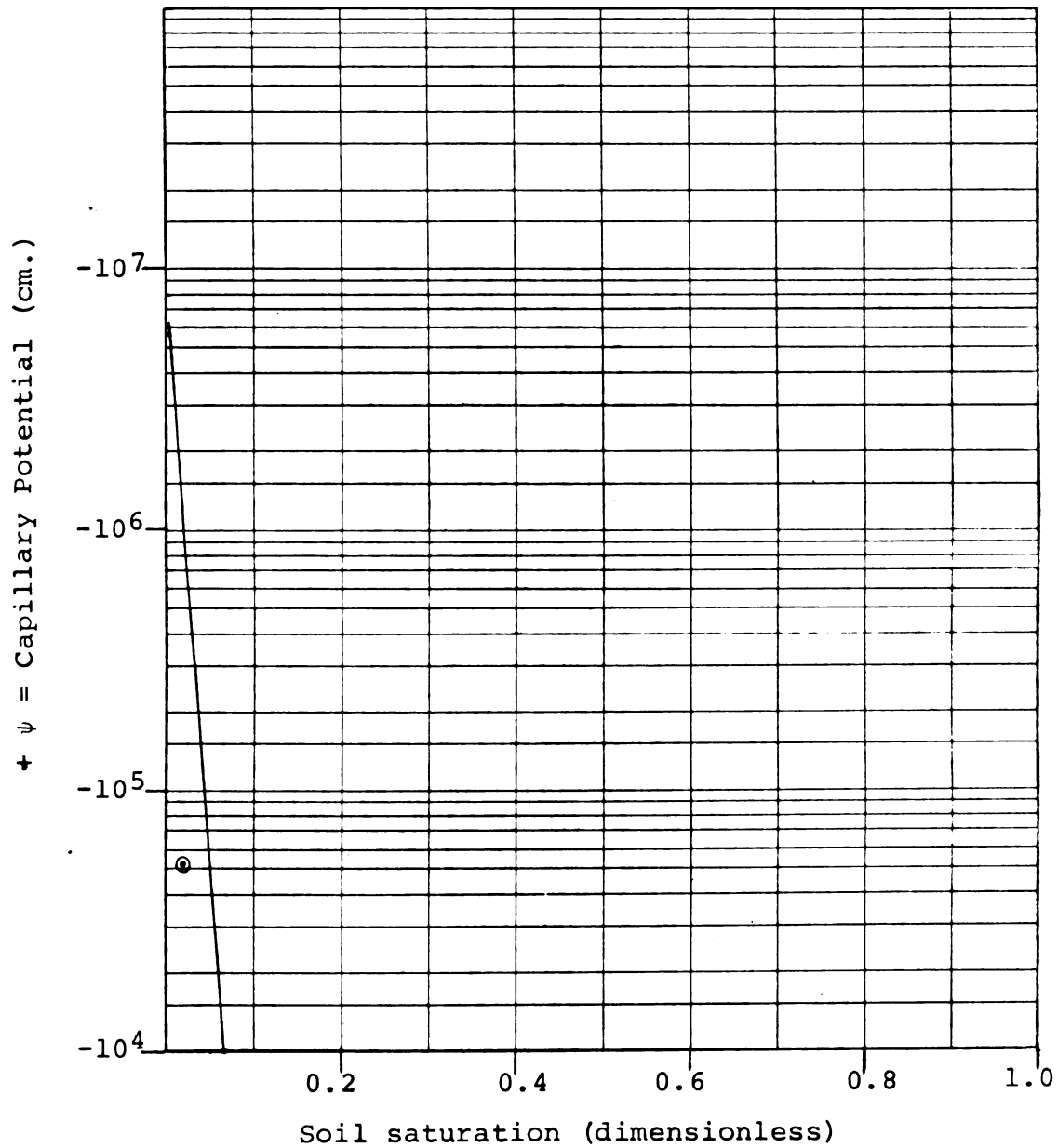


Figure 10.--Capillary potential versus soil saturation.

Water Vapor Diffusion Coefficient

In this study the water vapor diffusion coefficient in soil has been assumed equal to the ordinary diffusion coefficient of water vapor in air. Philip and De Vries have suggested a value of two thirds of the ordinary diffusion coefficient [11]. Clearly the ratio of water vapor diffusion coefficient in soil to the ordinary diffusion coefficient will be a function of saturation and not constant. It has been shown that the assumption just made is an upper bound on the water vapor diffusion coefficient (D_{aw}) in soil [28]. The ordinary diffusion coefficient for water vapor in air has been fitted as a function of temperature using an empirical equation from the International Critical Tables.

$$(2.26) \quad \mathcal{D}_{aw} |_{T(^{\circ}K)} = \mathcal{D}_{aw} |_{0(^{\circ}C)} \left(\frac{T(^{\circ}K)}{273.15} \right)^{1.75}$$

Liquid Water Vapor Pressure and Enthalpy of Vaporization

Data on liquid water vapor pressure and enthalpy of vaporization was obtained from the Handbook of Chemistry and Physics. Vapor pressure and enthalpy of vaporization were curve fit as functions of temperature and vapor pressure was corrected for the effect of saturation described in Appendix D. The documented subroutines for these parameters are contained in Appendix F.

Thermal Parameters: Effective
Thermal Conductivity and
Volumetric Heat Capacity

The thermal parameters of effective thermal conductivity and heat capacity were obtained on Ottawa sand from Moench [29]. This data is presented in Figure 11, and Appendix F contains the documented subroutines which are curve fits of this data. The method of thermal conductivity measurement and volumetric heat capacity calculation is contained in Moench's thesis [29]. In summary, the thermal probe method was used to measure the apparent thermal conductivity. The theory of Philip and De Vries was used to estimate the energy flux due to the distillation effect. The effective thermal conductivity is then obtained by subtracting the energy flux due to the distillation effect from the apparent thermal conductivity.

General Model for Water Movement
in Soils Under the Condition of
Vapor-Liquid Equilibrium

Thus far the general model for water movement in soils has been presented along with the physical parameters contained in the model. If vapor-liquid equilibrium exists, the general model reduces to the equations of Philip and De Vries. The equations of continuity for the liquid phase water (2.2) and water vapor (2.5) are added to give

$$(2.27) \quad \frac{\partial \rho_w \bar{\theta}}{\partial t} = - \frac{\partial}{\partial z} (\rho_w V^O + \tilde{N}_w M_w)$$

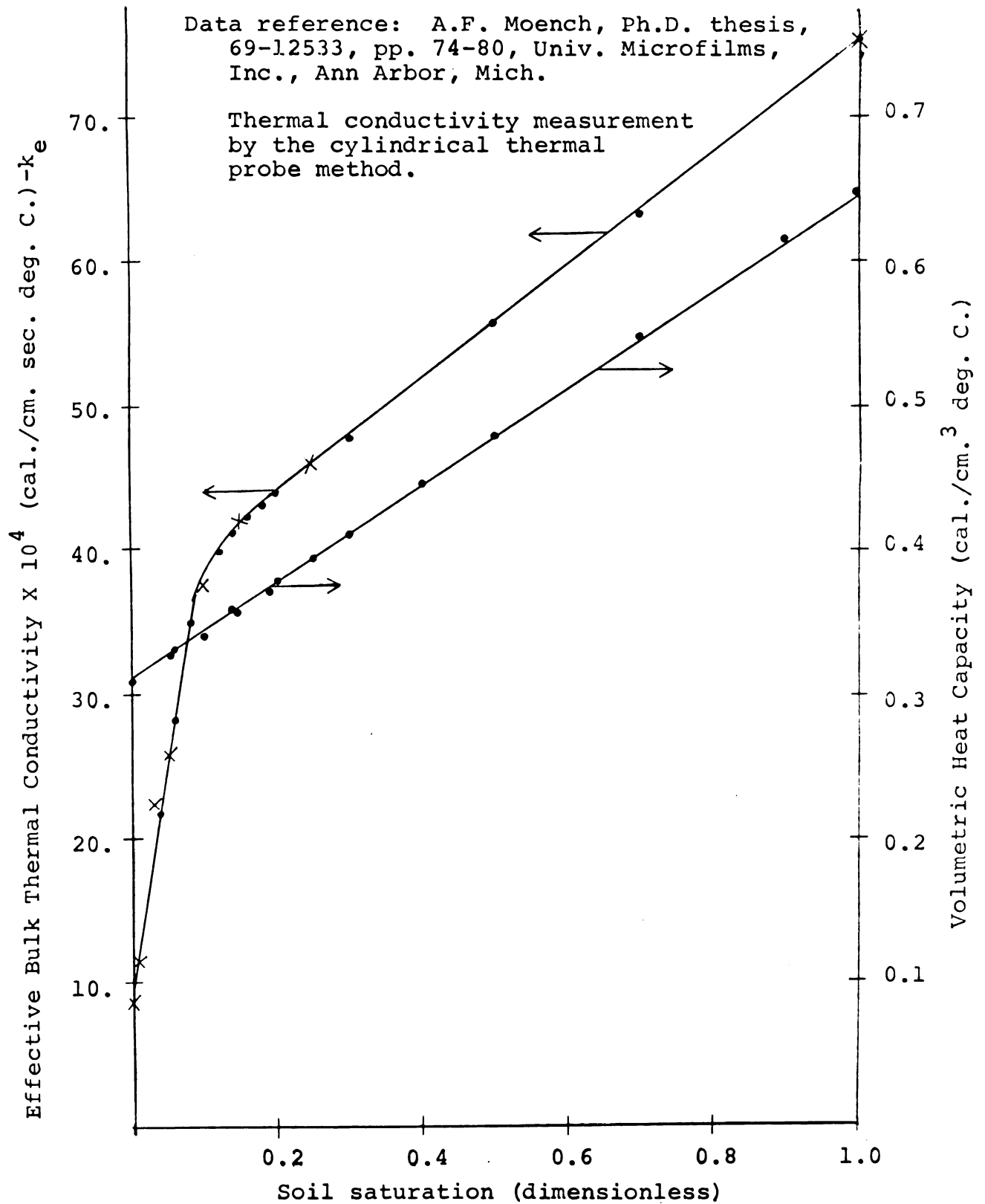


Figure 11.--Effective thermal conductivity and volumetric heat capacity versus soil saturation.

The energy balance (2.7) is modified to include the distillation effect.

$$(2.28) \quad c \frac{\partial T}{\partial t} = - \frac{\partial q}{\partial z} - \left(\frac{\partial \tilde{N}_w}{\partial z} \right) \Delta H_{\text{vap}} M_w.$$

In the next chapter, the general model for water movement in soils will be tested. A drying problem will be described and the numerical solution of the general model and earlier models will be developed. Using the numerical methods, some drying problems will be run using the new general model developed in this work, the theory of Philip and De Vries, and the isothermal equation of Gardner.

CHAPTER III

NUMERICAL SIMULATION

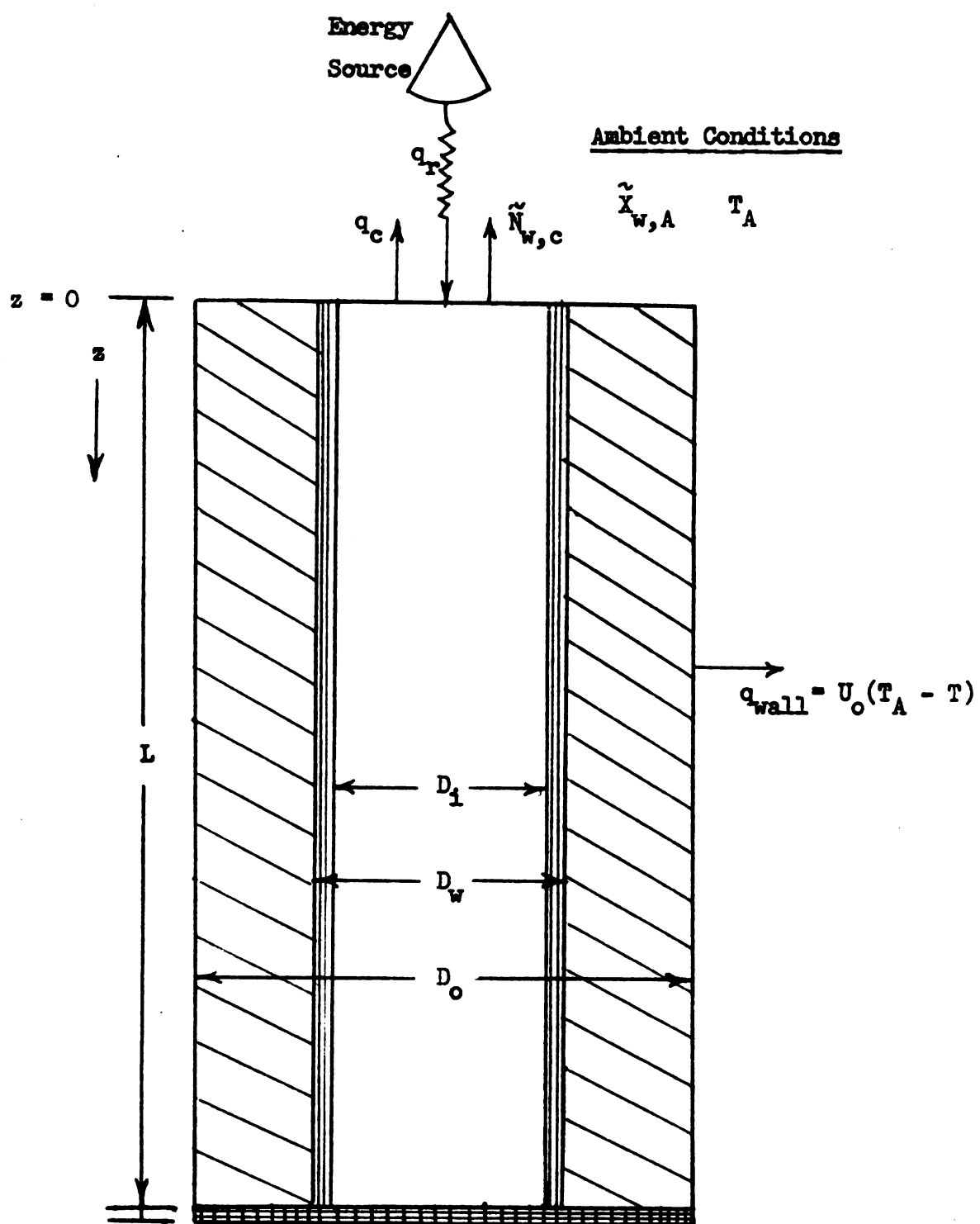
In this chapter, a general drying problem will be stated mathematically followed by the development of the numerical methods for simulation of the drying problem. The theory developed in Chapter II, the theory of Philip and De Vries, and the isothermal water movement equation will be used to simulate some drying problems. In Chapter IV, a number of drying problems will be defined and the simulation results will be presented and discussed.

Hanks et al. have published experimental data obtained from drying of Valentine sand by radiation [30]. The saturation and temperature profiles published are averages of two replicate experiments. Attempts by this author to obtain their original data were unsuccessful because they no longer had this data.

The complete set of boundary conditions for their drying experiments on Valentine sand were not published. In their experiments, ambient temperature was controlled at 25 ± 2 °C. but there was no control on humidity. Radiant energy was supplied by heat lamps and they attempted to minimize surface turbulence.

The following general drying problem is for a sand column of the same type and dimensions as the columns used by Hanks et al. Figure 12 is a diagram of the sand column with boundary conditions illustrated. Table 1 contains the legend for Figure 12.

In order to simulate a drying problem, the initial conditions and boundary conditions for the problem must be stated. The surface boundary conditions say that water can only be transported across the top surface of the column in the vapor state. Furthermore, the water flux is given by the product of a surface film mass transfer coefficient ($k_{m,s}$) and a concentration driving force. The driving force is the difference in water concentration between the atmosphere and soil surface. The film coefficient is a function of wind velocity and is calculated in Appendix K. The energy boundary condition contains a radiative flux (q_r) and a convective flux (q_c). The convective energy flux is given by a surface film heat transfer coefficient (h_s) and a temperature driving force. The temperature driving force is the temperature difference between the atmosphere and soil surface. Again, the film coefficient is a function of wind velocity and is calculated in Appendix K.



See Table 1 for the legend to Figure 12.

Figure 12.--Diagram of sand column for drying problems.

TABLE 1.--Legend for Figure 12.

Materials

	Styrofoam insulation
	Plexiglass column wall
	Valentine sand
	Column bottom; composed of a layer of plexiglass and wood

Column Dimensions

- $L = 45$ cm. (Column length)
 $D_i = 10$ cm. (Column inside diameter)
 $D_w = 11$ cm. (Outside diameter of column wall)
 $D_o = 27$ cm. (Outside diameter of column)

Definitions of Variables

- q_r = radiant flux of energy from heat lamps
 q_c = convective flux of energy at the top column surface
 q_{wall} = convective flux of energy at the column walls (radial direction)
 $\tilde{N}_{w,c}$ = molar flux of water vapor at the top column surface
 T_A = ambient temperature
 $\tilde{X}_{w,A}$ = ambient mole fraction of water vapor

Initial Conditions

- (3.1) $S(z,t) = S(z)$
 (3.2) $T(z,t) = T(z)$
 (3.3) $\tilde{X}_w(z,t) = \tilde{X}_w(z)$
- $\left. \begin{array}{l} z \in [0, L] \\ t = 0 \end{array} \right\}$

Boundary Conditions

At the top column surface,

- (3.4) $v^o(0,t) = 0$
 (3.5) $\tilde{N}_w(0,t) = \tilde{N}_{w,c} = \frac{k_{m,s} P}{RT} (\tilde{X}_{w,A} - \tilde{X}_w(0,t))$
 (3.6) $q(0,t) = q_r + q_c = q_r + h_s (T_A - T(0,t))$
- $\left. \begin{array}{l} \\ \\ \end{array} \right\} t \geq 0$

At the bottom column surface,

- (3.7) $v^o(L,t) = 0$
 (3.8) $\tilde{N}_w(L,t) = 0$
 (3.9) $q(L,t) = 0$
- $\left. \begin{array}{l} \\ \\ \end{array} \right\} t \geq 0$

The bottom boundary conditions say the column bottom is impervious to water flow and is a perfect insulator. Due to a lack of published information by Hanks et al., a column bottom heat transfer coefficient cannot be estimated. The validity of the perfect insulator assumption will have to be demonstrated by computer simulation.

The general model for water movement in soils (Equations (2.2), (2.5), (2.7)) is the set of equations of change written in terms of fluxes of mass and energy. These fluxes of mass and energy can be written in terms of macroscopic properties of the soil (Equations (1.3), (2.11), (2.12), (2.13)). The equations of change will now be written in terms of the macroscopic properties of the soil.

When the soil porosity and liquid water density are constant for the drying problems considered, Equations (2.2), (1.3), (1.4), (2.13) can be comined to give

$$(3.10) \quad \frac{\partial S}{\partial t} = - \frac{1}{\epsilon} \frac{\partial V^O}{\partial z} - \frac{K_O a P M_w}{\rho_w \epsilon R T} (\tilde{X}_w^* - \tilde{X}_w)$$

$$(3.11) \quad V^O = -K \left(\frac{\partial \Psi}{\partial z} - 1 \right)$$

When the gas phase pressure changes with time and position are negligible in comparison with other terms in the equation of continuity for the water vapor, Equations (2.5), (2.11), (2.13) combine to give

$$(3.12) \quad \frac{\partial \bar{C}}{\partial t} = - \frac{\partial \bar{N}_w}{\partial z} + \frac{K_o a}{\epsilon T} (\tilde{X}_w^* - \tilde{X}_w)$$

$$(3.13) \quad \bar{C} = \frac{\tilde{X}_w (1-S)}{T}$$

$$(3.14) \quad \bar{N}_w = - \frac{D_{aw} (1-S)}{T (1-\tilde{X}_w)} \frac{\partial \tilde{X}_w}{\partial z}$$

The energy balance equation with a term to include radial losses through the soil column becomes (see Appendix J for calculation of U_o)

$$(3.15) \quad C \frac{\partial T}{\partial t} = - \frac{\partial q}{\partial z} - \Delta H_{vap} \frac{K_o a}{RT} PM_w (\tilde{X}_w^* - \tilde{X}_w) - \frac{4D_o}{D_i} \frac{1}{2} (T - T_A) U_o$$

$$(2.12) \quad q = - k_e \frac{\partial T}{\partial z}$$

It can be seen that the three coupled partial differential equations are highly nonlinear. This fact precludes the use of successive linearization and implicit numerical techniques. Based on these considerations and the nature of the boundary conditions, it was decided to use the following explicit technique.

A first order forward difference formula on time was used.

$$(3.16) \quad \frac{S_{i,j+1} - S_{i,j}}{\delta t} \approx \frac{\partial S}{\partial t} \Big|_{i,j}$$

$$(3.17) \quad \frac{\bar{C}_{i,j+1} - \bar{C}_{i,j}}{\delta t} \cong \frac{\partial \bar{C}}{\partial t} \Big|_{i,j}$$

$$(3.18) \quad \frac{T_{i,j+1} - T_{i,j}}{\delta t} \cong \frac{\partial T}{\partial t} \Big|_{i,j}$$

On the spatial derivatives of the fluxes, a first order forward difference formula was used. A first order backward difference formula was then used on the spatial partial derivatives in the flux terms.

$$(3.19) \quad -\left(\frac{V_{i+1,j}^O - V_{i,j}^O}{\delta z}\right) \cong -\frac{\partial V^O}{\partial z} \Big|_{i,j}$$

$$(3.20) \quad -K_{i,j} \left(\frac{\Psi_{i,j} - \Psi_{i-1,j}}{\delta z} - 1\right) \cong V^O \Big|_{i,j}$$

$$(3.21) \quad -\left(\frac{\bar{N}_{w,i+1,j} - \bar{N}_{w,i,j}}{\delta z}\right) \cong -\frac{\partial \bar{N}_w}{\partial z} \Big|_{i,j}$$

$$(3.22) \quad -\left(\frac{D_{aw}(1-S_{i,j})}{T_{i,j}(1-\tilde{X}_{w,i,j})}\right) \frac{(\tilde{X}_{w,i,j} - \tilde{X}_{w,i-1,j})}{\delta z} \cong \bar{N}_w \Big|_{i,j}$$

$$(3.23) \quad -\left(\frac{q_{i+1,j} - q_{i,j}}{\delta z}\right) \cong -\frac{\partial q}{\partial z} \Big|_{i,j}$$

$$(3.24) \quad -k_{e_{i,j}} \left(\frac{T_{i,j} - T_{i-1,j}}{\delta z} \right) \cong q|_{i,j}$$

If Equation (3.20) were substituted into Equation (3.19) and the hydraulic conductivity were constant, the following second order difference formula would result.

$$(3.25) \quad K \left(\frac{\psi_{i+1,j} - 2\psi_{i,j} + \psi_{i-1,j}}{\delta z^2} \right) \cong K \frac{\partial^2 \psi}{\partial z^2} \quad i,j$$

The first order difference formulas on space were so chosen to obtain this type of a result. Equation (3.25) can be recognized as the second order difference formula for the second partial derivative of ψ with respect to z .

The numerical approximation to Equations (2.12), (3.10)-(3.15) is obtained by combining these equations with Equations (3.16)-(3.24). The resultant set of algebraic equations can then be solved on the digital computer. Appendix G contains the documented computer program which uses the above numerical techniques to solve the general model equations.

If vapor-liquid equilibrium exists, the general water model reduces to the equations of Philip and De Vries ((2.27), (2.28)). These equations subject to the constraints of constant porosity, liquid water density, and gas phase pressure reduce to

$$(3.26) \quad \frac{\partial \bar{S}}{\partial t} = - \frac{1}{\varepsilon} \frac{\partial}{\partial z} (V^O + \frac{\tilde{N}_w M_w}{\rho_w})$$

$$(3.27) \quad C \frac{\partial T}{\partial t} = - \frac{\partial q}{\partial z} - \left(\frac{\partial \tilde{N}_w}{\partial z} \right) \Delta H_{\text{vap}} M_w - \frac{4 D_o}{D_i^2} U_o (T - T_A)$$

where, gas phase pressure (P) appearing in $\tilde{N}_w$ is treated as a constant.

The initial conditions for the Philip and De Vries equations are:

$$\left. \begin{array}{l} (3.28) \quad \bar{S}(z, t) = \bar{S}(z) \\ (3.29) \quad T(z, t) = T(z) \end{array} \right\} \quad t = 0$$

The boundary conditions are the same as those given by Equations (3.4)-(3.9). The explicit numerical techniques used for the general problem (Equations (3.16), (3.17)-(3.24)) were used to transform the equations of Philip and De Vries into a set of algebraic equations which could be solved on the digital computer. The computer program which solves the equations of Philip and De Vries is listed in Appendix H.

The simplest water model for unsteady state flow in soils is the isothermal equation of Gardner. For a constant porosity Gardner's equation and Darcy's law combine to give

$$(3.30) \quad \frac{\partial \bar{S}}{\partial t} = - \frac{1}{\varepsilon} \frac{\partial \bar{V}^O}{\partial z}$$

$$(3.31) \quad \bar{V}^O = -K \left(\frac{\partial \Psi}{\partial z} - 1 \right)$$

These equations cannot predict the constant drying rate during the constant rate period, and so to run a simulation experimental data must be available to determine the constant rate. If the boundary conditions at the soil surface were known, the constant drying rate could be calculated from the controlling transfer process: that is heat transfer or mass transfer.

The initial conditions for the drying problem using the isothermal equation are

$$(3.28) \quad \bar{S}(z,t) = \bar{S}(z) \quad t = 0$$

The boundary conditions are

$$(3.32) \quad \bar{V}^O = \text{constant, during the constant rate drying period.}$$

When the surface saturation reaches the irreducible saturation, the drying rate begins to decrease and the boundary condition becomes

$$(3.33) \quad \bar{S}(0,t) = \bar{S}_{\text{Irreducible}}$$

Appendix I contains a listing of the documented computer program which solves the isothermal equation for a drying problem.

CHAPTER IV

RESULTS AND DISCUSSION

Using the numerical method outlined in Chapter III, a number of drying problems were simulated. Table 2 contains a listing of the simulated drying problems. It can be seen from Table 2 that a number of simulations were run for each of the models: (1) isothermal Equation (3.30), (2) Philip and De Vries model (3.26, 3.27), and (3) general model (3.10, 3.12, 3.15). For simplicity, in the future the above models will be denoted as: (1) IE, (2) P&DVM, and (3) GM respectively. All of the simulations are for the soil column described in Figure 12 and Table 1.

A numerical solution to any of these models brings up questions of stability and convergence. A numerical solution is stable if the difference between the real solution and numerical solution does not have large oscillations or grow large with time. A convergent solution is one where the difference between the real solution and numerical solution is very small.

In this work the experimental drying data of Hanks et al. gives an indication about the general shape of the solution. This information is useful for a stability

TABLE 2.--Simulation Problems.

Simulation Number	1	2	3	4	5	6
Unsteady State Models						
Isothermal (Gardner)	X		X	X		X
Nonisothermal - equilibrium (Philip & De Vries)		X			X	
Thermal conductivity & heat capacity data (Moench)	-	X	-	-	X	-
Ottawa sand						
Capillary Potential Data						
Uplands sand (Staple)	X	X				
Valentine sand (Hanks)			X	X	X	X
Hydraulic conductivity data						
Uplands sand (Staple)	X	X	X			
0.1 X Uplands sand (Staple)				X	X	
0.01 X Uplands sand (Staple)						X
Boundary Conditions						
Ambient temp. = 25°C.	X	X	X	X	X	X
Ambient mole fraction $X_{w,A}=0.01$	X	X	X	X	X	X
Surface wind velocity = 4 miles/hr.	X	X	X	X	X	X
Radiation input = $q_r=870 \text{ cal./cm.}^2\text{day}$	X	X	X	X	X	X
Simulation time (days)	X	X				
0-10			X	X	X	X
0-40						

TABLE 2.--Continued.

Simulation Number	7	8	9	10	11
Unsteady State Models					
Nonisothermal, Equilibrium (Philip & De Vries)					X
Nonisothermal, Nonequilibrium (Novak)	X	X	X	X	
Thermal conductivity & heat capacity data (Moench) Ottawa sand	X	X	X	X	X
Capillary potential data					
Uplands sand (Staple)	X	X			
Valentine sand (Hanks)			X	X	X
Hydraulic conductivity data					
Uplands sand (Staple)	X	X			
0.1 X Uplands sand (Staple)			X	X	X
Boundary Conditions					
Constant	X	X	X	X	
Time varying					
Simulation time (days)	2.0 sec	0.2 sec	2.0 sec	0.02 sec	7
Initial Conditions	-	-	-	-	Wet
Sherwood Number (Sh)	0.002	2.0	0.002	2.0	-

criterion. If a solution deviates largely from the general solution shape it can be judged unstable.

The real solution will be the solution converged to by adjustment of the finite difference sizes used in the numerical solutions. In this work, the procedure used to arrive at stable, convergent solutions was the following. A space increment of 9 cm. was chosen and 5 space increments were used for the 45 cm. column. The time increment was then changed until a stable solution was obtained. Using the stable time increment as a base value, the time increment was decreased until the solutions converged. By changing the time increments while holding the space increment fixed the ratio of time increment to space increment was changed. It was found that time increments differing by a couple orders of magnitude gave solutions which agreed out to 7-10 significant figures. For the long simulation runs, the larger time increments which gave convergent solutions were used to minimize computation cost. It was felt that 7-10 significant figure agreement was sufficient.

The Michigan State University CDC-6500 computer was used to simulate the drying problems. A number of compiler options were available and the FTN compiler was chosen since it is guaranteed against system errors by CDC and has about 13 significant figures in single precision. In contrast the RUNT compiler which generates a poorer code matched only 9 significant figures of some sample FTN calculations and overlooked a fortran program syntax error.

A drying experiment was chosen to be an "acid test" for the different models. This is because water movement would occur in two phases and there would be temperature gradients to affect the water movement. The porous media chosen was a sand.

A literature search did not turn up any references which contained the saturation and temperature profiles for a drying experiment and a complete set of physical properties data. However, the drying data on Valentine sand by Hanks et al. [30] did contain the saturation and temperature profiles and some capillary potential data. Since the data needed on Valentine sand could not be found in the literature, data on other sands was found to supplement the information provided by Hanks et al. Hydraulic conductivity and capillary potential for Uplands sand was published by Staple [6]. Effective thermal conductivity and volumetric heat capacity was published by Moench for Ottawa sand [29]. With this data simulation numbers 1 and 2 were run. Table 2, 3, and 4 and Figures 13-15 contain the simulation parameters and results [33].

The unsteady state solution of the P&DVM has not previously been obtained. However, the constant and falling rate drying periods have been studied numerically for the IE [14,15]. In the P&DVM it was found that the material balance on water determined the maximum allowable time increment. During simulation numbers 1 and 2 it was found

TABLE 3.--Simulation parameters for simulation number 1.

<u>Numerical Information</u>			
Maximum Simulation Time (Days)	.50000000E+01		
Size of Time Increment (Days)	.34652222E-03		
The Number of Time Increments	115432		
Column Length (Cm.)	.45000000E+02		
Size of Space Increment (Cm.)	.90000000E+01		
Number of Space Increments	5		
Ratio of Delt to Delz	.38502469E-04		
<u>***</u>			
<u>The Initial Conditions Are</u>			
.6792339E+00	.7687889E+00	.8315037E+00	.8824673E+00 .9314091E+00
z = 0	z = 9	z = 18	z = 27 z = 36 cm. (Soil Depth)
Column Length			.450000E+02 cm
Porosity			.305000E+00
Drying Rate During Constant Rate Period			-.47213E+01 cm/day
Surface Saturation During Falling Rate			.150000E-01
Drainage Rate Thru Column Bottom			.0

TABLE 4.--Simulation parameters for simulation number 2.

Numerical Information	
Maximum Simulation Time (Days)	.500000000E+01
Size of Time Increment (Days)	.34652222E-03
The Number of Time Increments	115432
Column Length (Cm.)	.450000000E+02
Size of Space Increment (Cm.)	.900000000E+01
Number of Space Increments	5
Ratio of Delt to Delz	.38502469E-04

The Following is a List of Physical Parameters for the System	
Column OD (Cm.)	.260000000E+02
Column ID (Cm.)	.100000000E+02
Porosity (Dim.)	.305000000E+00
Ordinary Diffusion Coef. Air-Water ($\frac{\text{Cm}^2}{\text{day}}$)	.190000000E+05
Over All Mass Transfer Coef. (1/day)	.380000000E+06
Pressure (Atm.)	.100000000E+01
Molecular Wt. of Water	.180000000E+02
Gas Constant (CC.Atm/Gm.Mole-Deg.K.)	.82057000E+02

The Following is a List of Boundary Conditions	
Ambient Temperature (Deg.C.)	.250000000E+02
Ambient Mole Fraction of Water Vapor	.100000000E-01
Radiation Flux ($\text{Cal}/\text{Cm}^2\text{-Day}$)	.870000000E+03
Wall Over All Heat Transfer Coef.	.548000000E+00
Filmh ($\text{Cal.}/\text{Cm.}^2\text{-Day-Deg.}$)	.211000000E+02

The Following is a Listing of the Initial Conditions			
Increment	Position (Cm.)	Saturation (Dim.)	Temperature (Deg.C.)
1	.0	.6792339E+00	.2500000E+02
2	.90E+01	.7687889E+00	.2500000E+02
3	.18E+02	.8315037E+00	.2500000E+02
4	.27E+02	.8824673E+00	.2500000E+02
5	.36E+02	.9314091E+00	.2500000E+02

Mole Fraction of Water Vapor (Dim.)			
1	.3117188E-01		
2	.3117188E-01		
3	.3117188E-01		
4	.3117188E-01		
5	.3117188E-01		

CURVE

- 1. - Initial Condition
- 2. - time = 1 day
- 3. - time = 2 days
- 4. - time = 6 days
- 5. - time = 10 days

See Tables 2, 3 and 4 for simulation conditions.

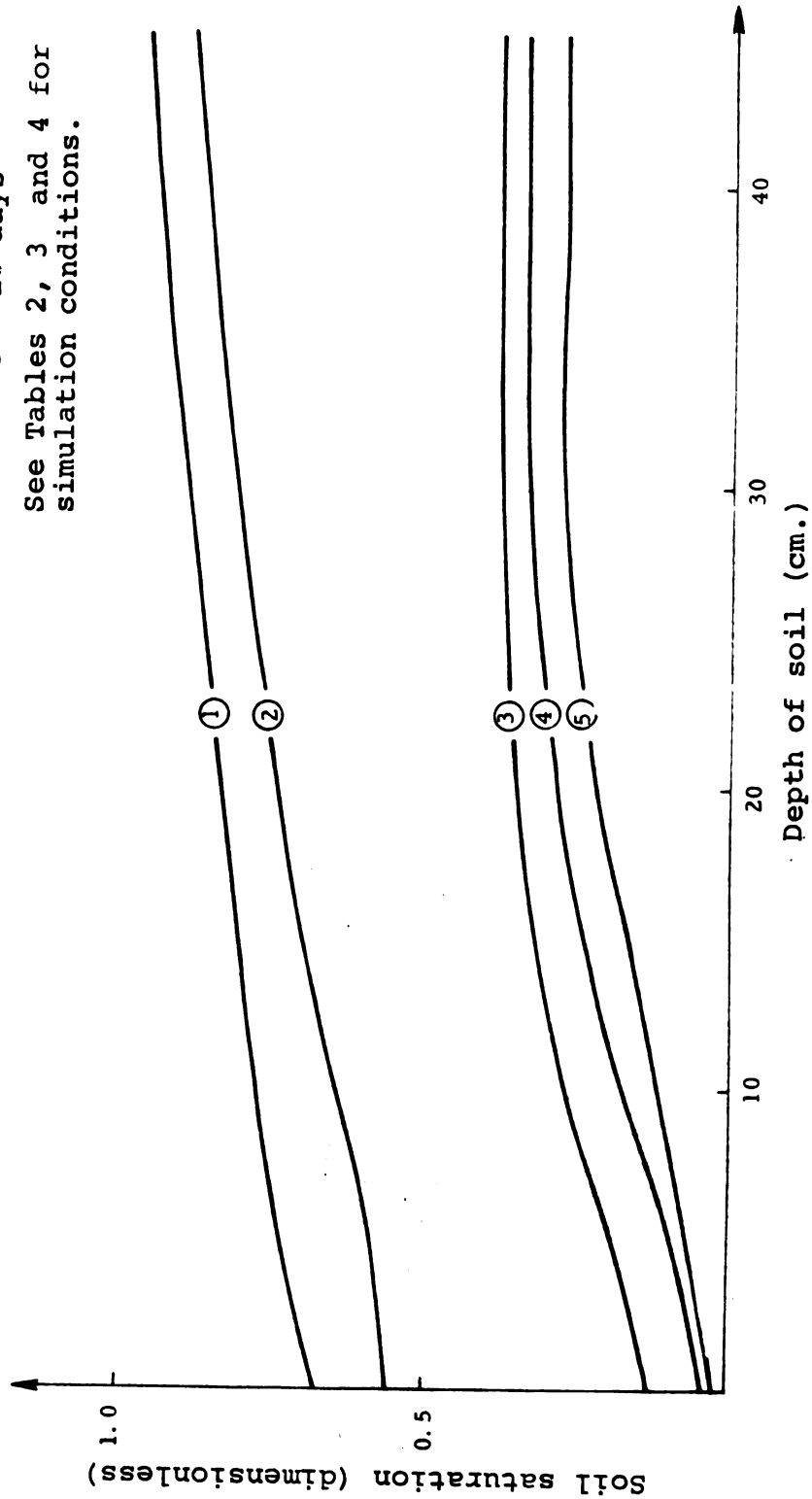


Figure 13.--Soil saturation versus depth of soil (simulation numbers 1 and 2).

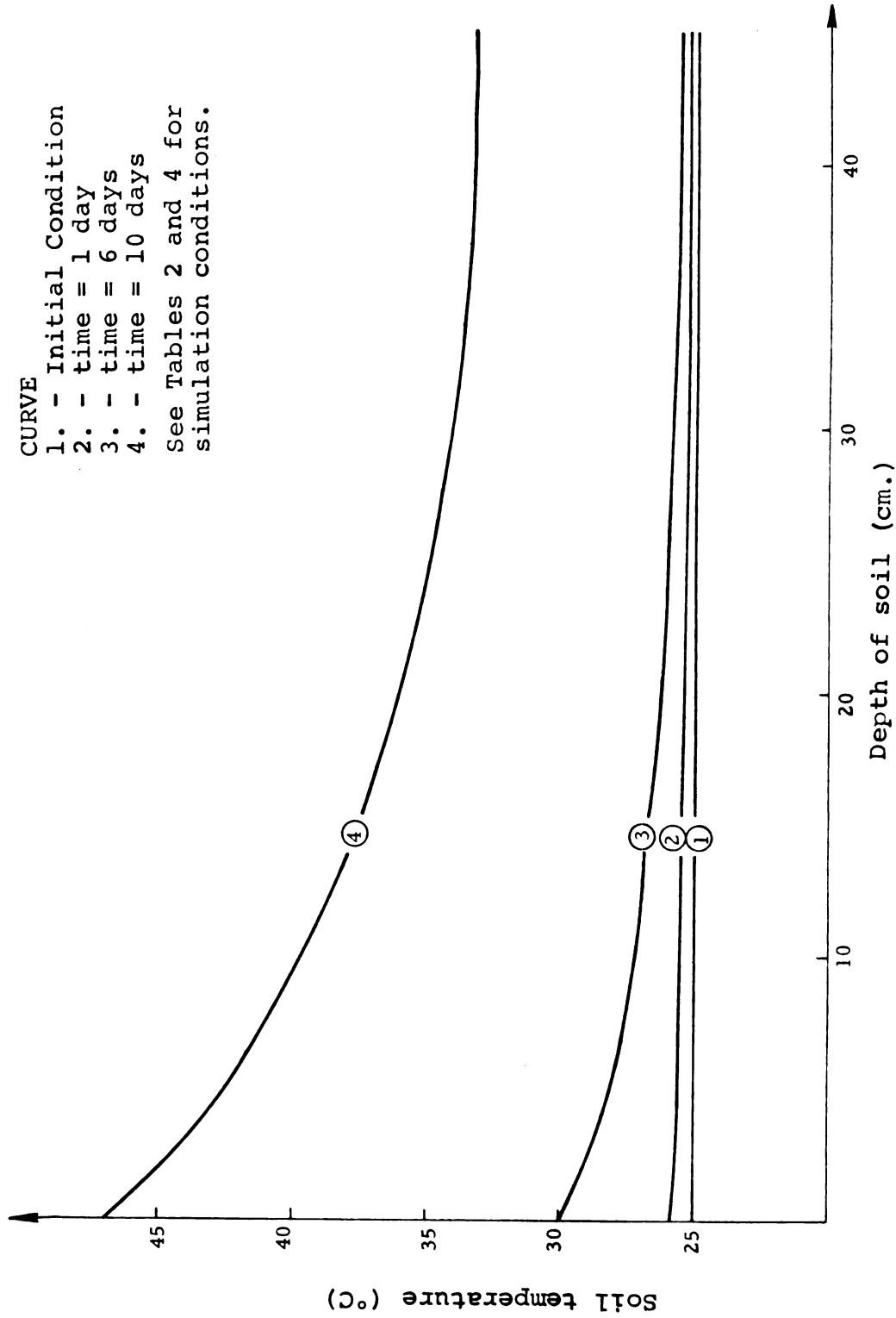


Figure 14.--Soil temperature versus depth of soil (simulation number 2).

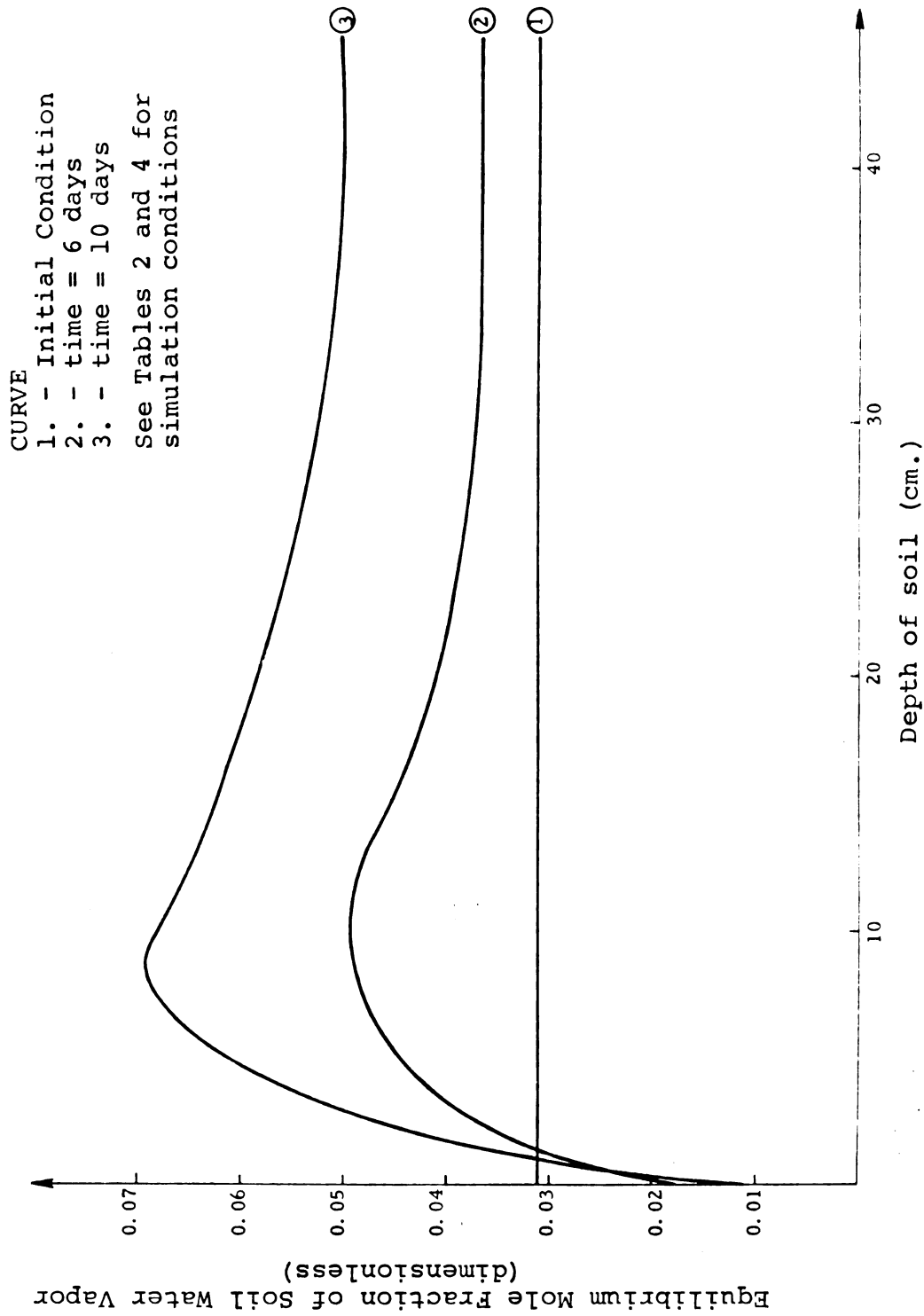


Figure 15.--Equilibrium mole fraction of soil water vapor versus depth of soil (simulation number 2).

that the time increment could be increased with time. For example the time increment used between 0 and 1 day was 1 sec. After 1 day a 30 sec. time increment was used.

Simulation numbers 1 and 2 used the hydraulic conductivity and capillary potential (drying curve) for Uplands sand. From Figure 13 it is obvious that the simulation results do not fit the experimental drying data (Figure 16) on valentine sand. This gives an idea of how sensitive the hydraulic parameters are to the specific soil or porous media type. Uplands sand is a soil in which liquid water has a high capillary conductivity. This type of soil has a very slight S-shape saturation profile during drying because the liquid water movement is so rapid.

The IE gives only the saturation profiles whereas the P&DVM gives the saturation, temperature, and equilibrium mole fraction of water vapor profiles. The saturation profiles calculated by both models were found to be the same and these results are contained in Figure 13. The equilibrium mole fraction of water vapor profile contains a peak (Figure 15). This is because the temperature is monotonically decreasing with depth and the saturation is monotonically increasing with depth. The result is that although the surface temperature is the largest and hence would yield the largest free water vapor pressure, the surface saturation is low enough to depress the vapor pressure far enough

below the free water vapor pressure to give the profile peak (see Appendix D).

Since the Uplands sand data did not fit the experimental drying data, the capillary potential function for Valentine sand was obtained. The capillary potential was measured by Hanks at low saturations and as discussed in Appendix L, the capillary potential could be calculated at the higher saturations from data published by Hanks et al. [30].

Simulation number 3 was run with the IE to illustrate the effect of the capillary potential function on the drying saturation profiles. Tables 2 and 5 show that simulation number 3 contains slightly different initial conditions than simulation 1. Also, the Valentine sand capillary potential function is used in simulation number 3. Figure 16 demonstrates that the Valentine capillary potential function results in a less water conductive soil and a more pronounced S-shape saturation profile. It also takes less real time in simulation number 3 to reach the irreducible saturation. Even with the Valentine sand capillary potential function, the simulation did not fit the experimental drying data on Valentine sand.

Since the hydraulic conductivity of Uplands sand appeared to be too large, simulation numbers 4 and 6 were run

Table 5: Simulation Parameters for Simulation Numbers 3, 4, & 6

NUMERICAL INFORMATION

MAXIMUM SIMULATION TIME (DAYS) .400000040E+02

SIZE OF TIME INCREMENT (DAYS) .694444444E-03

THE NUMBER OF TIME INCREMENTS 57600

COLUMN LENGTH (CM.) .450000040E+02

SIZE OF SPACE INCREMENT (CM.) .900000040E+01

NUMBER OF SPACE INCREMENTS 5

RATIO OF DELT TO DELZ .77160494E-04

THE INITIAL CONDITIONS ARE*****

.5715551E+00 .8424127E+00 .9057420E+00 .9636097E+00 .9916412E+00
Z = 0 Z = 9 Z = 18 Z = 27 Z = 36 cm. (Soil Depth)

COLUMN LENGTH = .45000000000E+02 CM

POROSITY = .305000000000E+00

DRYING RATE DURING CONSTANT RATE PERIOD = -.472130000000E+01 CM/DAY

SURFACE SATURATION DURING FALLING RATE PERIOD = .150000000000E-01

DRAINAGE RATE THRU COLUMN BOTTOM = 0.

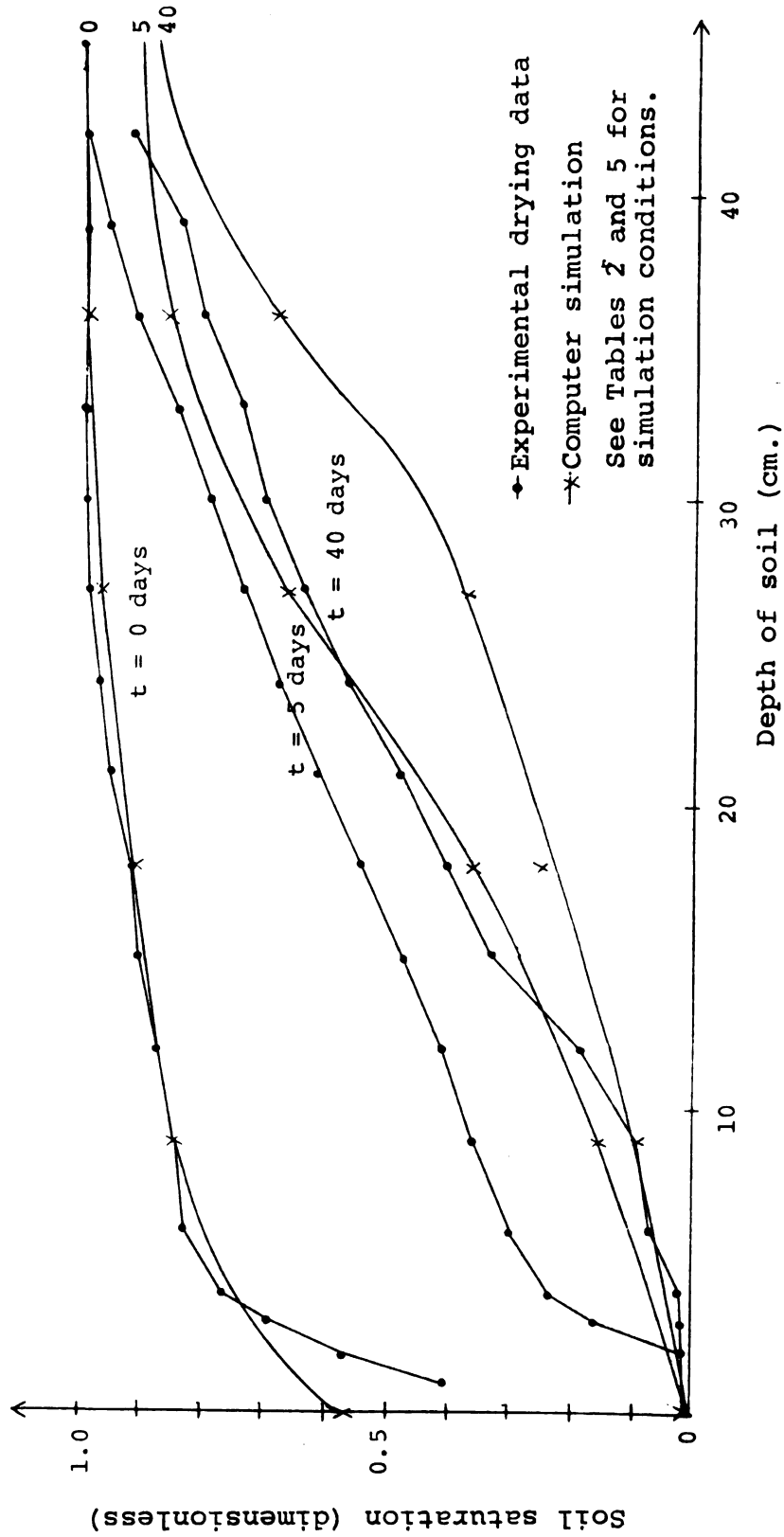


Figure 16.--Soil saturation versus depth of soil (simulation number 3).

to investigate decreasing the hydraulic conductivity by 0.1 and 0.01 respectively. Tables 2 and 5 contain the simulation parameters and Figures 17-19 contain the simulation results compared with the experimental data. Simulation number 4 fits the experimental drying saturation profiles the best and also fits the cumulative evaporation data the best. By decreasing the hydraulic conductivity of Staple, the over all drying rate is decreased and the S-shape of the saturation profile becomes more pronounced and skewed. The S-shape saturation profiles obtained during the drying simulations are very similar in shape to the drying saturation profiles for sands and clays that are presented by Larian [8]. The data presented by Larian is experimental data taken by engineers concerned with the drying phenomenon back in the 1930's. Unfortunately no capillary potential or hydraulic conductivity data was taken on these porous media.

The Blake-Kozeny equation for saturated flow in porous media at low particle Reynolds numbers indicates that the saturated hydraulic conductivity is proportional to the effective particle diameter squared. This implies that by cutting the hydraulic conductivity by 0.1, the effective particle diameter of the porous media is cut by $1/\sqrt{10}$. Since sands range in particle sizes from 2.0 mm. through 0.10 mm. in diameter and Staple's saturated hydraulic conductivity of 188 cm/day corresponds to an

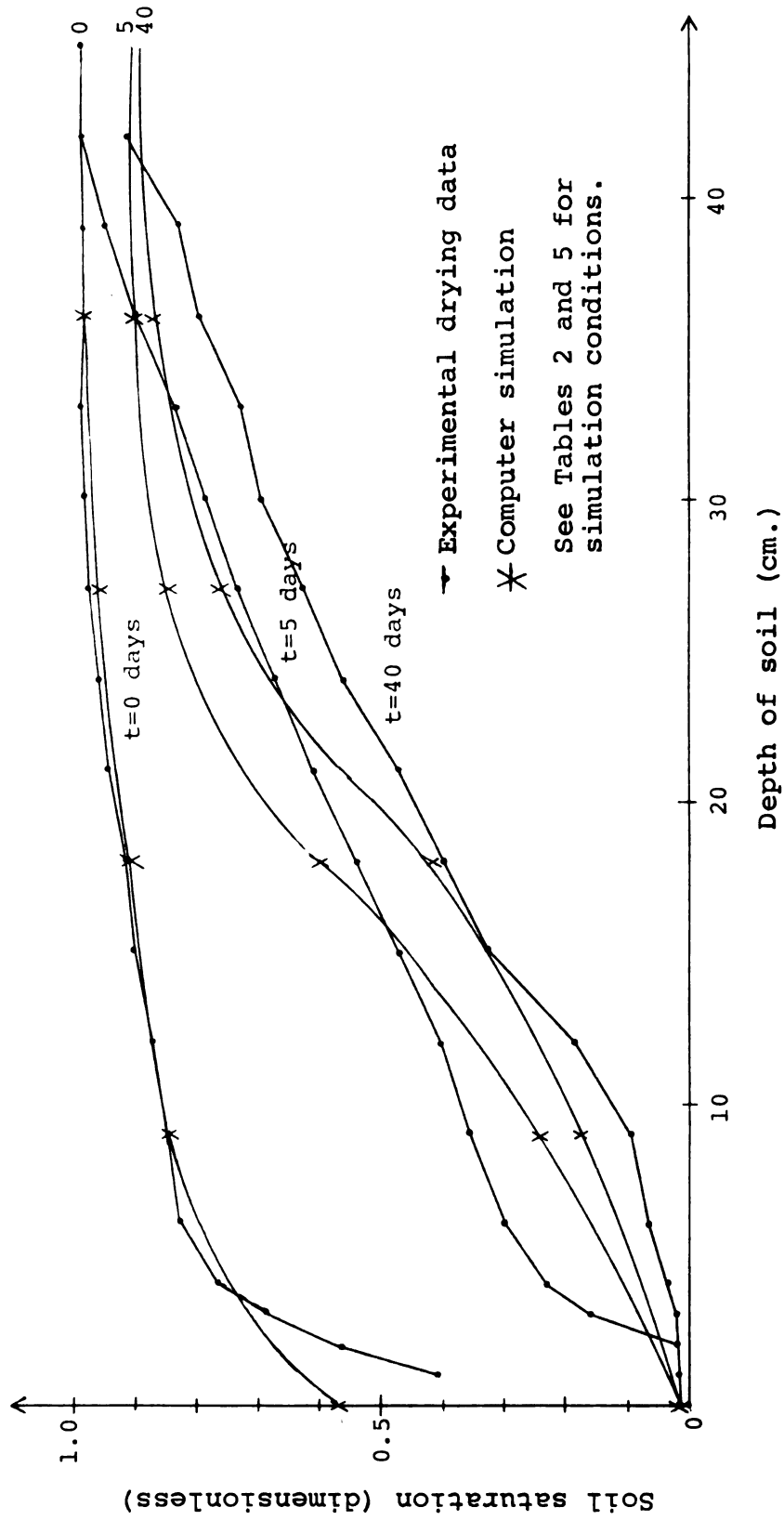


Figure 17.--Soil saturation versus depth of soil (simulation number 6).

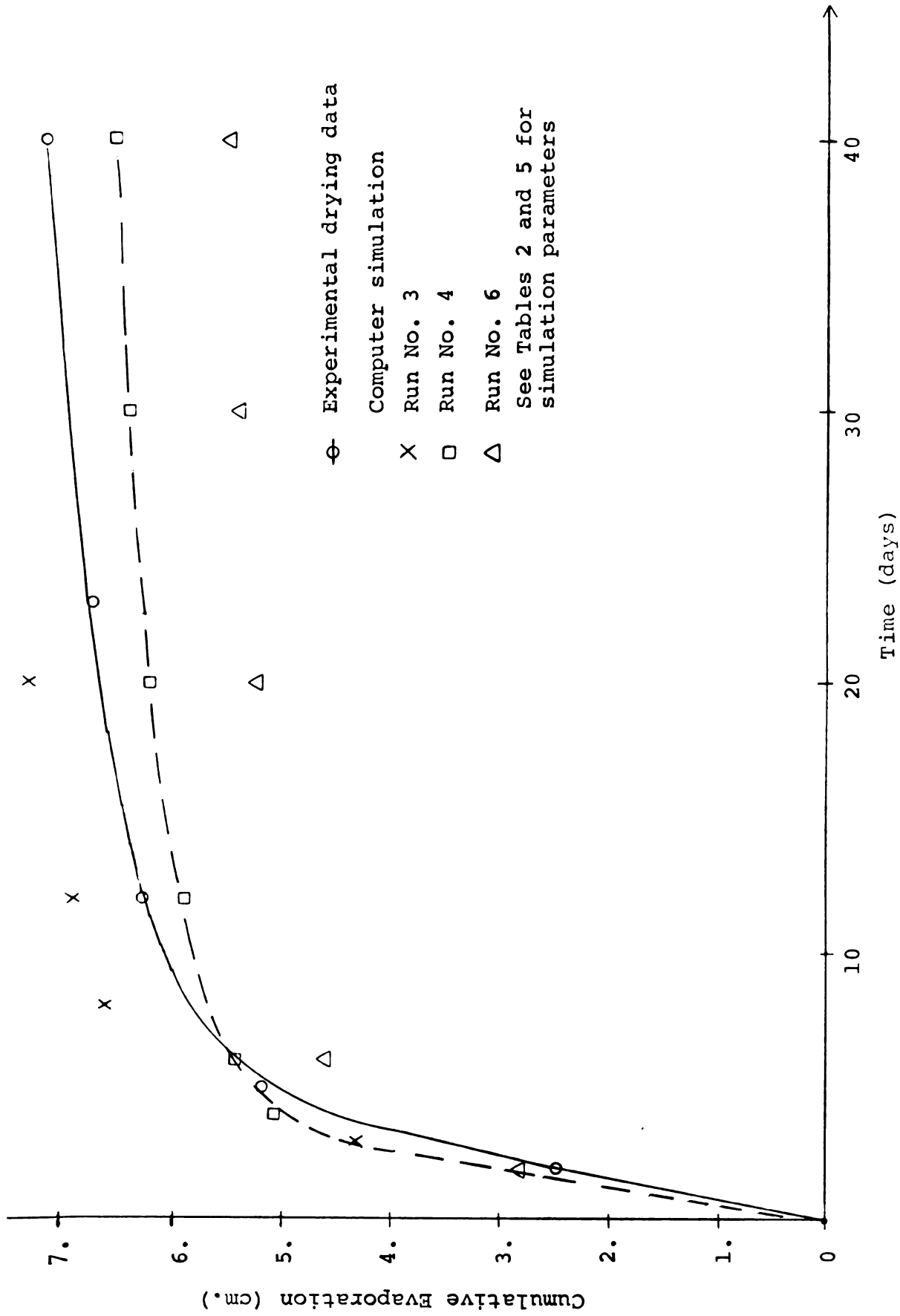


Figure 18.--Cumulative evaporation versus time (simulation numbers 3, 4, and 6).

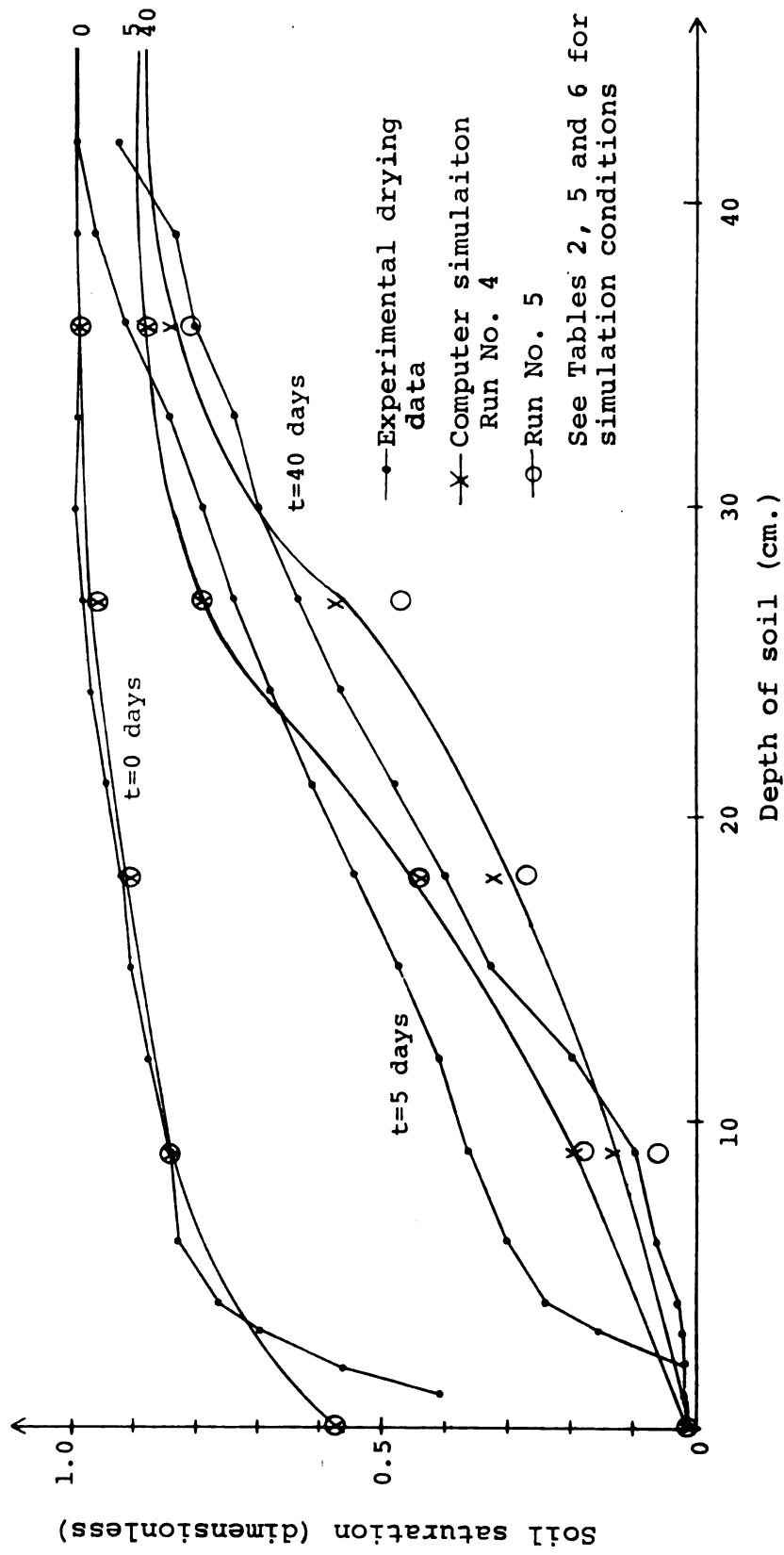


Figure 19.--Soil saturation versus depth of soil (simulation numbers 4 and 5).

effective particle diameter of .62 mm. we have the following: By cutting Staple's hydraulic conductivity by 0.1, the effective particle diameter turns out to be 0.20 mm. which is still in the sand classification. Then, the hydraulic conductivity in simulation number 4 does correspond in magnitude to a sand.

The data reported by Hanks et al. on drying of Valentine sand [30] are an "average" of two replicate drying runs. The saturation measurements were by γ -ray transmission. The work of Fritton et al. indicates that the accuracy of the saturation profiles measured by this technique is not too good. There are differences between gravimetric and γ -ray measurements which are probably due to slight inhomogeneities in the soil column compared to the soil used to standardize the γ -ray measurements [16]. Considering the scatter in the saturation profiles of Fritton et al., Hanks et al. have probably published an eyeball curve fit of the actual data. Attempts by this author to obtain more experimental data on Valentine sand were unsuccessful because the original data had been lost. With the accuracy of the γ -ray measurements, simulation 4 is considered to be a good fit.

As in simulation numbers 1 and 2, it was found in simulation numbers 3-6 that the time increment could be increased as the simulation proceeded. In simulation numbers

3, 4, and 6, a time increment of 6 secs. was used to 1 day and after 1 day a 60 sec. time increment was used.

Using the capillary potential and hydraulic conductivity data which gave a good fit of the experimental data in simulation number 4, simulation number 5 was run to compare the IE and P&DVM. In addition to the hydraulic parameters required for the IE, the P&DVM requires the effective thermal conductivity and volumetric heat capacity data. The data on Ottawa sand by Moench [29] was used. It was assumed that this thermal data would not vary much from one sand type to another. Tables 2 and 6 contain the simulation parameters for simulation number 5. The size increment between 0 and 1 day was 6 sec. and the time increment after 1 day was 240 sec.

The saturation, temperature, and equilibrium mole fraction of water vapor profiles from simulation number 5 can be found in Figures 19, 20, and 21 respectfully. After 5 days of drying there is good agreement between the IE and P&DVM. However, after 40 days of drying, there are some differences between the IE (No. 4) and P&DVM (No. 5) (refer to Figure 19). The irreducible saturation in simulation number 4 was set at $S=0.015$ which is the value reported by Hanks et al. for the drying of Valentine sand. The P&DVM calculates an irreducible saturation of $S=0.00977$ at 40 days of drying time. If the P&DVM is restrained to $S=0.015$, the

TABLE 6:--Simulation Parameters for Simulation Number 5

NUMERICAL INFORMATION	
MAXIMUM SIMULATION TIME (DAYS)	.10000000E+02
SIZE OF TIME INCREMENT (DAYS)	.6944444E-04
THE NUMBER OF TIME INCREMENTS	144000
COLUMN LENGTH (CM.)	.45000000E+02
SIZE OF SPACE INCREMENT (CM.)	.90000000E+01
NUMBER OF SPACE INCREMENTS	5
RATIO OF DELT TO DELZ	.77160494E-05

THE FOLLOWING IS A LISTING OF THE INITIAL CONDITIONS

*** ***** ** * ***** ** * ***** *****

INCREMENT	POSITION (CM.)	SATURATION (DIM.)	TEMPERATURE (DEG.C.)	MOLE FRACTION OF WATER VAPOR (DIM.)
1	0.	.5715551140370E+00	.2500000000000E+02	.3117210828660E-01
2	.9000000000000E+01	.8424126800080E+00	.2500000000000E+02	.3117210828660E-01
3	.1800000000000E+02	.9057419528010E+00	.2500000000000E+02	.3117251177090E-01
4	.2700000000000E+02	.9636096508660E+00	.2500000000000E+02	.3117271351490E-01
5	.3600000000000E+02	.9916411683000E+00	.2500000000000E+02	.3117300000000E-01

The following is a list of physical parameters for the system.

COLUMN LENGTH (CM.)	.45000000E+02
COLUMN OD (CM.)	.26000000E+02
COLUMN ID (CM.)	.10000000E+02
POROSITY (DIM.)	.30500000E+00
ORDINARY DIFFUSION COEF. AIR-WATER (CM**2/DAY)	.19000000E+05
OVER ALL MASS TRANSFER COEF. (1/DAY)	.38000000E+06
PRESSURE (ATM.)	.10000000E+01
MOLECULAR WT. OF WATER	.18000000E+02
GAS CONSTANT (CC.-ATM/GM.MOLE-DEG.D.)	.82057000E+02

THE FOLLOWING IS A LIST OF BOUNDARY CONDITIONS

AMBIENT TEMPERATURE (DEG.C.)	.25000000E+02
AMBIENT MOLE FRACTION OF WATER VAPOR (DIM.)	.10000000E-01
RADIATION FLUX (CAL/CM**2-DAY)	.87000000E+03
WALL OVER ALL HEAT TRANSFER COEF. (CAL/CM**2-DAY-DEG.C.)	.54800000E+00
FILMH (CAL./CM.**2-DAY-DEG.)	.21100000E+02

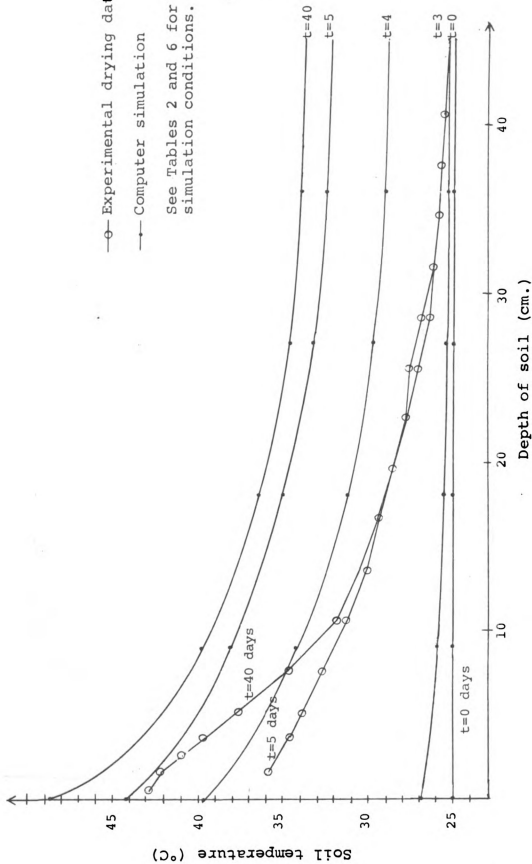


Figure 20.--Soil temperature versus depth of soil (simulation number 5).

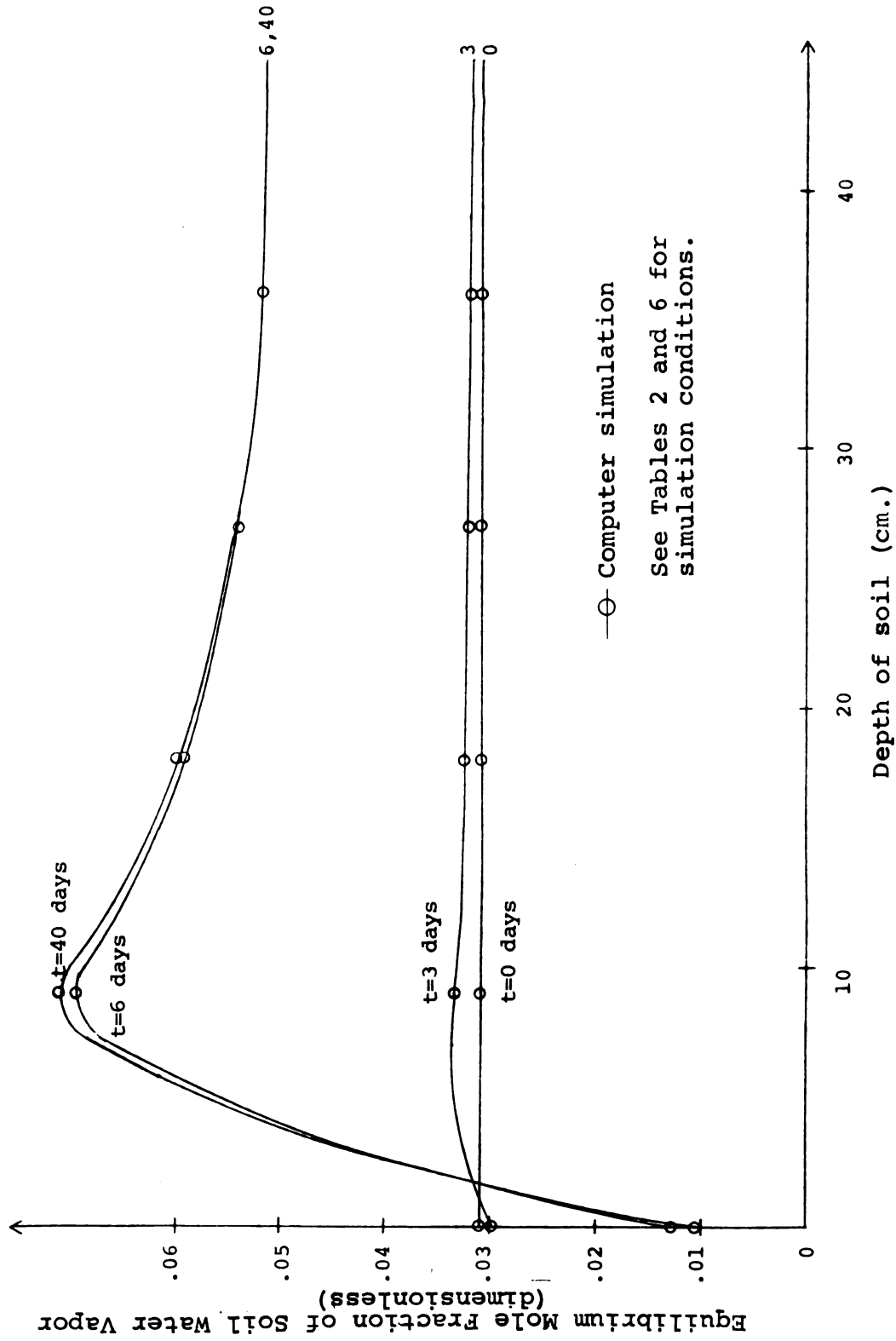


Figure 21.--Equilibrium mole fraction of soil water versus depth of soil (simulation number 5).

saturation profiles obtained are in good agreement with those obtained in simulation number 4 using the IE. And so the differences at 40 days in Figure 19 between the IE and P&DVM are due mainly to the differences in the irreducible saturation used in the IE and calculated in the P&DVM.

Since the irreducible saturation appears in the surface evaporation rate Equation (3.5), there is the following explanation for why the P&DVM results in a lower irreducible saturation and greater overall drying rate. First, the ambient humidity used by Hanks et al. is not known. If a higher humidity was used in simulation number 5, the higher irreducible saturation would have been calculated in the P&DVM. Second, if the capillary potential function for Valentine sand is on the low side at $S=0.015$, the irreducible saturation calculated would turn out to be lower than $S=0.015$.

The temperature profiles calculated in simulation number 5 have shapes similar to the experimental temperature profiles. However, the calculated temperatures are larger than the experimental temperatures. For example, at a drying time of 40 days the surface temperature calculated is 5 deg.C. larger than the experimental value. The calculated values are larger because the zero heat flux boundary condition at the column bottom apparently was not met during the drying experiment. As mentioned earlier, the temperature profiles have very little influence on the calculated saturation profiles. This was demonstrated by comparison of the

calculated saturation profiles using the IE and P&DVM with identical irreducible saturations.

Since the calculated temperature profile was similar in shape to the experimental temperature profile, the equilibrium mole fraction of water vapor profile in Figure 21 is expected to be correct in shape. As a result the water vapor flux by diffusion as calculated in the P&DVM should be correct.

Figure 22 contains the surface evaporation rate as a function of time. It is interesting to note that the P&DVM predicts the startup until the "constant rate" period is reached and then it predicts the falling rate period.

Table 7 contains a tabulation of the material and energy fluxes during drying (simulation number 5). This data illustrates what is happening during the drying of porous media. During the first hour of drying, the evaporation rate increases to the so called constant rate. During the constant rate period the liquid and vapor fluxes in the top 18 cm. of the column increase. The energy flux at the surface decreases due to convective losses to a lower temperature environment. The energy fluxes into the greater depths begin to increase.

Between the third and fourth day, the falling rate period begins and the evaporation rate drops rapidly during the next day, as shown in Figure 22. It can be seen from

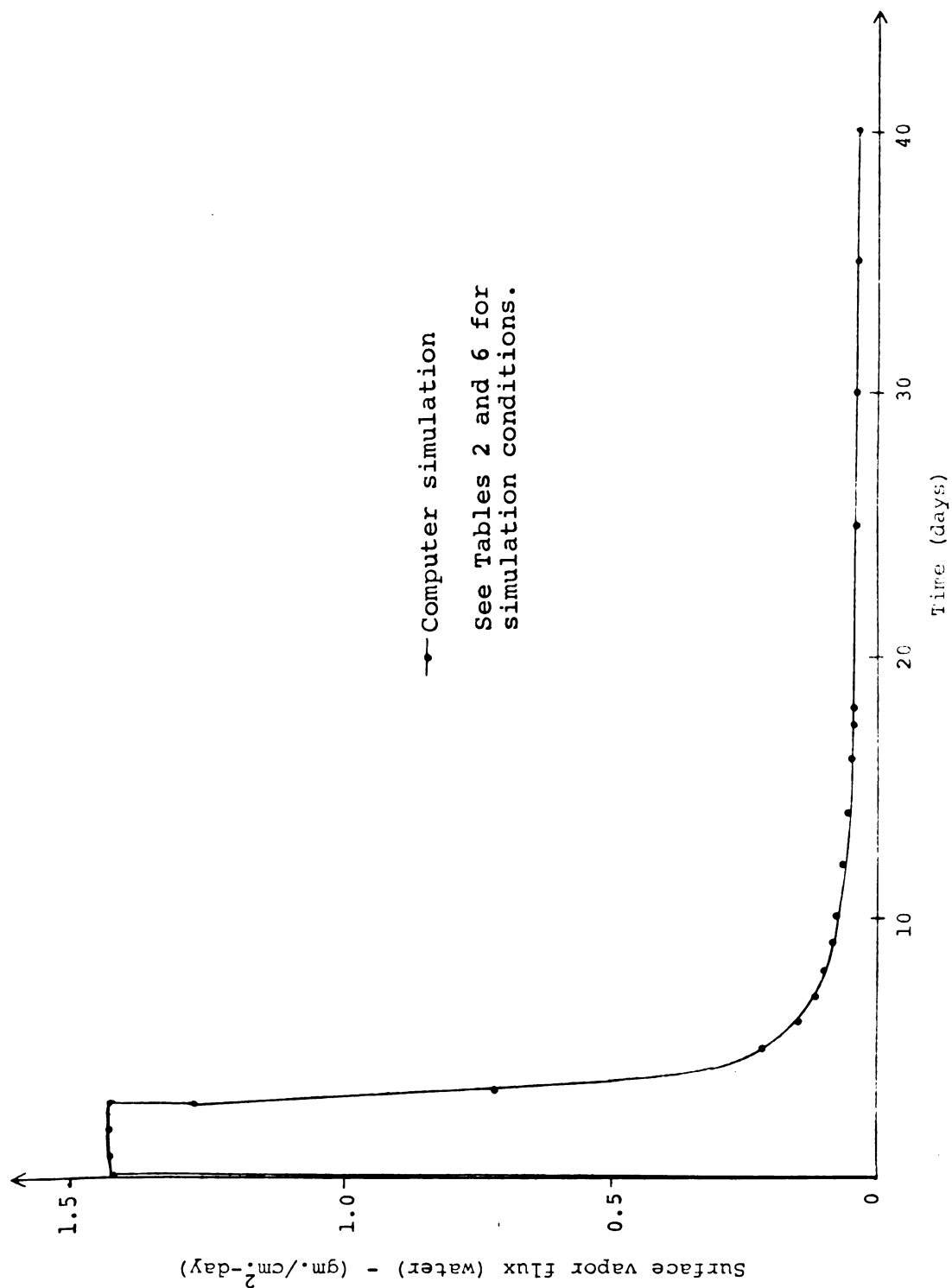


Figure 22.-- Surface vapor flux versus time (simulation number 5).

TABLE 7.--Material and energy fluxes during drying (simulation number 5).

Time (days)	Liquid Flux Profile (gm/cm ² -day)	Vapor Flux Profile (gm/cm ² -day)	Energy Flux Profile (cal/cm ² -day)
1/24 = 1 hour	0 -.46369E+00 -.25982E+00 -.13915E+00 -.65285E-02	-.14129E+01 .63111E-04 .15354E-04 .18587E-05 .93506E-07	.85801E+03 z=0 cm. .23667E+02 z=9 cm. .10188E+02 z=18cm. .31995E+01 z=27cm. .75314E+00 z=36cm.
1	0 -.88040E+00 -.30021E+00 -.19946E+00 -.11651E+00	-.14388E+01 .72146E-04 .18900E-04 .66912E-05 .58193E-06	.85335E+03 z=0 cm. .11885E+02 z=9 cm. .85283E+01 z=18cm. .55225E+01 z=27cm. .27264E+01 z=36cm.
2	0 -.10207E+01 -.42355E+00 -.19684E+00 -.99388E-01	-.14409E+01 .11700E-03 .22522E-04 .79525E-05 .18328E-05	.85289E+03 .10140E+02 etc. .70477E+01 .44487E+01 .21548E+01
3	0 -.11182E+01 -.70782E+00 -.18273E+00 -.79696E-01	-.12793E+01 -.13005E-02 .17790E-03 .30663E-04 .71885E-05	.82407E+03 .45391E+02 .24730E+02 .12806E+02 .53402E+01
4	0 -.38723E+00 -.31114E+00 -.99323E-01 -.34819E-01	-.41641E+00 -.16920E-01 .23710E-02 .38676E-03 .10210E-03	.56079E+03 .23402E+03 .15406E+03 .99201E+02 .47797E+02
5	0 -.18575E+00 -.17023E+00 -.67437E-01 -.18150E-01	-.21450E+00 -.25756E-01 .34746E-02 .55468E-03 .14136E-03	.46602E+03 .25299E+03 .16180E+03 .10391E+03 .50424E+02
40	0 -.10892E-02 -.35984E-01 -.23704E-01 -.62395E-02	-.36044E-01 -.34923E-01 .49758E-02 .17778E-02 .22893E-03	.37104E+03 .24895E+03 .15033E+03 .93742E+02 .45435E+02

See Tables 2 and 6 for simulation conditions.

Table 7 that during this period the liquid flux in the top 18 cm. drops rapidly. This is accompanied by a sharp decrease in the surface vapor flux. However, the vapor fluxes at the $z=9$ and 18 cm. levels begin to increase rapidly. The energy fluxes at depths of $z=9$ cm. or more begin to increase at a rate faster than before the start of the falling rate period.

It should be noted that the difference in magnitude between the liquid and vapor fluxes is usually an order of magnitude or more throughout the simulation (Table 7). This coupled with the fact that the effect of temperatures on capillary potential is small explains why good agreement is obtained between the IE and P&DVM. The IE is a one phase model and the P&DVM demonstrates that it is the liquid flux which is controlling the drying process in simulation number 5.

In Chapter II it was assumed that the convective flow energy fluxes were negligible in comparison to the conductive energy flux. The data in Table 7 was used in calculations contained in Appendix M to justify this assumption. The assumption was found valid.

Simulation numbers 7-10 contain the results of simulations using the general model (GM) developed in Chapter II. These simulations were run to investigate the interphase vapor-liquid equilibrium assumption which is the basis for the P&DVM. As mentioned in Chapter II, there

is some disagreement in the literature about the value of the particle Sherwood number at very low particle Reynolds numbers. Since the interphase mass transfer coefficient is contained in the dimensionless particle Sherwood number and will have an affect on the calculated value of the gas phase mole fraction of water vapor, it was decided to investigate how sensitive the gas phase humidity ($\tilde{X}_w/\tilde{X}_w^*$) was to the particle Sherwood number.

Simulations 7-10 used initial conditions for a dry soil. The drying simulation results from the P&DVM supplied the saturation and temperature profile initial conditions for the general model (GM). The GM initial condition for the gas phase mole fraction of water vapor was taken to be the equilibrium mole fraction of water vapor calculated by the P&DVM. Simulations 7-10 then show the unsteady state response of the gas phase mole fraction of water vapor from the initial conditions. A larger deviation from the interphase vapor-liquid equilibrium assumption would be found in a dry soil as opposed to a wet soil.

Tables 2 and 8 contain the simulation parameters for simulation number 7. A particle Sherwood number of 0.002 was used as opposed to the generally accepted value of 2.0. A lower value of the particle Sherwood number would result in a lower gas phase humidity. Figure 23 shows the simulation number 7 results. It can be seen that the surface mole fraction of water vapor in the gas

TABLE 8.--Simulation Parameters for Simulation Number 7

NUMERICAL INFORMATION

MAXIMUM SIMULATION TIME (DAYS) .10000000E+02
 SIZE OF TIME INCREMENT (DAYS) .11574074E-07
 THE NUMBER OF TIME INCREMENTS 864000000
 COLUMN LENGTH (CM.) .45000000E+02
 SIZE OF SPACE INCREMENT (CM.) .90000000E+01
 NUMBER OF SPACE INCREMENTS 5
 RATIO OF DELT TO DELZ .12860082E-08

THE FOLLOWING IS A LISTING OF THE INITIAL CONDITIONS
 *** ***** ** * ***** ** *** ***** *****

INCREMENT	POSITION (CM.)	SATURATION (DIM.)	TEMPERATURE (DEG.C.)	MOLE FRACTION OF WATER VAPOR (DIM.)
1	0.	.2191073463361E-01	.4783856850506E+02	.1105469302093E-01
2	.9000000000000E+01	.8920791427854E-01	.4058982740232E+02	.6571641823167E-01
3	.1800000000000E+02	.1668295532955E+00	.3684252610178E+02	.6062012880899E-01
4	.2700000000000E+02	.2221975151559E+00	.3469122914914E+02	.5424743100584E-01
5	.3600000000000E+02	.2502908859055E+00	.3369637362956E+02	.5139153569702E-01

1

The following is a list of physical parameters for the system.

COLUMN LENGTH (CM.)	.45000000E+02
COLUMN OD (CM.)	.26000000E+02
COLUMN TD (CM.)	.10000000E+02
POROSITY (DIM.)	.30500000E+00
ORDINARY DIFFUSION COEF. AIR-WATER (CM**2/DAY)	.19000000E+05
OVER ALL MASS TRANSFER COEF. (1/DAY)	.38000000E+03
PRESSURE (ATM.)	.10000000E+01
MOLECULAR WT. OF WATER	.18000000E+02
GAS CONSTANT (CC.-ATM/GM.MOLE-DEG.K.)	.82057000E+02

THE FOLLOWING IS A LIST OF BOUNDARY CONDITIONS

AMBIENT TEMPERATURE (DEG.C.)	.25000000E+02
AMBIENT MOLE FRACTION OF WATER VAPOR (DIM.)	.10000000E-01
RADIATION FLUX (CAL/CM**2-DAY)	.87000000E+03
WALL OVER ALL HEAT TRANSFER COEF. (CAL/CM**2-DAY-DEG.C.)	.54800000E+00
FILMH (CAL./CM.**2-DAY-DEG.)	.21100000#+02

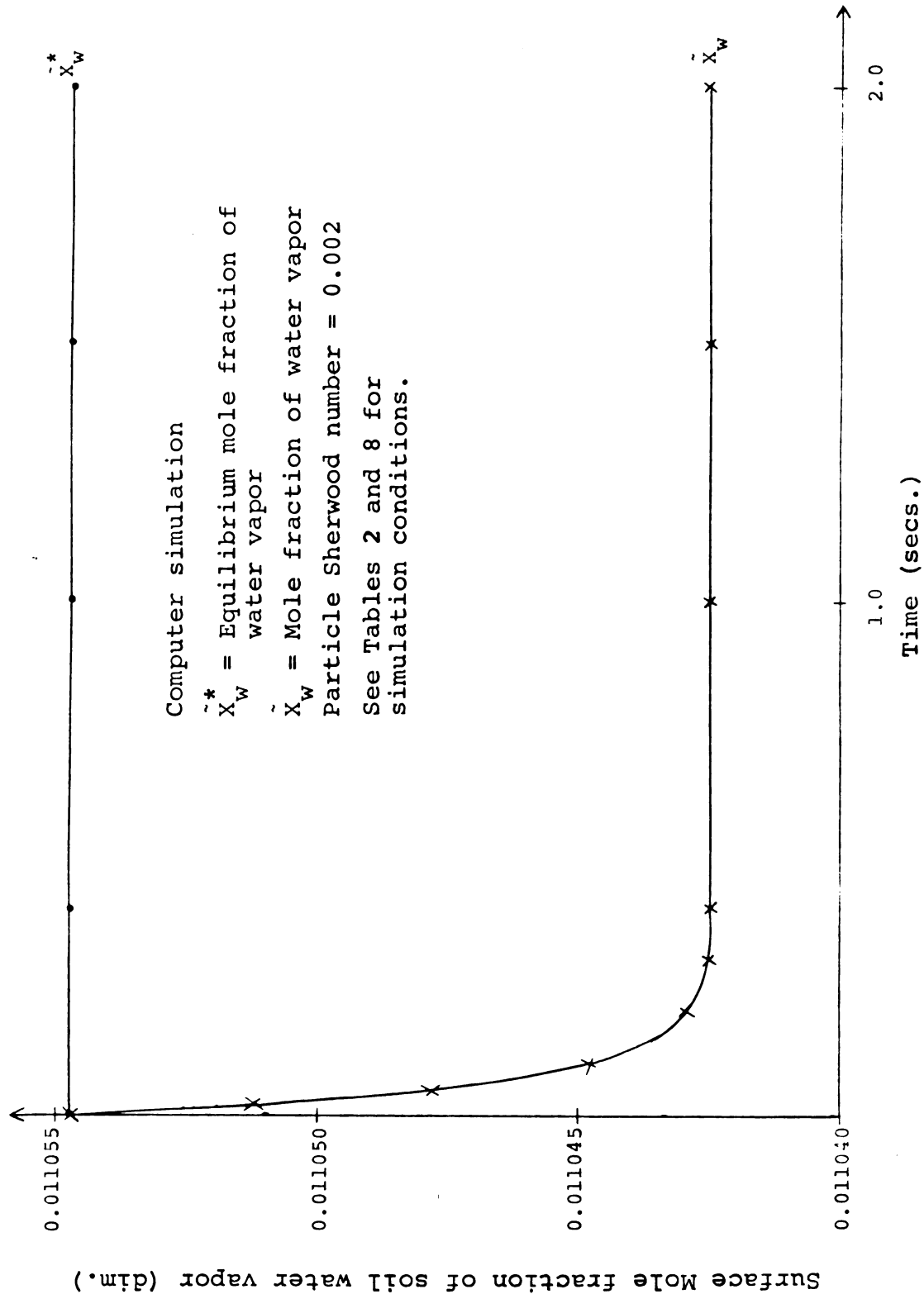


Figure 23.--Surface mole fraction of soil water vapor versus time (simulation number 7).

phase quickly approaches a pseudo steady state value close to 100% humidity. At lower column depths, the gas phase humidity is even closer to 100%. This means that even under dry soil conditions, the interphase vapor-liquid equilibrium assumption is valid. Also, the dynamics of the gas phase mole fraction of water vapor are very fast.

Simulation number 8 was run with the generally accepted value for the particle Sherwood number of 2.0. Tables 2 and 9 contain the simulation parameters and Table 10 contains the results. These results show that at all column depths the gas phase humidity is very close to 100%. Also the gas phase equilibrium mole fraction dynamics are much faster than in simulation number 7. Evaporation is taking place near the surface and condensation is taking place near the column bottom. This is to be expected from the profiles in Figures 15 and 21. These figures indicate that water vapor diffuses away from the peak, toward the surface, and toward the column bottom. This type of result has not previously been obtained either by experiment or theory.

Simulation numbers 9 and 10 are analagous to numbers 7 and 8 and were run to investigate what affect the soil hydraulic properties might have on the interphase vapor-liquid equilibrium assumption. Tables 2, 11, and 12 contain the simulation parameters for simulation number 9 and 10.

TABLE 9.--Simulation parameters for simulation number 8.

Numerical Information	
Maximum Simulation Time (Days)	.23148148E-05
Size of Time Increment (Days)	.11574074E-08
Column Length (Cm.)	.45000000E+02
Size of Space Increment (Cm.)	.90000000E+01
Ratio of Delt to Delz	.12860082E-09

The Following is a List of Physical Parameters for the System	
Column OD (Cm.)	.260000000E+02
Column ID (Cm.)	.100000000E+02
Porosity (Dim.)	.305000000E+00
Ordinary Diffusion Coef. Air-Water (Cm ² /day)	.190000000E+05
Over All Mass Transfer Coef. (l/day)	.380000000E+06
Pressure (Atm.)	.100000000E+01
Molecular Weight of Water	.180000000E+02
Gas Constant (CC.Atm/Gm.Mole-Deg.K.)	.82057000E+02

The Following is a List of Boundary Conditions	
Ambient Temperature (Deg.C.)	.250000000E+02
Ambient Mole Fraction of Water Vapor	.100000000E-01
Radiation Flux (Cal/Cm ² -Day)	.870000000E+03
Wall Over All Heat Transfer Coef.	.548000000E+00 (Cal/Cm ² -Day-Deg.K.)
Filmh (Cal./Cm.2-Day-Deg.)	.211000000E+02

The Following is a Listing of the Initial Conditions				
Increment	Position (Cm.)	Saturation (Dim.)	Temperature (Deg.C.)	Mole Fraction of Water Vapor (Dim.)
1	.0	.2191074E-01	.4783857E+02	.1105469E-01
2	.90E+01	.8920791E-01	.4058983E+02	.6571642E-01
3	.18E+02	.1668296E+00	.3684253E+02	.6062013E-01
4	.27E+02	.2221975E+00	.3469123E+02	.5425743E-01
5	.36E+02	.2502909E+00	.3369637E+02	.5139154E-01



TABLE 10.--Simulation number 8 results.

Mole Fraction of Soil Water Vapor vs. Time

Particle Sherwood Number = 2.0

Time = 0.0 Secs.

Position	Mole Fraction of Soil Water Vapor	Equilibrium Mole Fraction of Soil Water Vapor
0.	.11054655E-01	.11054655E-01
.900E+01	.65715938E-01	.65715938E-01
.180E+02	.60620075E-01	.60620075E-01
.270E+02	.54257406E-01	.54257406E-01
.360E+02	.51391514E-01	.51391514E-01

Time = 0.002 Secs.

0.	.11054643E-01	.11054655E-01
.900E+01	.65715919E-01	.65715938E-01
.180E+02	.60620075E-01	.60620075E-01
.270E+02	.54257407E-01	.54257406E-01
.360E+02	.51391515E-01	.51391514E-01

Time = 0.196 Secs.

0.	.11054642E-01	.11054655E-01
.900E+01	.65715916E-01	.65715935E-01
.180E+02	.60620075E-01	.60620075E-01
.270E+02	.54257407E-01	.54257405E-01
.360E+02	.51391515E-01	.51391514E-01

See Tables 2 and 9 for simulation conditions.

TABLE 11.--Simulation Parameters for Simulation Number 9.

NUMERICAL INFORMATION

MAXIMUM SIMULATION TIME (DAYS) .10000000E+02
 SIZE OF TIME INCREMENT (DAYS) .11574074E-07
 THE NUMBER OF TIME INCREMENTS 864000000
 COLUMN LENGTH (CM.) .45000000E+02
 SIZE OF SPACE INCREMENT (CM.) .90000000E+01
 NUMBER OF SPACE INCREMENTS 5
 RATIO OF DELT TO DELZ .12860082E-08

THE FOLLOWING IS A LISTING OF THE INITIAL CONDITIONS

*** ***** ** * ***** ** * ***** *****

INCREMENT	POSITION (CM.)	SATURATION (DIM.)	TEMPERATURE (DEG.C.)	MOLE FRACTION OF WATER VAPOR (DIM.)
1	0.	.1773193299240E-01	.3424828796551E+02	.2162857193566E-01
2	.90000000000000E+01	.2314836178658E+00	.3012889219399E+02	.4203837454039E-01
3	.18000000000000E+02	.544266904483E+00	.2897321463635E+02	.3734013506830E-01
4	.27000000000000E+02	.8367829337971E+00	.2703686611619E+02	.3515031302005E-01
5	.36000000000000E+02	.9022167868357E+00	.2658015037253E+02	.3422162695744E-01

The following is a list of physical parameters for the system.

COLUMN LENGTH (CM.)	.45000000E+02
COLUMN OD (CM.)	.26000000E+02
COLUMN ID (CM.)	.10000000E+02
POROSITY (DIM.)	.30500000E+00
ORDINARY DIFFUSION COEF. AIR-WATER (CM**2/DAY)	.19000000E+05
OVER ALL MASS TRANSFER COEF. (1/DAY)	.38000000E+03
PRESSURE (ATM.)	.10000000E+01
MOLECULAR WT. OF WATER	.18000000E+02
GAS CONSTANT (CC.-ATM/GM.MOLE-GEG.K.)	.82057000E+02

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THE FOLLOWING IS A LIST OF BOUNDARY CONDITIONS

AMBIENT TEMPERATURE (DEG.C.)	.25000000E+02
AMBIENT MOLE FRACTION OF WATER VAPOR (DIM.)	.10000000E-01
RADIATION FLUX (CAL/CM**2-DAY)	.87000000E+03
WALL OVER ALL HEAT TRANSFER COEF. (CAL/CM**2-DAY-DEG.C.)	.54800000E+00
FILMH *CAL./CM.**2-DAY-GEG.)	.21100000E+02

TABLE 12.--Simulation Parameters for Simulation Number 10

NUMERICAL INFORMATION

MAXIMUM SIMULATION TIME (DAYS) .10000000E+02
 SIZE OF TIME INCREMENT (DAYS) .11574074E-09
 THE NUMBER OF TIME INCREMENTS 86400000030
 COLUMN LENGTH (CM.) .45000000E+02
 SIZE OF SPACE INCREMENT (CM.) .90000000E+01
 . NUMBER OF SPACE INCREMENTS 5
 RATIO OF DELT TO DELZ .12860082E-10

THE FOLLOWING IS A LISTING OF THE INITIAL CONDITIONS

*** ***** ** * ***** ** *** ***** *****

INCREMENT	POSITION (CM.)	SATURATION (DIM.)	TEMPERATURE (DEG.C.)	MOLE FRACTION OF WATER VAPOR (DIM.)
1	0.	.1773193299250E-01	.3424828796551E+02	.2161857193566E-01
2	.90000000000000E+01	.2314836178658E-00	.3012889219399E+02	.4203837454039E-01
3	.18000000000000E+02	.5442669044483E-00	.2807321463635E+02	.3734013506830E-01
4	.27000000000000E+02	.8367829337971E+00	.2703686611619E+02	.3515031302005E-01
5	.36000000000000E+02	.9022167868357E+00	.2658015037253E+02	.3422162695744E-01

The following is a list of physical parameters for the system.

COLUMN LENGTH (CM.)	.45000000E+02
COLUMN OD (CM.)	.26000000E+02
COLUMN ID (CM.)	.10000000E+02
POROSITY (DIM.)	.30500000E+00
ORDINARY DIFFUSION COEF. AIR-WATER (CM**2/DAY)	.19000000E+05
OVER ALL MASS TRANSFER COEF. (1/DAY)	.38000000E+06
PRESSURE (ATM.)	.10000000E+01
MOLECULAR WT. OF WATER	.18000000E+02
GAS CONSTANT (CC.-ATM/GM.MOLE-DEG.K.)	.82057000E+02

THE FOLLOWING IS A LIST OF BOUNDARY CONDITIONS

AMBIENT TEMPERATURE (DEG.C.)	.25000000E+02
AMBIENT MOLE FRACTION OF WATER VAPOR (DIM.)	.10000000E-01
RADIATION FLUX (CAL/CM**2-DAY)	.87000000E+03
WALL OVER ALL HEAT TRANSFER COEF. (CAL/CM**2-DAY-DEG.C.)	.54800000E+00
FILMH (CAL./CM.**2-DAY-DEG.)	.21100000E+02

The results of these simulations are contained in Figures 24 and 25. Again, as in simulation numbers 7 and 8, the gas phase humidity is close to 100% and the interphase vapor-liquid assumption is valid.

The factor controlling the allowable time increment in simulation numbers 7-10 is the mass transfer coefficient. For lower particle Sherwood numbers the interphase mass transfer coefficient is smaller, and a larger time increment can be used. Although it is not economical to run the GM for long periods of real time, it can be run for a few seconds to check out the interphase vapor-liquid equilibrium assumption. If the assumption is valid, then the P&DVM is valid and can be run for long periods of real time. If the assumption is not valid, the P&DVM is only an approximation and the GM should be run. It may be possible to develop a numerical procedure for the GM which would be more economical than the existing numerical procedure.

With the interphase equilibrium assumption validated, it was decided to use the P&DVM to simulate the response of the soil column to time varying boundary conditions. This type of simulation also has not been run previous to this work.

The simulation parameters are listed in Table 13 and the time varying boundary conditions are given in Figures 26-29. Natural weather conditions existing in

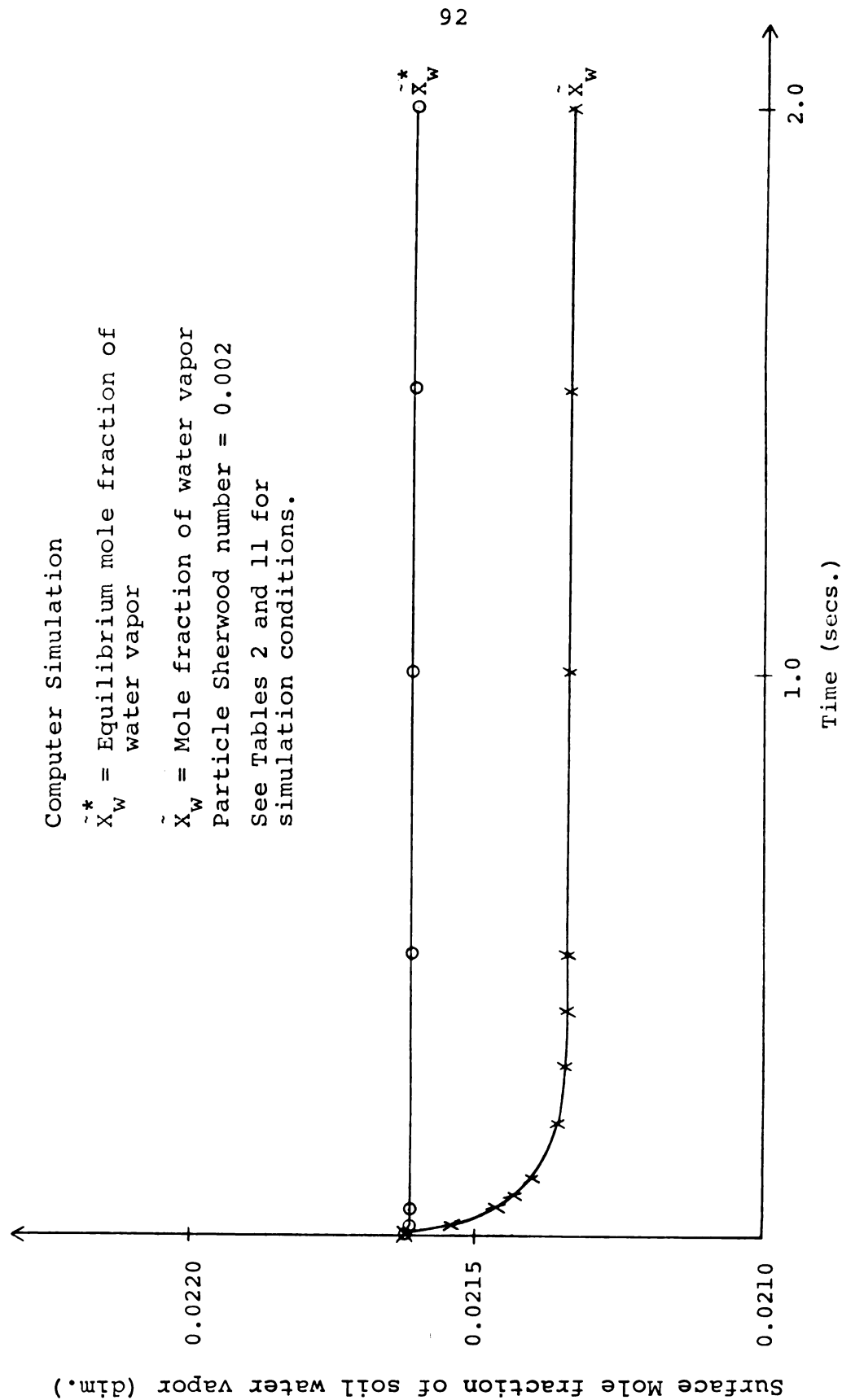


Figure 24.--Surface mole fraction of soil water vapor versus time (simulation number 9).

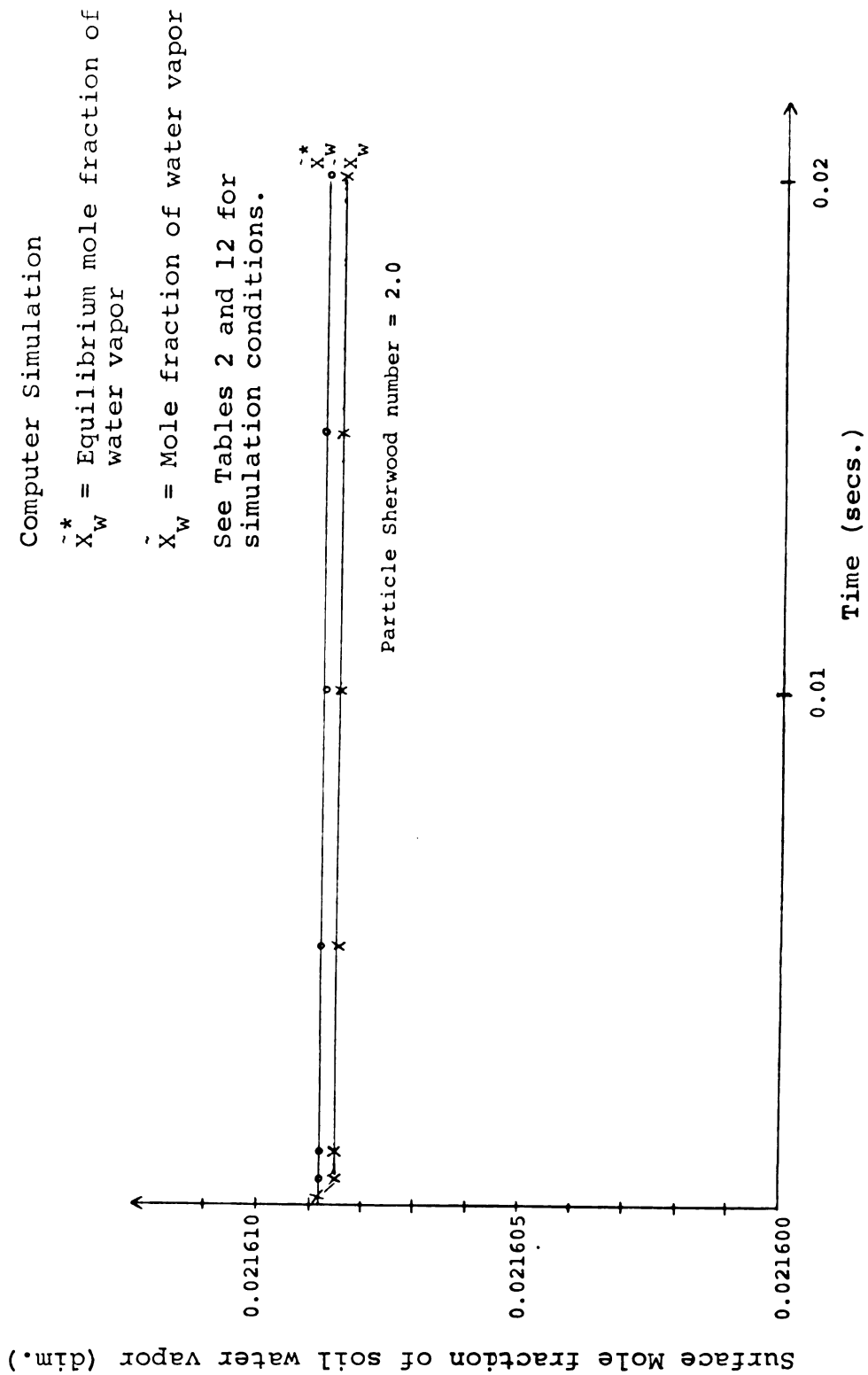


Figure 25.--Surface mole fraction of soil water vapor versus time (simulation number 10).

TABLE 13.--Simulation parameters for simulation number 11.

<u>Numerical Information</u>				
Size of Time Increment				.69444444E-04 for 0-1 day real time
				.27777777E-02 for greater than 1 day
Column Length				.45000000E+02
Size of Space Increment				.90000000E+01
Number of Space Increments				.50000000E+01

<u>The Following is a List of Physical Parameters for the System</u>				
Column OD (Cm.)				.26000000E+02
Column ID (Cm.)				.10000000E+02
Porosity (dim.)				.30500000E+00
Ordinary Diffusion Coef. Air-Water (cm ² /day)				.19000000E+05
Over All Mass Transfer Coef. (1/day)				.38000000E+06
Pressure (Atm.)				.10000000E+01
Molecular Weight of Water				.18000000E+02
Gas Constant (CC.-Atm/Gm.Mole-Deg.K.)				.82057000E+02

<u>The Following is a Listing of the Initial Conditions</u>				
Increment	Position (Cm.)	Saturation (dim.)	Temperature (Deg.C.)	Mole Fraction of Water Vapor (dim.)
0	.90E+01	.5715511E+00	.2500000E+02	.3117211E-01
2	.18E+02	.8424127E+00	.2500000E+02	.3117231E-01
3	.27E+02	.9057420E+00	.2500000E+02	.3117271E-01
4	.36E+02	.9916412E+00	.2500000E+02	.3117300E-01

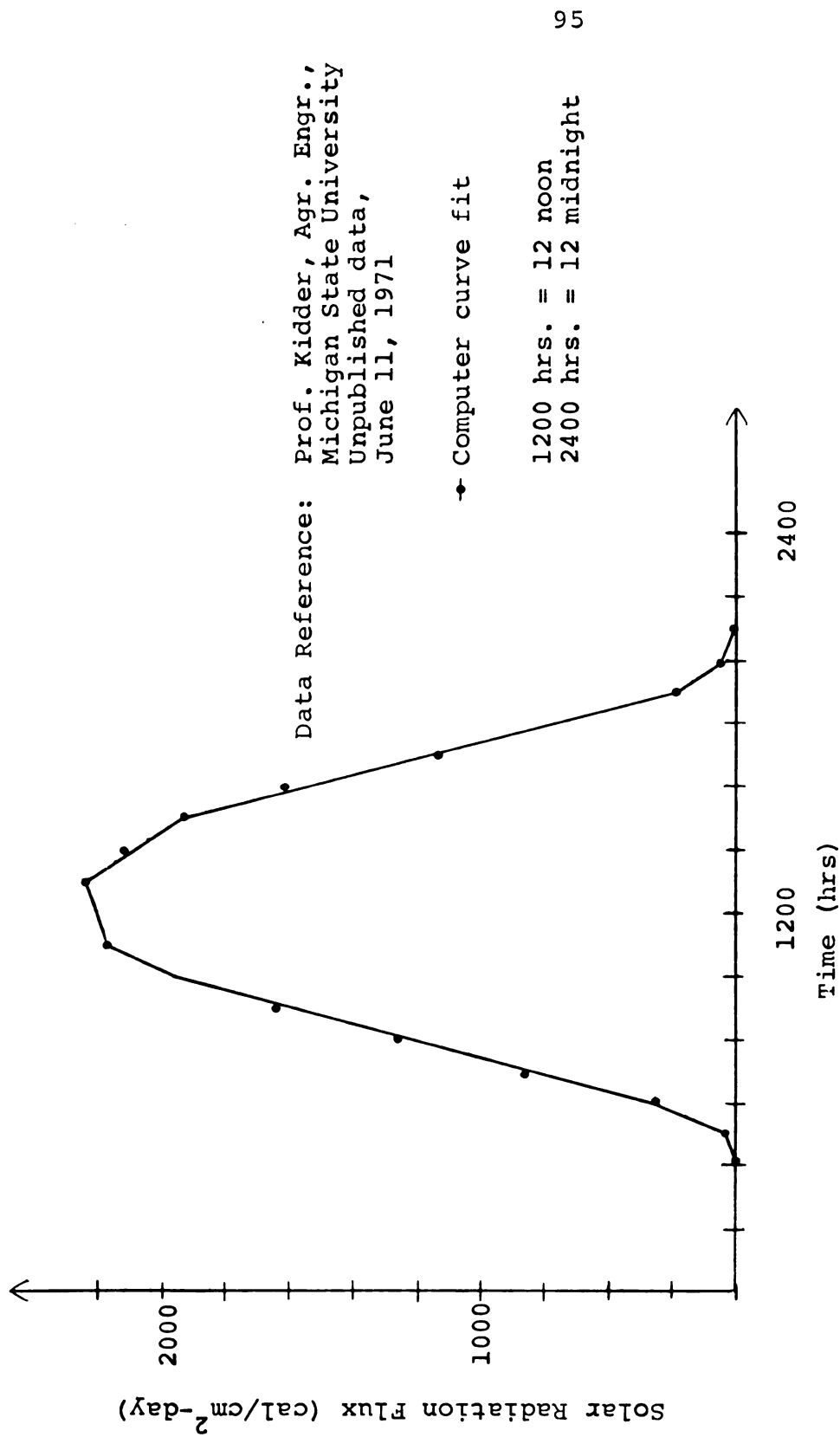


Figure 26.--Boundary conditions for simulation number 11 (solar radiation flux versus time).

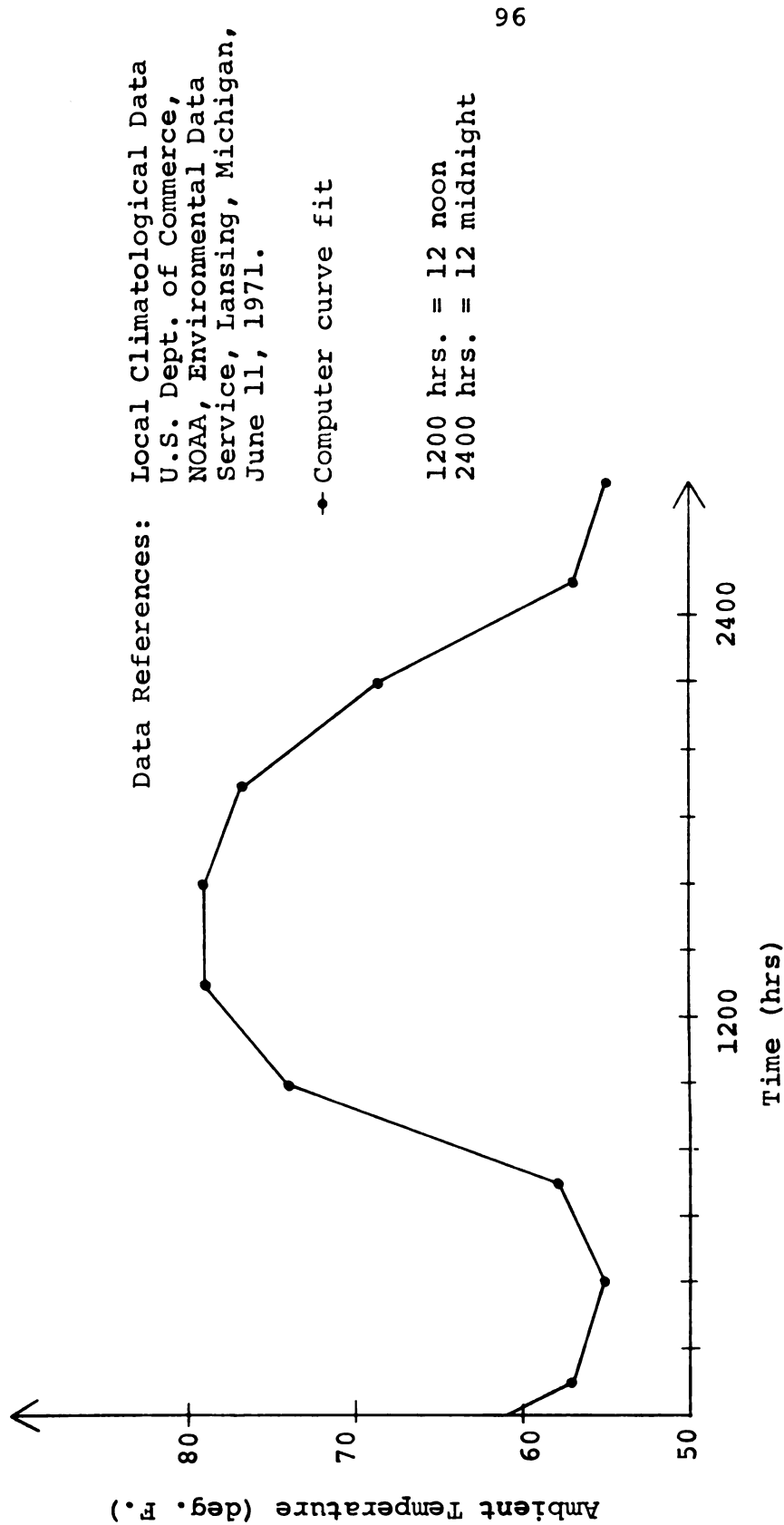
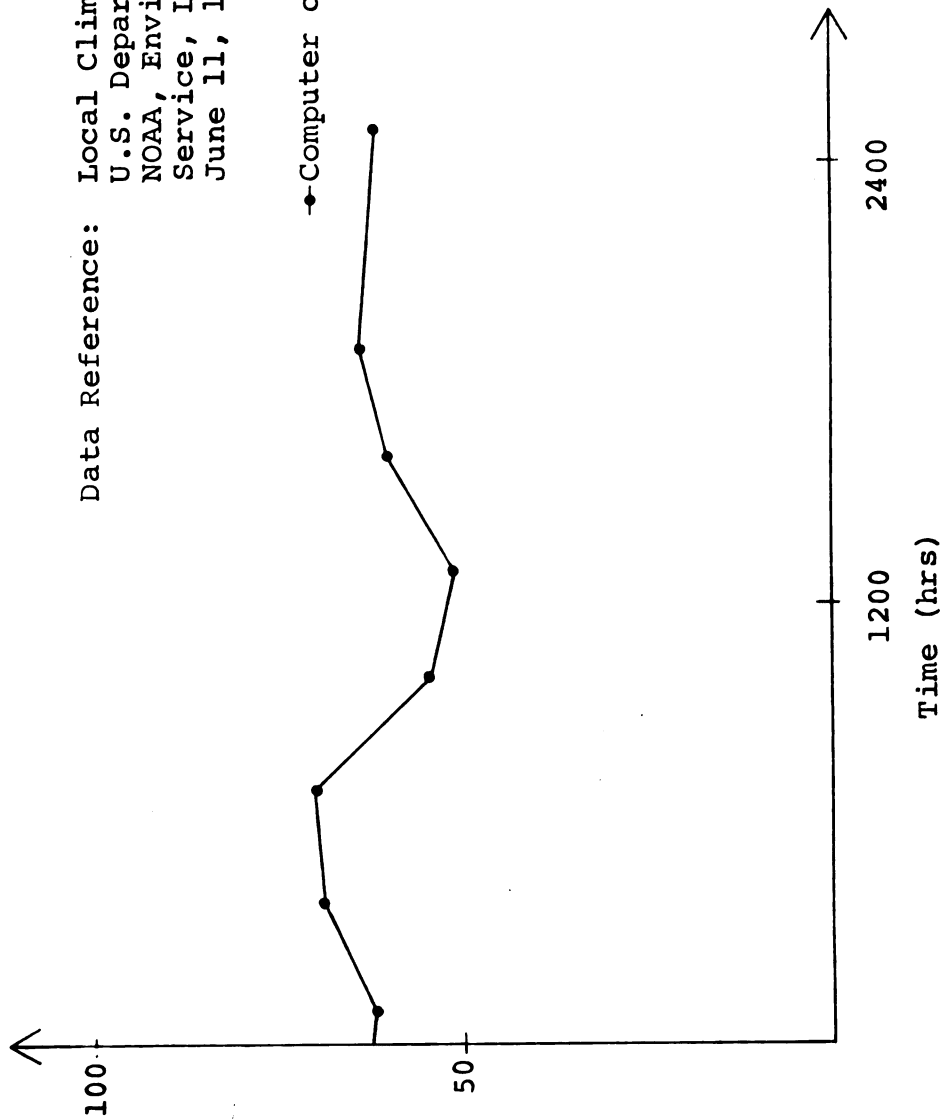


Figure 27.--Boundary conditions for simulation number 11 (ambient temperature versus time).

$$\frac{X_{w,A}}{X_{w,A}^*} = 100 \times \text{Ambient Relative Humidity (dim.)}$$



Data Reference: Local Climatological Data,
U.S. Department of Commerce,
NOAA, Environmental Data
Service, Lansing, Michigan,
June 11, 1971.

•—Computer curve fit

1200 hrs. = 12 noon
2400 hrs. = 12 midnight

Figure 28.--Boundary conditions for simulation number 11 (ambient relative humidity versus time).

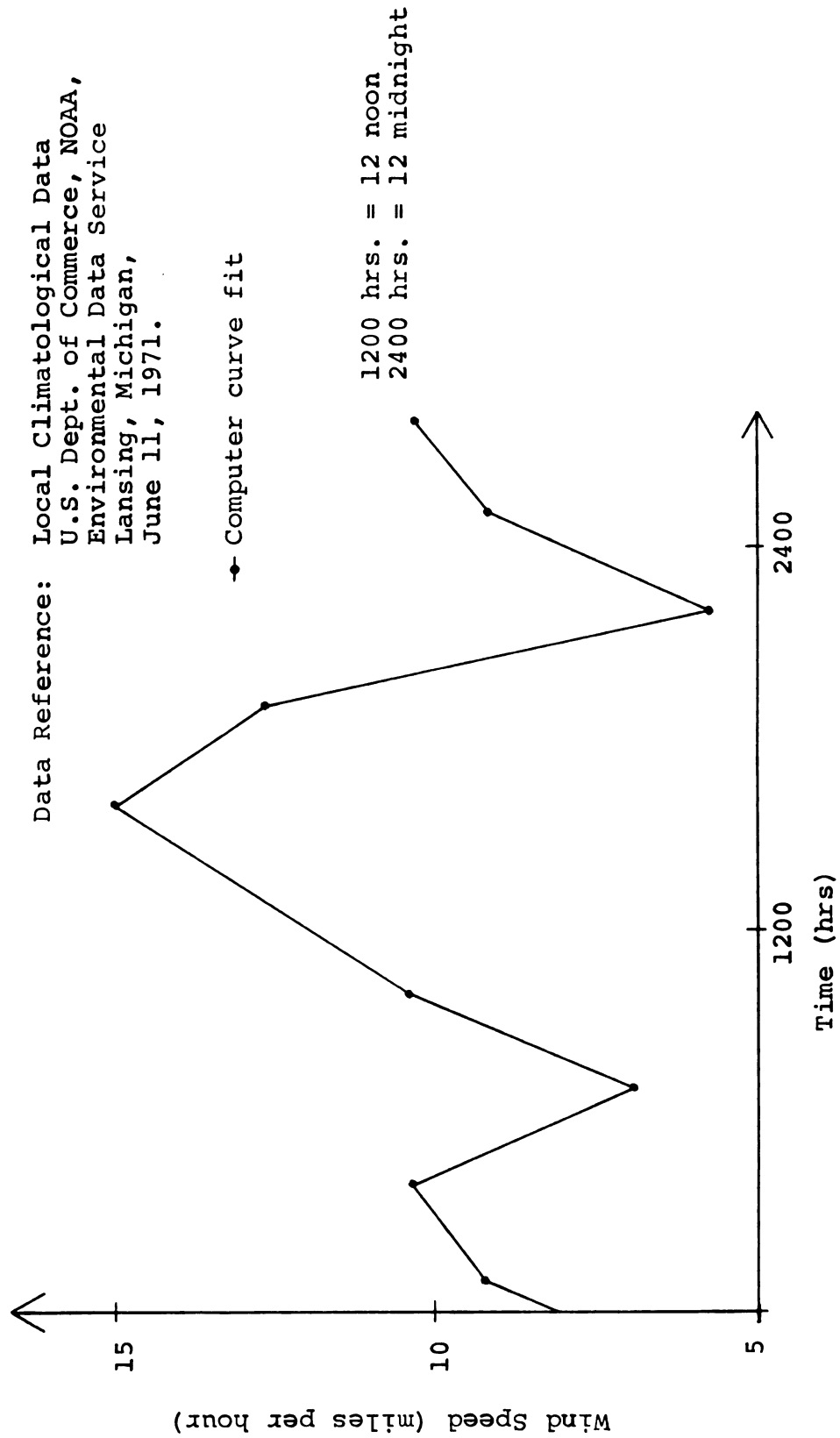


Figure 29.--Boundary conditions for simulation number 11 (wind speed versus time).

Lansing, Michigan on June 11, 1971 were used to construct a daily weather cycle which was repeated day after day for the duration of the simulation.

The temperatures at the soil surface, 9 cm., and 18 cm. soil depths were plotted as functions of time in Figures 30-35. The saturation profiles are given in Figure 36. From Figures 30-36 it can be seen that between the second and third day the falling rate period begins and the surface saturation is near the irreducible saturation.

The amplitude of the temperature oscillations increases with time at all depths. For example, before the falling rate period, the magnitude of the surface variation is about 15 deg. C., whereas during the falling rate period the magnitude increases to about 30 deg.C. At lower depths the magnitude of the temperature variation decreases. Also, there is a lag between temperature peaks in comparison to the surface temperature peak. The temperature peak at the surface occurs at about 1300 hrs., whereas the temperature peak for $z=9$ cm. occurs at about 1330 hrs. At a depth of $z=18$ cm., the temperature peak occurs at about 1500 hrs.

Simulation number 11 illustrates the moderating affect that soil water has on the soil temperature variations and magnitude of the soil temperature. During the nighttime

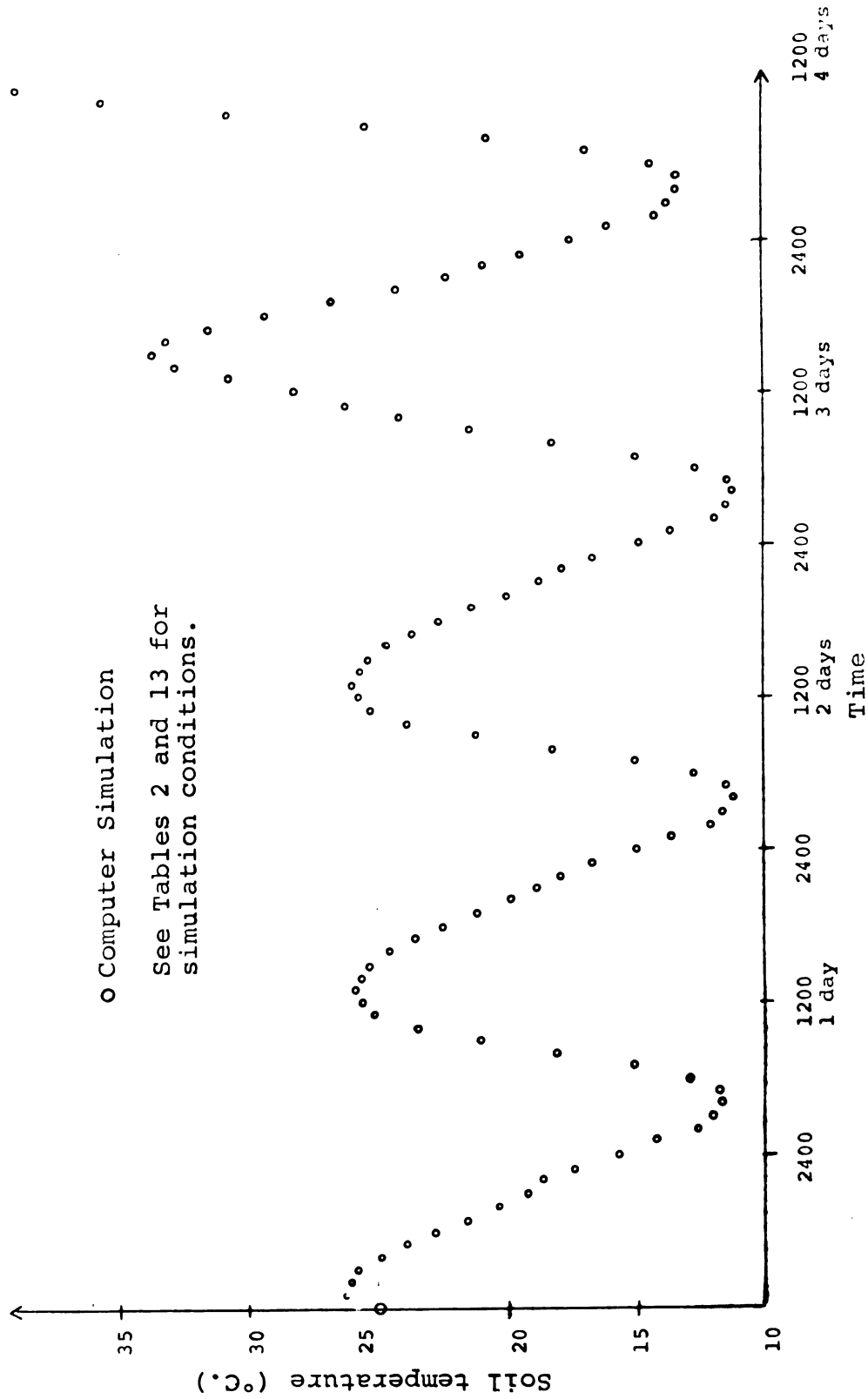


Figure 30.--Soil temperature versus time, $z=0$ (simulation number 11).

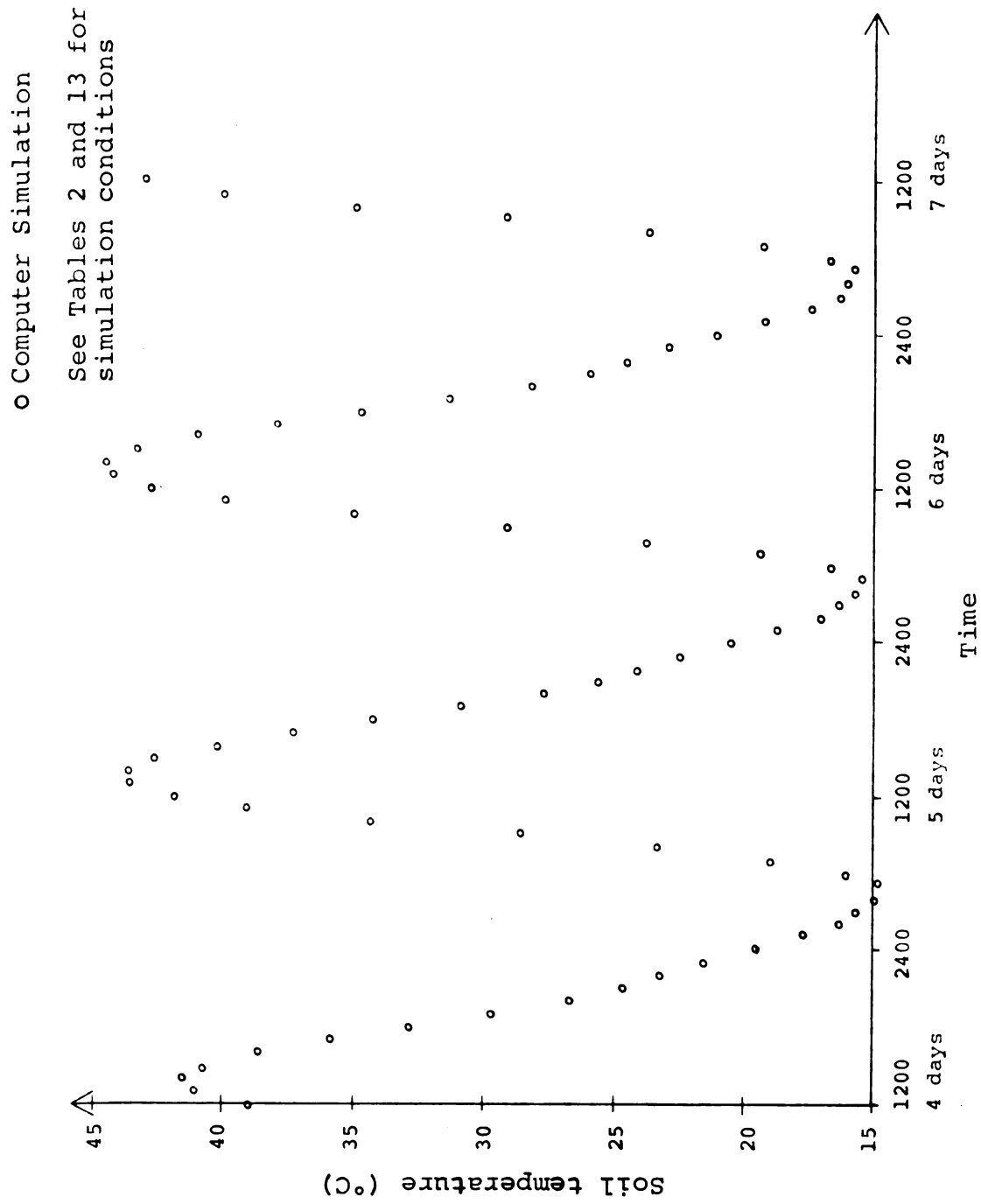


Figure 31.--Soil temperature versus time, z=0 (simulation number 11).

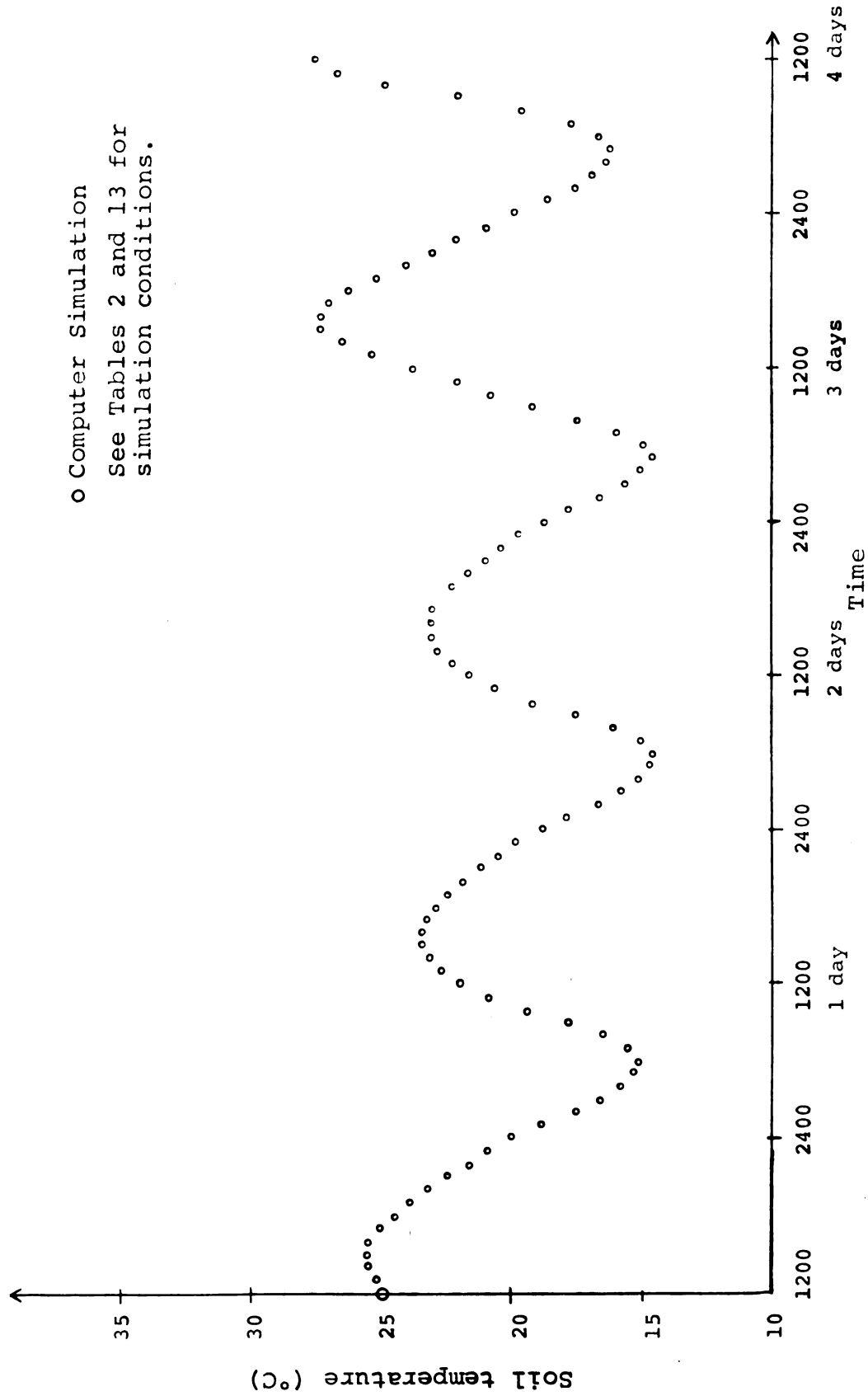


Figure 32.--Soil temperature versus time, $z=9$ cm. (simulation number 11).

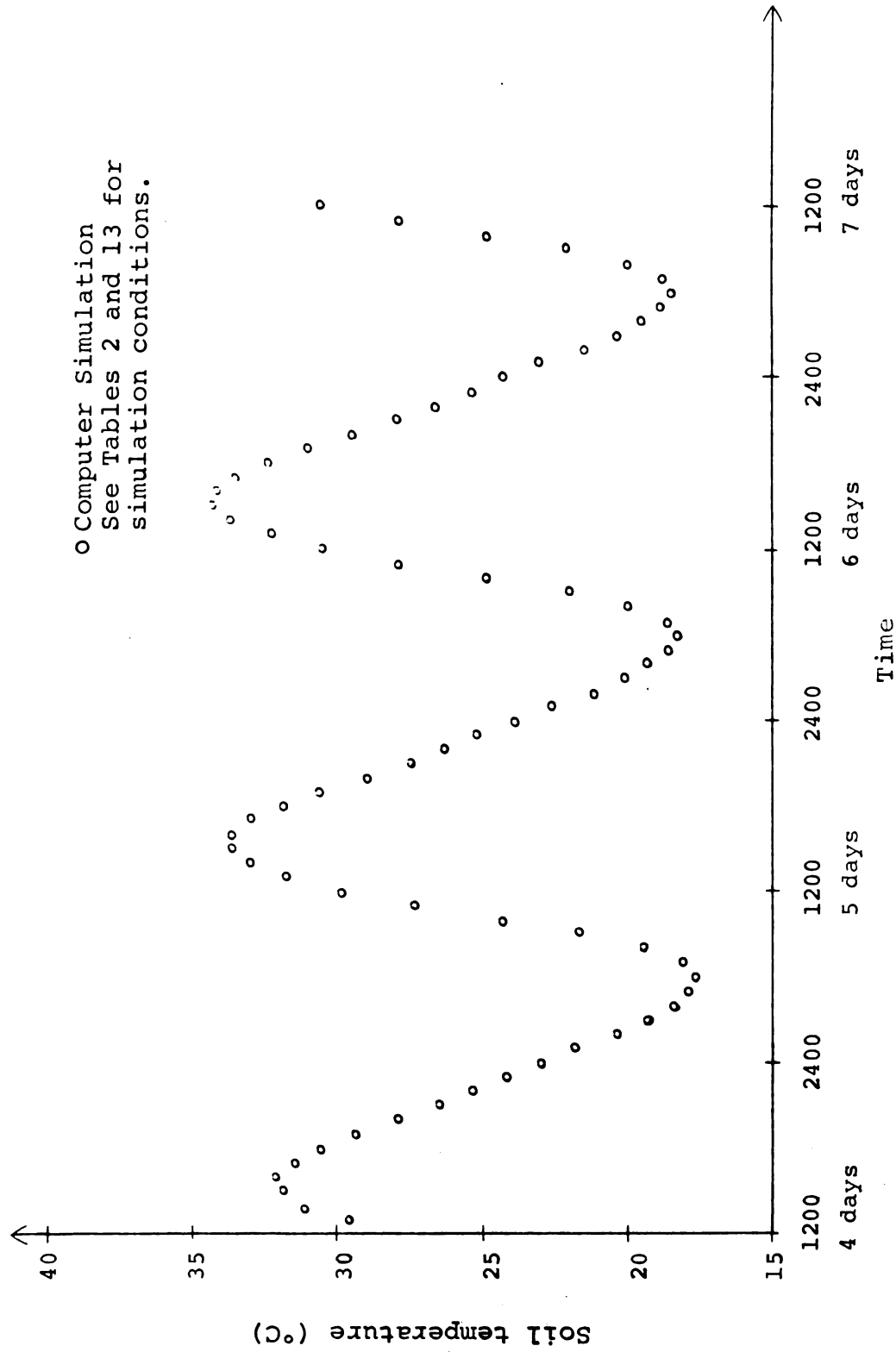


Figure 33.--Soil temperature versus time, $z=9$ cm. (simulation number 11).

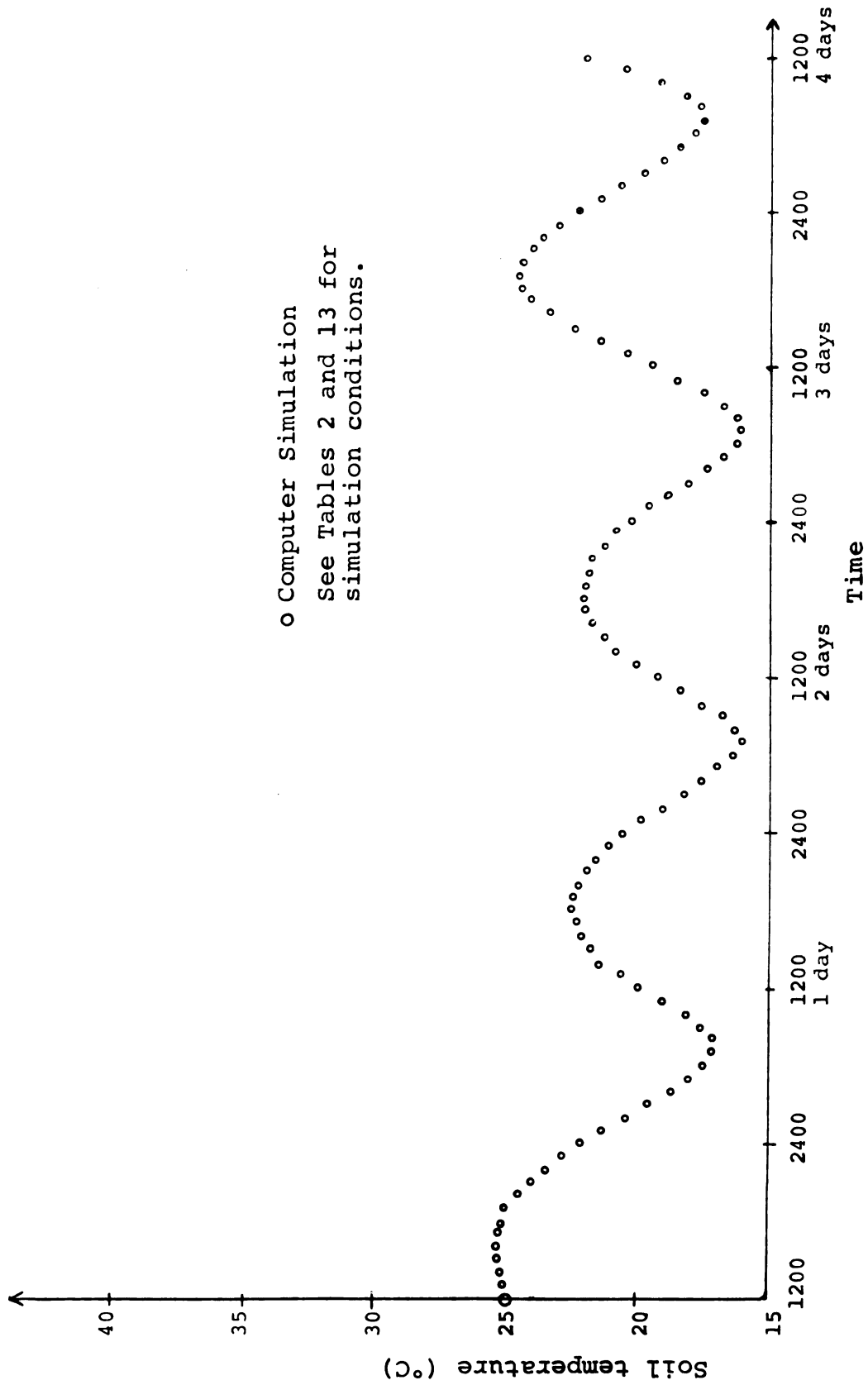


Figure 34.--Soil temperature versus time, $z=18$ cm. (simulation number 11).

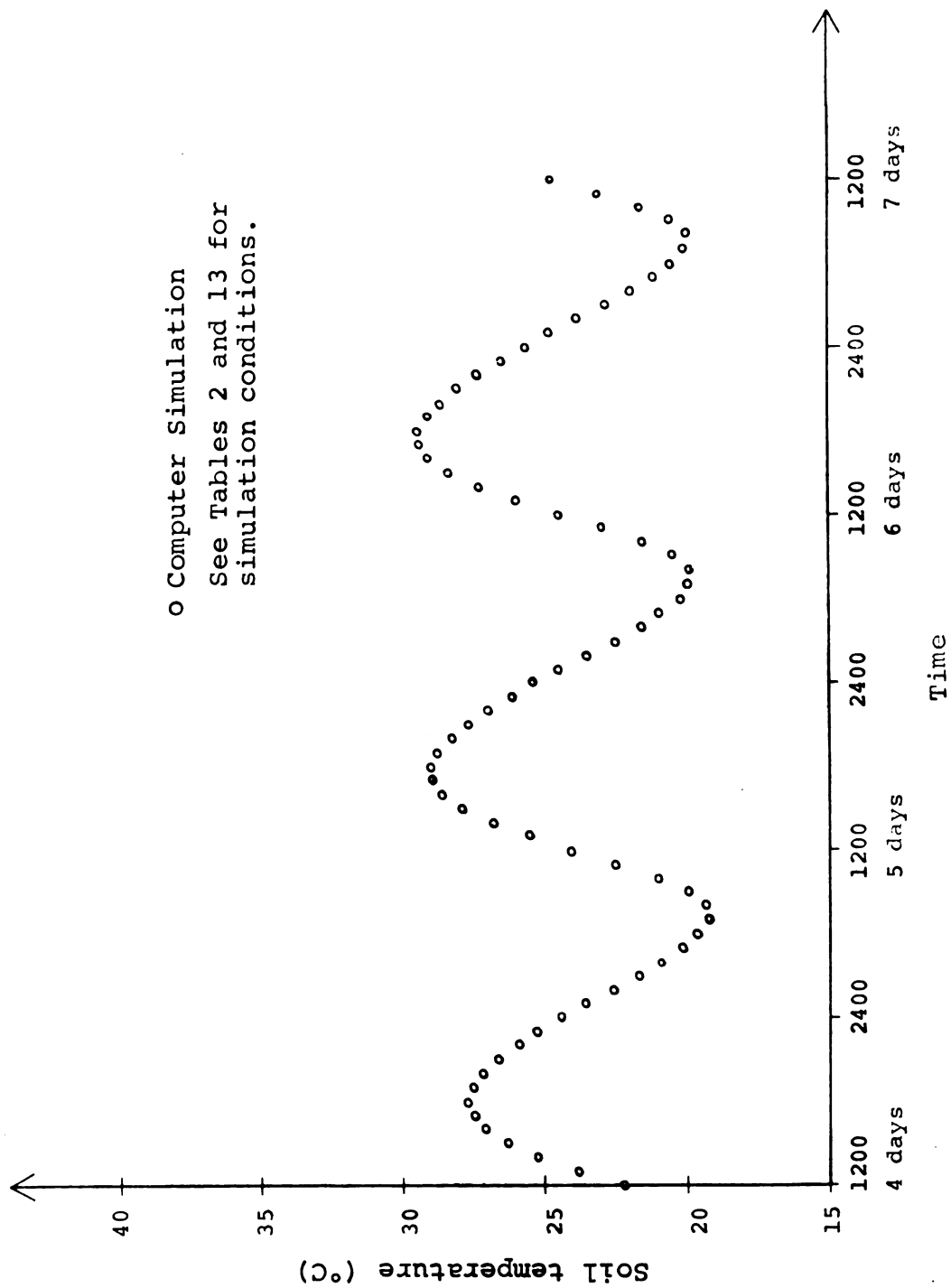


Figure 35.--Soil temperature versus time, $z=18$ cm. (simulation number 11).

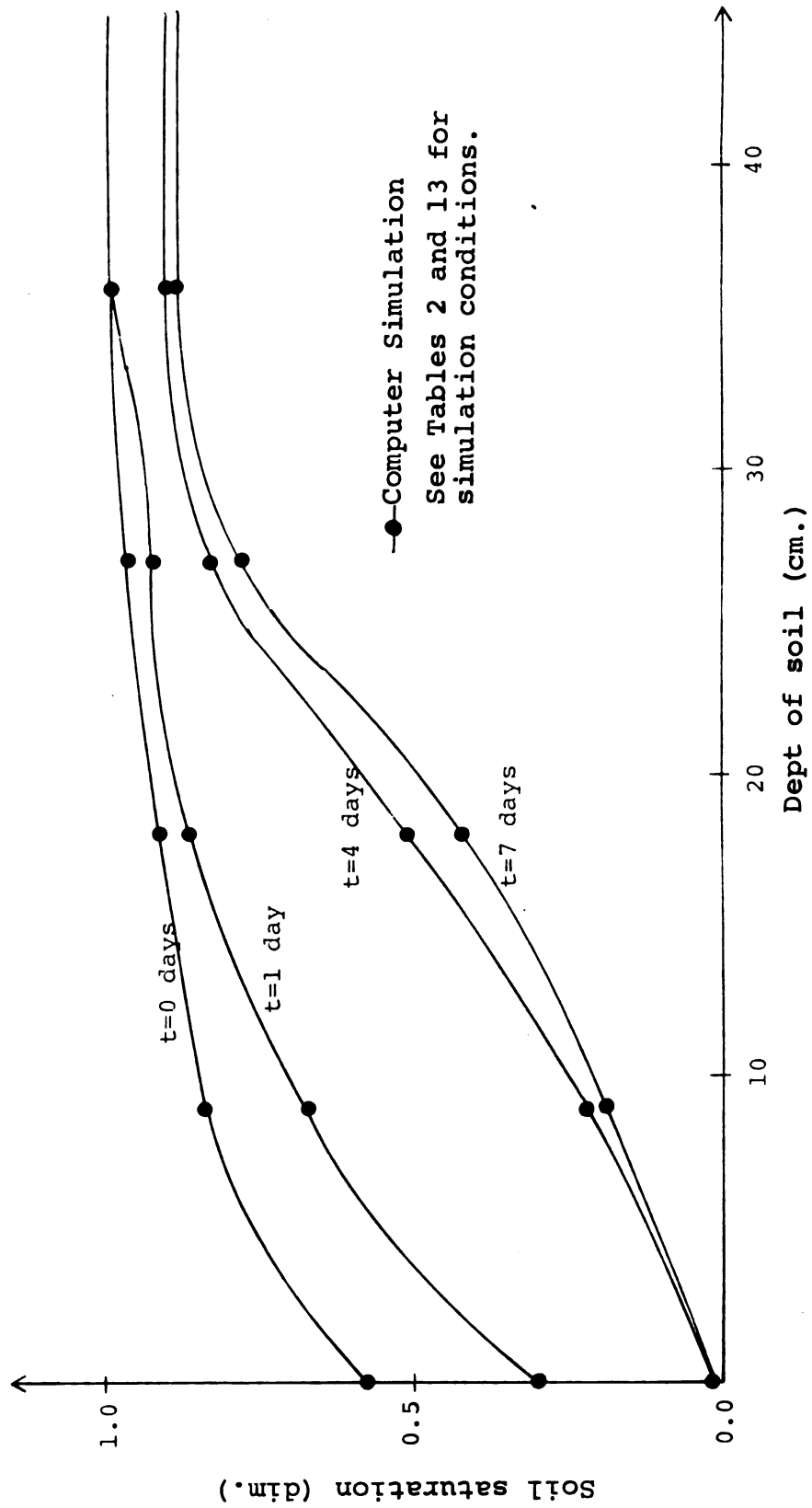


Figure 36.---Soil saturation versus depth of soil (simulation number 11).

hours the soil temperature dropped below the ambient temperature when the soil surface saturation was high. This was because evaporation was taking place at night with the subsequent cooling of the surface.

Although the bottom column boundary condition and radial column energy loss do not represent exactly the boundary conditions in an open field of soil, simulation number 11 does give a reasonable estimate of the temperature variations. Cary has reported data on maximum daily variations in soil temperatures at various depths for Argonne, Illinois [32]. Table 14 shows these variations. If the soil is wet, these simulation results are close to those reported for Argonne daily maximums.

TABLE 14.--Maximum daily soil temperature changes over an annual cycle at Argonne, Ill.

Depth (cm.)	Maximum daily soil temperature variation (deg.C.)
1	12
10	9
20	3
50	0.5

If the soil is very dry the simulation results are off by a factor of two on the large side.

CHAPTER V

CONCLUSIONS

The objectives of this work, outlined in Chapter I, have been met. A general model to describe water movement in soils has been developed. This new model and earlier models for water movement in soils have been used in digital computer simulations. The different models have been compared with one another and with experimental drying data.

Using the general model developed in Chapter II, it was shown that even under dry soil conditions, the inter-phase vapor-liquid equilibrium assumption was valid. This assumption is the foundation for the Philip and De Vries model and has not previously been justified by soil air humidity measurements, or by theoretical analysis. The general model can indicate the validity of the assumption for a given situation defined by the following information: (1) saturation profile, (2) temperature profile, and (3) boundary conditions.

The unsteady state solution of the Philip and De Vries equations has been obtained for both constant and

time varying boundary conditions. Previous to this work, the Philip and De Vries equations have not been solved for unsteady state problems. Simulations on identical drying problems using the Philip and De Vries model and the isothermal equation has shown the following. When the irreducible saturations (during the drying falling rate period) used in both models are the same, there is good agreement between the saturation profiles calculated by each model.

An advantage of the Philip and De Vries model is that it can be used to calculate saturation, temperature, and equilibrium mole fraction of water vapor profiles during the drying of soil or porous media. With the hydraulic and thermal properties of the porous media, the irreducible saturation can be calculated for a given set of boundary conditions. The isothermal equation cannot predict the irreducible saturation. This is because the surface temperature is not known since this model does not predict temperature.

Current use of the isothermal equation for drying has mainly been in fitting experimental cumulative evaporation data. Experimental information on the values of irreducible saturation is used in the simulations. Now for the first time the Philip and De Vries model has been solved in this work to yield a predictive model.

A time varying boundary condition problem was run with the Philip and De Vries model. Natural weather conditions were used as the surface boundary conditions. The temperature variations in the soil which were calculated were reasonably close to the experimental data. The simulations also showed that soil water acts to minimize the maximum soil temperature reached in a daily cycle. Also a dry soil has a daily temperature variation almost double that of a wet soil under the weather conditions studied.

Literature physical property data was used with the isothermal equation and the Philip and De Vries model in an attempt to fit experimental drying data. The saturation profiles calculated fitted the experimental saturation profiles. Although the calculated temperature profiles were similar in shape to the experimental temperature profiles, the calculated temperatures were larger than the experimental temperatures. This is because the column bottom boundary condition on energy flux was not a close enough approximation to the drying experiment boundary condition.

The solution to the Philip and De Vries model developed in this work should be useful in problems involving drying of soils or porous media where a predictive capability is needed. The general model will also be useful in these types of problems to evaluate the interphase vapor-liquid equilibrium assumption upon which the Philip and De Vries model is based. The following is a brief listing of some

problems where the Philip and De Vries model and the general model would be useful.

- (1) Drying of a porous media where a certain temperature or dryness must not be exceeded in the porous media.
- (2) Management strategies for irrigation practices.
- (3) Management strategies for insect pest control (example, cereal leaf beetle) where the insect hatching is strongly dependent on soil moisture and temperature.
- (4) Meteorological studies.

For soils which are above the irreducible saturation, the isothermal equation for water movement would be the most expedient model to use if soil temperature information was not desired. In particular, the isothermal equation would be a good base for structuring models to describe the movement of chemical compounds in soils subjected to spray irrigation with liquid wastes.

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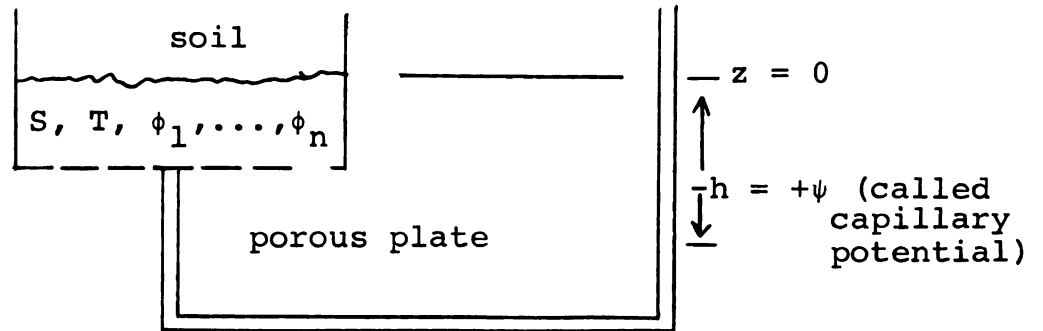
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APPENDIX A
CAPILLARY POTENTIAL AS A FUNCTION OF
SATURATION, TEMPERATURE, HISTORY,
AND COMPOSITION



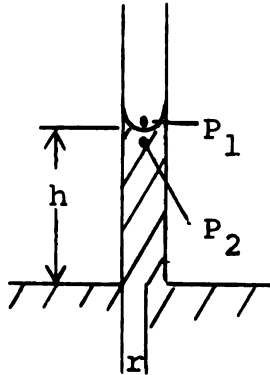
The free energy of water per weight of water in soil is a function of saturation, temperature, and composition. It can be calculated as follows:

$$(A.1) \quad d\psi = \left(\frac{\partial \psi}{\partial S}\right)_{T, \phi_i} dS + \left(\frac{\partial \psi}{\partial T}\right)_{S, \phi_i} dT + \sum_i \left(\frac{\partial \psi}{\partial \phi_i}\right)_{S, T} d\phi_i$$

where, ψ = free energy per weight of water = dyne-cm/dyne

ψ^0 = standard state ($S = 0, T, \phi_1, \phi_2, \dots, \phi_n$) = 0

An analogy has been made between the soil drawing water as shown above, and a capillary tube drawing water.



$$(A.2) \quad P_c = P_1 - P_2 = h = \frac{2\sigma}{r} = -\psi$$

The capillary tube analogy appears to be the source for calling Ψ the capillary potential.

When the capillary potential (Ψ) is due to surface phenomenon such as curved gas-liquid interfaces in soil capillaries, the effect of temperature can be calculated from the surface tension (or free energy) as follows:

$$(A.3) \quad \frac{\partial \Psi}{\partial T} = - \frac{\partial P_c}{\partial T} = - \frac{2}{r} \frac{\partial \sigma}{\partial T} = - \frac{P_c}{\sigma} \frac{\partial \sigma}{\partial T} = \frac{\Psi}{\sigma} \frac{\partial \sigma}{\partial T}$$

Integration of Equation (A.3) gives capillary potential as a function of temperature. This integration is contained in the physical property subroutine for capillary potential (see Appendix F).

It was mentioned that capillary potential is also a function of history. This is because there is a hysteresis in the capillary potential--saturation function which is dependent on the drying--wetting history of the soil. From the discussion in Appendix E on the interfacial area model, it is evident that the way in which the water distributes itself beyond the drainage point will affect the interfacial area--saturation function. The water distribution phenomenon likewise affects the capillary potential--saturation function, and hence the hysteresis. For a drying process, there is no hysteresis as long as the soil saturation is monotonically decreasing. In this case a unique curve exists for the capillary potential--saturation function.

APPENDIX B
ANALOGY BETWEEN THE ISOTHERMAL EQUATION
OF GARDNER AND THE UNSTEADY STATE
DIFFUSION EQUATION

The isothermal equation of Gardner and Darcy's law can be combined to give an equation of a form similar to the unsteady state diffusion equation. Assuming capillary potential (Ψ) is only a function of saturation, Darcy's law can be written

$$(B.1) \quad v^o = -K \left(\frac{\partial \Psi}{\partial S} \frac{\partial \bar{S}}{\partial z} - 1 \right) = -D \frac{\partial \bar{S}}{\partial z} + K.$$

Substituting Equation (D.1) into Gardner's equation for constant porosity (ϵ),

$$(B.2) \quad \epsilon \frac{\partial \bar{S}}{\partial t} = \frac{\partial}{\partial z} \left(D \frac{\partial \bar{S}}{\partial z} \right) - \frac{\partial K}{\partial z}$$

In the absence of gravity Equation (B.2) is analogous in form to the unsteady state diffusion equation written with a variable diffusivity.

APPENDIX C
THREE DIMENSIONAL EQUATIONS OF CHANGE
FOR POROUS MEDIA

The three dimensional equations of change can be obtained by making material and energy balances which include the possibility for variation in three spatial directions. The equations of continuity (Equations (2.2), (2.5), (2.7) in three dimensional form are:

$$(C.1) \quad \frac{\partial \rho_w \theta}{\partial t} = -\nabla \cdot \rho_w V^O - E$$

$$(C.2) \quad \frac{\partial (\tilde{C}_w \varepsilon (1-S))}{\partial t} = -\nabla \cdot \tilde{N}_w + \frac{E}{M_w}$$

$$(C.3) \quad C \frac{\partial T}{\partial t} = -\nabla \cdot q - \nabla H_{vap} E$$

where,

$$(C.4) \quad \nabla = \left(\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z} \right)$$

In the above equations the flux quantities (V^O , $\tilde{N}_w$, q) are vectors.

APPENDIX D

LIQUID WATER VAPOR PRESSURE AS A FUNCTION
OF TEMPERATURE, SATURATION,
AND COMPOSITION

The vapor pressure of water in soil is dependent on temperature, saturation, and water phase composition. Based on free energy considerations, it can be shown that the vapor pressure--temperature relationship should obey the Clapeyron equation [31].

$$(D.1) \quad \frac{d \ln P_{\text{vap}}}{d\left(\frac{1}{T}\right)} = - \frac{\tilde{\Delta H}_{\text{vap}}}{R}$$

This equation can be intergrated to give

$$(D.2) \quad \ln\left(\frac{P_{\text{vap}}(T_2)}{P_{\text{vap}}(T_1)}\right) = - \frac{\tilde{\Delta H}_{\text{vap}}}{R} \left(\frac{1}{T_2} - \frac{1}{T_1}\right).$$

where, $\tilde{\Delta H}_{\text{vap}} = \text{constant over } [T_1, T_2]$

This equation is not accurate over a wide range of temperatures because the enthalpy of vaporization is a function of temperature. For purposes of this study a quadratic relationship between $\ln P_{\text{vap}}$ and $\left(\frac{1}{T}\right)$ was used to obtain a good fit of vapor pressure over a range of 20-60°C.

Saturation is another variable which affects the vapor pressure of water in soils. If a wet soil is dried under isothermal conditions, the vapor pressure is reduced

as the soil dries out. This is due to capillary and adsorption forces. The adsorption forces predominate in very dry soil. The phenomenon can be quantified based on free energy considerations.

Consider the following states for soil water.

State 1 - pure water in soil at 25°C., saturation = $S_1 = 1.0$

State 2 - pure water in soil at 25°C., saturation = S_2

The change of free energy of soil water between states one and two is

$$(D.3) \quad \Delta G = -RT \ln \frac{P_{\text{vap}}(S_2)}{P_{\text{vap}}(S_1)} .$$

The free energy change can also be written as

$$(D.4) \quad \Delta G = \tilde{V} \Delta P = \frac{\tilde{V} \rho g (-\Psi)}{\gamma}$$

where, $\Delta P = -\Psi$

The combination of Equations (D.3) and (D.4) give the relationship between capillary potential (and saturation) and water vapor pressure. This equation is used to determine capillary potential under low moisture conditions in the soil by making water vapor pressure measurements.

$$(D.5) \quad P_{\text{vap}}(S_2) = P_{\text{vap}}(S_1) \exp\left(\frac{\tilde{V}\rho g\Psi}{RT\gamma}\right), \quad \Psi \leq 0$$

When the water in soil is not pure, the soluble compounds affect the water vapor pressure. Methods for handling this situation will not be covered here as they are covered in standard thermodynamics textbooks [31].

APPENDIX E

INTERFACIAL AREA MODEL (SIMPLE CUBIC
PACKING OF RODS) AND COMPUTER PROGRAM

Figure 37 on the next page defines the terms in the following equations which are not defined in the nomenclature.

The solid and void fractions are calculated as follows for the simple cubic packing of rods.

$$(E.1) \quad 1 - \epsilon = \frac{\pi D_L^2}{4D^2} = \frac{\pi}{4}$$

$$(E.2) \quad \epsilon = 1 - \frac{\pi}{4} = 0.21460$$

Before drainage is reached:

$$(E.3) \quad S\epsilon = \frac{8L}{D^2} \int_0^{x^*} (y^* - \bar{y}) \, dx = \frac{8}{D^2} \int_0^{x^*} (y^* - \bar{y}) \, dx$$

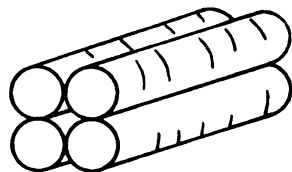
$$(E.4) \quad a = \frac{\pi DL}{D^2} + \frac{8L}{D^2} \int_0^{x^*} \sqrt{1 + \left(\frac{dy^*}{dx}\right)^2} \, dx - \frac{8L}{D^2} \int_0^{x^*} \sqrt{1 + \left(\frac{d\bar{y}}{dx}\right)^2} \, dx$$

The equation of a rod cross section:

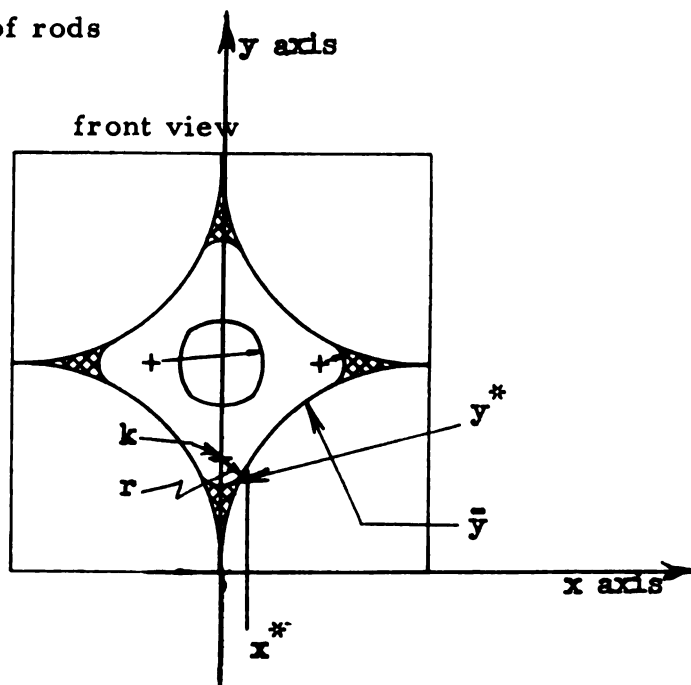
$$(E.5) \quad (x-R)^2 + y^2 = R^2$$

The equation of the gas-liquid interface:

$$(E.6) \quad x^2 + (y-k)^2 = r^2$$



simple cubic packing of rods



Rod diameter = $D = 2R$

Rod length = L

r = radius of curvature of liquid-gas interface

y^* = y distance from x axis to the gas-liquid interface

$\bar{y}$ = y distance from x axis to the rod surface

Figure 37.--Interfacial area model (simple cubic packing of rods).

so,

$$(E.7) \quad \bar{y} = + R^2 - (x-R)^2$$

$$(E.8) \quad y^* = - r^2 - x^2 + k$$

Before drainage the liquid interface is tangent to the solid interface at the gas-liquid-solid contact point ($x=x^*$).

so,

$$(E.9) \quad x^* = R(1-\cos\theta)$$

$$(E.10) \quad r = R(-1 + \sqrt{1 + \tan^2\theta}), \quad 0 \leq \theta \leq \frac{\pi}{4}$$

$$(E.11) \quad k = R \tan\theta$$

Combining Equations (E.3)-(E.8) and integrating we get

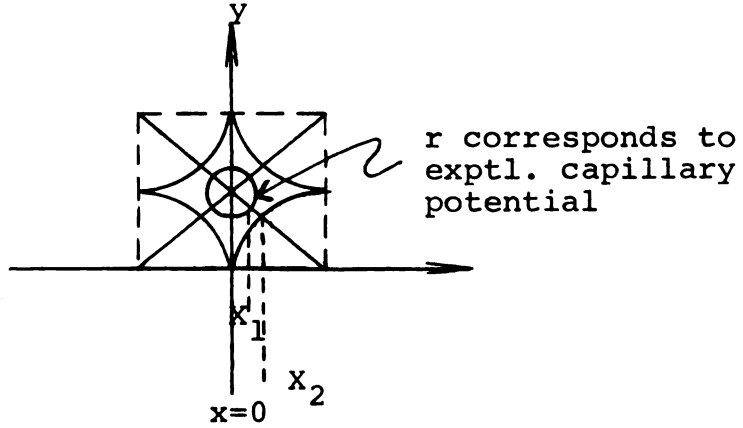
$$(E.12) \quad S = \frac{8}{D^2 \epsilon} \left[kx^* - \frac{1}{2} [x^* \sqrt{r^2 - x^{*2}} + r^2 \sin^{-1}(\frac{x^*}{r})] \right. \\ \left. - \frac{1}{2} [(x^* - R) \sqrt{R^2 - (x^* - R)^2} + R^2 \sin^{-1}(\frac{x^* - R}{R})] \right. \\ \left. + \frac{1}{2} R^2 \sin^{-1}(-1) \right]$$

$$(E.13) \quad a = \frac{\pi}{D} + \frac{8}{D^2} [r[\sin^{-1}(\frac{x^*}{r}) - \sin^{-1}(0)] \\ - R[\sin^{-1}(\frac{x^* - R}{R}) - \sin^{-1}(-1)]]$$

After drainage the following water distribution is assumed:

Drainage occurs at $\theta = 45^\circ$ or $x_1 = x_2 = \frac{R}{\sqrt{2}}$

$$-\psi = P_c = \frac{2\sigma}{r\gamma}$$



The equations for saturation and interfacial area after drainage are given below.

$$(E.14) \quad S = \frac{8L}{D^2 L} \int_0^{x_1} (y^* - \bar{y}) \, dx + \int_{x_1}^{x_2} (y^* - \bar{y}) \, dx$$

$$(E.15) \quad a = \frac{8L}{D^2 L} \int_0^{x_1} \sqrt{1 + \left(\frac{dy^*}{dx}\right)^2} \, dx$$

where,

$$(E.16) \quad (y^* - \bar{y}) = k - \sqrt{r^2 - x^2} - \sqrt{R^2 - (x-R)^2}$$

$$(E.17) \quad (y^* - \bar{y}) = -(x-R) - \sqrt{R^2 - (x-R)^2}$$

$$(E.18) \quad y^* = -(x-R)$$

Substitution of Equations (E.16)-(E.18) into Equations (E.14) and (E.15) and integration give the following equations which apply after drainage.

$$(E.19) \quad S = \frac{1}{\epsilon_D^2} [kx_1 - \frac{1}{2}(x_1 \sqrt{r^2 - x_1^2} + r^2 \sin^{-1}(\frac{x_1}{r})) - \frac{1}{2}(x_2^2 - x_1^2 - 2(x_2 - x_1)R) - \frac{1}{2}[(x_2 - R) \sqrt{2x_2 R - x_2^2} + R^2(\sin^{-1}(\frac{x_2 - R}{R}) - \sin^{-1}(-1))]]$$

$$(E.20) \quad a = \frac{8r}{D^2} [\sin^{-1}(\frac{x_1}{r}) - \sin^{-1}(0)]$$

To find x_1 , consider the intersection of the line ($y = -(x-R)$) with the circle ($x^2 + (y-k)^2 = r^2$). Then,

$$(E.21) \quad x_1 = -\frac{1}{2}(k-R) \pm \sqrt{\frac{1}{2}r^2 - \frac{1}{4}(k-R)^2}, \text{ where } r = \frac{1}{2}(k-R)^2$$

The location of the radius of the radius of curvature (r) on the y axis will be at $y = k$. The following conditions must be satisfied by this location.

1. The saturation calculated for a given k must be equal to the experimental saturation associated with the experimental capillary potential represented by the radius of curvature (r).
2. A solution must exist for a given k . That is the radius of curvature must intersect the rod or the line $y = -(x-R)$.

The existence of a solution is also dependent on the rod radius. The following is the documented computer program which calculates the interfacial area versus saturation curve over the entire saturation range. Beyond drainage, logic statements are used to insure a solution exists and a Newton-Raphson iteration is used to locate the radius of curvature at $y = k$.

```

C      PROGRAM AREA3(INPUT,OUTPUT,TAPE60=INPUT,TAPE61=OUTPUT)
C
C      L.T. NOVAK,      28 JAN 72      NEW VERSION *****
C      PROGRAM AREA3 DOES CALCULATIONS ON THE SIMPLE CUBIC PACKING ROD
C      MODEL.  THE PROGRAM CALCULATES INTERFACIAL AREA PER VOLUME AND
C      ASSUMES THAT THE CONTACT ANGLE BETWEEN THE LIQUID AND SOLID AT
C      CAPILLARY PRESSURE AS A FUNCTION OF SATURATION.  THE MODEL
C      AIR-LIQUID-SOLID CONTACT POINT IS ZERO
C
C      EXTERNAL EXP,ASIN,SQRT
C      REAL K,KG,KGO
C
C      READ IN PARTICLE DIAMETER, POROSITY, AND THE UPPER VALUE OF THETA
C      FOR WHICH THE EQUATIONS APPLY.
C
C      READ(60,50) D,THETM,EPS
C      50 FORMAT(3F10.0)
C      WRITE(61,54)
C
C      54 FORMAT(1H1,118HPROGRAM AREA3 DOES CALCULATIONS ON THE SIMPLE CUBIC
C      2PACKING ROD MODEL.  THE PROGRAM CALCULATES INTERFACIAL AREA PER
C      3R ,/1H ,118HVOLUME AND CAPILLARY PRESSURE AS A FUNCTION OF SATU
C      4RATION.  THE MODEL ASSUMES THAT THE ANGLE BETWEEN THE LIQUID AND
C      5 ,/1H , 63HSOLID INTERFACES AT THE AIR-LIQUID-SOLID CONTACT POIN
C      6T IS ZERO.,////)
C      WRITE(61,51) D,EPS,THETM
C      51 FORMAT(1H ,20HPARTICLE DIAMETER = ,E14.6,5H CM.,/12H POROSITY =
C      2E14.6,/,13H THETA MAX = ,E14.6,9H DEGREES,///)
C      WRITE(61,52)
C      52 FORMAT(1H0,5H1H1,5H1H2H1,5H1H3H1,5H1H4H1,5H1H5H1,5H1H6H1,5H1H7H1,5H1H8H1,5H1H9H1,5H1H10H1,5H1H11H1,5H1H12H1,5H1H13H1,5H1H14H1,5H1H15H1,5H1H16H1,5H1H17H1,5H1H18H1,5H1H19H1,5H1H20H1,5H1H21H1,5H1H22H1,5H1H23H1,5H1H24H1,5H1H25H1,5H1H26H1,5H1H27H1,5H1H28H1,5H1H29H1,5H1H30H1,5H1H31H1,5H1H32H1,5H1H33H1,5H1H34H1,5H1H35H1,5H1H36H1,5H1H37H1,5H1H38H1,5H1H39H1,5H1H40H1,5H1H41H1,5H1H42H1,5H1H43H1,5H1H44H1,5H1H45H1,5H1H46H1,5H1H47H1,5H1H48H1,5H1H49H1,5H1H50H1,5H1H51H1,5H1H52H1,5H1H53H1,5H1H54H1,5H1H55H1,5H1H56H1,5H1H57H1,5H1H58H1,5H1H59H1,5H1H60H1,5H1H61H1,5H1H62H1,5H1H63H1,5H1H64H1,5H1H65H1,5H1H66H1,5H1H67H1,5H1H68H1,5H1H69H1,5H1H70H1,5H1H71H1,5H1H72H1,5H1H73H1,5H1H74H1,5H1H75H1,5H1H76H1,5H1H77H1,5H1H78H1,5H1H79H1,5H1H80H1,5H1H81H1,5H1H82H1,5H1H83H1,5H1H84H1,5H1H85H1,5H1H86H1,5H1H87H1,5H1H88H1,5H1H89H1,5H1H90H1,5H1H91H1,5H1H92H1,5H1H93H1,5H1H94H1,5H1H95H1,5H1H96H1,5H1H97H1,5H1H98H1,5H1H99H1,5H1H100H1,5H1H101H1,5H1H102H1,5H1H103H1,5H1H104H1,5H1H105H1,5H1H106H1,5H1H107H1,5H1H108H1,5H1H109H1,5H1H110H1,5H1H111H1,5H1H112H1,5H1H113H1,5H1H114H1,5H1H115H1,5H1H116H1,5H1H117H1,5H1H118H1,5H1H119H1,5H1H120H1,5H1H121H1,5H1H122H1,5H1H123H1,5H1H124H1,5H1H125H1,5H1H126H1,5H1H127H1,5H1H128H1,5H1H129H1,5H1H130H1,5H1H131H1,5H1H132H1,5H1H133H1,5H1H134H1,5H1H135H1,5H1H136H1,5H1H137H1,5H1H138H1,5H1H139H1,5H1H140H1,5H1H141H1,5H1H142H1,5H1H143H1,5H1H144H1,5H1H145H1,5H1H146H1,5H1H147H1,5H1H148H1,5H1H149H1,5H1H150H1,5H1H151H1,5H1H152H1,5H1H153H1,5H1H154H1,5H1H155H1,5H1H156H1,5H1H157H1,5H1H158H1,5H1H159H1,5H1H160H1,5H1H161H1,5H1H162H1,5H1H163H1,5H1H164H1,5H1H165H1,5H1H166H1,5H1H167H1,5H1H168H1,5H1H169H1,5H1H170H1,5H1H171H1,5H1H172H1,5H1H173H1,5H1H174H1,5H1H175H1,5H1H176H1,5H1H177H1,5H1H178H1,5H1H179H1,5H1H180H1,5H1H181H1,5H1H182H1,5H1H183H1,5H1H184H1,5H1H185H1,5H1H186H1,5H1H187H1,5H1H188H1,5H1H189H1,5H1H190H1,5H1H191H1,5H1H192H1,5H1H193H1,5H1H194H1,5H1H195H1,5H1H196H1,5H1H197H1,5H1H198H1,5H1H199H1,5H1H200H1,5H1H201H1,5H1H202H1,5H1H203H1,5H1H204H1,5H1H205H1,5H1H206H1,5H1H207H1,5H1H208H1,5H1H209H1,5H1H210H1,5H1H211H1,5H1H212H1,5H1H213H1,5H1H214H1,5H1H215H1,5H1H216H1,5H1H217H1,5H1H218H1,5H1H219H1,5H1H220H1,5H1H221H1,5H1H222H1,5H1H223H1,5H1H224H1,5H1H225H1,5H1H226H1,5H1H227H1,5H1H228H1,5H1H229H1,5H1H230H1,5H1H231H1,5H1H232H1,5H1H233H1,5H1H234H1,5H1H235H1,5H1H236H1,5H1H237H1,5H1H238H1,5H1H239H1,5H1H240H1,5H1H241H1,5H1H242H1,5H1H243H1,5H1H244H1,5H1H245H1,5H1H246H1,5H1H247H1,5H1H248H1,5H1H249H1,5H1H250H1,5H1H251H1,5H1H252H1,5H1H253H1,5H1H254H1,5H1H255H1,5H1H256H1,5H1H257H1,5H1H258H1,5H1H259H1,5H1H260H1,5H1H261H1,5H1H262H1,5H1H263H1,5H1H264H1,5H1H265H1,5H1H266H1,5H1H267H1,5H1H268H1,5H1H269H1,5H1H270H1,5H1H271H1,5H1H272H1,5H1H273H1,5H1H274H1,5H1H275H1,5H1H276H1,5H1H277H1,5H1H278H1,5H1H279H1,5H1H280H1,5H1H281H1,5H1H282H1,5H1H283H1,5H1H284H1,5H1H285H1,5H1H286H1,5H1H287H1,5H1H288H1,5H1H289H1,5H1H290H1,5H1H291H1,5H1H292H1,5H1H293H1,5H1H294H1,5H1H295H1,5H1H296H1,5H1H297H1,5H1H298H1,5H1H299H1,5H1H300H1,5H1H301H1,5H1H302H1,5H1H303H1,5H1H304H1,5H1H305H1,5H1H306H1,5H1H307H1,5H1H308H1,5H1H309H1,5H1H310H1,5H1H311H1,5H1H312H1,5H1H313H1,5H1H314H1,5H1H315H1,5H1H316H1,5H1H317H1,5H1H318H1,5H1H319H1,5H1H320H1,5H1H321H1,5H1H322H1,5H1H323H1,5H1H324H1,5H1H325H1,5H1H326H1,5H1H327H1,5H1H328H1,5H1H329H1,5H1H330H1,5H1H331H1,5H1H332H1,5H1H333H1,5H1H334H1,5H1H335H1,5H1H336H1,5H1H337H1,5H1H338H1,5H1H339H1,5H1H340H1,5H1H341H1,5H1H342H1,5H1H343H1,5H1H344H1,5H1H345H1,5H1H346H1,5H1H347H1,5H1H348H1,5H1H349H1,5H1H350H1,5H1H351H1,5H1H352H1,5H1H353H1,5H1H354H1,5H1H355H1,5H1H356H1,5H1H357H1,5H1H358H1,5H1H359H1,5H1H360H1,5H1H361H1,5H1H362H1,5H1H363H1,5H1H364H1,5H1H365H1,5H1H366H1,5H1H367H1,5H1H368H1,5H1H369H1,5H1H370H1,5H1H37
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C      CALCULATE SATURATION, INTERFACIAL AREA/VOLUME, CAPILLARY PRESSURE AREA3 37
C      AND DIMENSIONLESS CAPILLARY PRESSURE AS A FUNCTION OF THETA. AREA3 38
C      THEN PRINT THESE RESULTS. AREA3 39
C      AREA3 40
C      AREA3 41
C      AREA3 42
C      AREA3 43
C      S = 37.278338/(D*D)*(K*X - 0.5*(X*SQRT(R*R - X*X) + R*R*ASIN(X/R))) AREA3 44
C      2 - 0.5*((X - D/2.)*SQRT(X*D - X*X) + D*D/4.*(ASIN(2.*X/D - 1.0) - AREA3 45
C      3 ASIN(-1.0))) AREA3 46
C      A = 3.1415927/D + 8./(D*D)*(R* ASIN(X/R) - D/2.*(ASIN(2.*X/D - 1.0) AREA3 47
C      2 - ASIN(-1.))) AREA3 48
C      SI = 0.1483687/R AREA3 49
C      DIM = (D/2.)/R AREA3 50
C      10 WRITE(61,53) THETA,S,A,SI,DIM AREA3 51
C      53 FORMAT(1H ,F9.5,X,F7.4,11X,E14.6,12X,E14.6,8X,E14.6) AREA3 52
C      AREA3 53
C      AREA3 54
C      AREA3 55
C      ADDITION TO AREA3
C      THE FOLLOWING PORTION OF THIS PROGRAM CALCULATES INTERFACIAL AREA AREA3 56
C      PER VOLUME, CAPILLARY PRESSURE, AND DIMENSIONLESS CAPILLARY AREA3 57
C      PRESSURE AS A FUNCTION OF SATURATION BEYOND THE DRAINAGE POINT. AREA3 58
C      THE RADIUS OF CURVATURE OF THE AIR-LIQUID INTERFACE IS CHOSEN AREA3 59
C      TO CORRESPOND TO EXPERIMENTAL DATA AT EACH GIVEN SATURATION BEYOND AREA3 60
C      THE DRAINAGE POINT OF SATURATION = 0.37 (APPROXIMATELY). AREA3 61
C      AREA3 62
C      WRITE(61,56) AREA3 63
C      56 FORMAT(1H1,81HDRAINAGE HAS BEEN REACHED AND CALCULATIONS WILL CONTINUE AREA3 64
C      2INUE UNDER THE ASSUMED MODEL. ,/119H BEYOND DRAINAGE THE INTERFACIAL AREA3 65
C      3IAL AREA PER VOLUME IS CALCULATED BY ASSUMING THE WATER PHASE IS DAREA3 66
C      4ISTRIBUTED ACCORDING TO ,/23H THE FOLLOWING DIAGRAM.,/////////) AREA3 67
C      WRITE(61,57) AREA3 68
C      57 FORMAT(1H0,5HERROR,5X,10HSATURATION,5X,30HINTERFACIAL AREA/VOLUME AREA3 69
C      2(CM-1),3X,26H- CAPILLARY PRESSURE (CM.),3X,32HDIMENSIONLESS CAPILLARY AREA3 70
C      3ARY PRESSURE ,/)) AREA3 71
C      READ(60,58) CHECK,KODE2 AREA3 72

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```

58 FORMAT( F10.0,I1)
C
C CALCULATE CYLINDRICAL DIAMETER SUCH THAT DRAINAGE OCCURS AT 0.38
C SATURATION. IF YOU CALCULATE THE CYLINDRICAL DIAMETER (D) AT
C S = 0.38 SO THAT R = RC, THEN FOR S .GT. 0.38, R.GT.RC. AND WE CAN
C ALWAYS FIND A SOLUTION IN SUBROUTINE NEWTON FOR THE INTERSECTION
C OF THE LIQUID INTERFACE WITH EITHER THE CYLINDER OR THE 45 DEG.
C LINE. THIS SOLUTION WILL GIVE A CORRESPONDENCE BETWEEN THE MODEL
C VALUES FOR CAPILLARY POTENTIAL-SATURATION AND THE EXPERIMENTAL
C VALUES. WITH THIS INFORMATION THE INTERFACIAL AREA IS CALCULATED.
C
C CALL CAPPO(0.380,SI)
C D = (2.0*0.1483687/(-SI))/(-1.0 + SQRT(2.0))
C WRITE(61,106) D
106 FORMAT(1H0,62HTHE CYLINDER DIAMETER USED IN THE FOLLOWING CALCULATIONS IS = ,E15.8)
C
C CALCULATE X2 AND RC.
C
C X2 = D/2.*(1. - 1./SQRT(2.0))
C RC = D/2.*(-1. + SQRT(2.0))
C
C BEGIN DO LOOP TO CALCULATE SATURATION (S) AND INTERFACIAL AREA
C (A) BEYOND THE DRAINAGE POINT. *****
C
C DO 11 I = 1,32
C S1 = I
C S1 = 0.36 + 0.02*S1
C
C CALL THE EXPERIMENTAL CAPILLARY POTENTIAL = - CAPILLARY PRESSURE.
C
C CALL CAPPO(S1,SI)
C
C CALCULATE THE RADIUS OF CURVATURE (R) FOR THE LIQUID INTERFACE AND
C KG AND KGO. THE FOLLOWING IF STATEMENTS ARE LOGIC CHECKS TO
C INSURE THAT A REAL SOLUTION IS FOUND.

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AREA3 73
AREA3 74
AREA3 75
AREA3 76
AREA3 77
AREA3 78
AREA3 79
AREA3 80
AREA3 81
AREA3 82
AREA3 83
AREA3 84
AREA3 85
AREA3 86
AREA3 87
AREA3 88
AREA3 89
AREA3 90
AREA3 91
AREA3 92
AREA3 93
AREA3 94
AREA3 95
AREA3 96
AREA3 97
AREA3 98
AREA3 99
AREA3100
AREA3101
AREA3102
AREA3103
AREA3104
AREA3105
AREA3106
AREA3107
AREA3108

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AREA3145
AREA3146
AREA3147
AREA3148
AREA3149
AREA3150
AREA3151
AREA3152
AREA3153
AREA3154
AREA3155
AREA3156
AREA3157
AREA3158
AREA3159
AREA3160
AREA3161
AREA3162
AREA3163
AREA3164
AREA3165
AREA3166
AREA3167
AREA3168
AREA3169
AREA3170
AREA3171
AREA3172
AREA3173
AREA3174
AREA3175
AREA3176
AREA3177
AREA3178
AREA3179
AREA3180

IF(R.GE.X1) GO TO 27
WRITE(61,71) R,X1,MODE
71 FORMAT(1H0,55HLOOK FOR ERROR IN SUBROUTINE NEWTON, R IS LESS THAN
2X1.,4HR = ,E15.8,2X,5HX1 = ,E15.8,2X,7HCODE = ,I3)
GO TO 11
27 K = D/2. - X1 + SQRT(R*R - X1*X1)
S = 37.278338/(D*D)*(K*X1 - 0.5*(X1*SQRT(R*R - X1*X1) + R*R*ASIN
2(X1/R)) - 0.5*(X2*X2 - X1*X1 - D*(X2 - X1)) - 0.5*((X2 - D/2.)*
3SQRT(D*X2 - X2*X2) + D*D/4.*(ASIN(2.*X2/D - 1.) - ASIN(-1.)))
GO TO 40
23 CODE = 2
C
C DETERMINE X, THE POINT OF INTERSECTION BETWEEN THE LIQUID INTERFAC
C AND THE CYLINDER CIRCULAR CROSS-SECTION (X-D/2)**2 + Y**2 =D*D/4.
C
CALL NEWTON(KODE,KODE2,CHECK,R,D,S1,X2,Y,X)
C*****
WRITE(61,103) KODE,KODE2,CHECK,R,D,S1,X2,Y,X
103 FORMAT(1H ,11HDEBUG CARD5,2I3,4X,7E14.7)
IF(R.GE.X)GO TO 28
WRITE(61,72) R,X,MODE
72 FORMAT(1H0,54HLOOK FOR ERROR IN SUBROUTINE NEWTON, R IS LESS THAN
2X.,4HR = ,E15.8,2X,4HX = ,E15.8,2X,7HCODE = ,I3)
28 IF(D.GE.X) GO TO 29
WRITE(61,73) D,X,MODE
73 FORMAT(1H0,54HLOOK FOR ERROR IN SUBROUTINE NEWTON, D IS LESS THAN
2X.,4HD = ,E15.8,2X,4HX = ,E15.8,2X,7HCODE = ,I3)
GO TO 11
29 K = SQRT(R*R - X*X) + SQRT(D*X - X*X)
S = 37.278338/(D*D)*(K*X - 0.5*(X*SQRT(R*R - X*X) + R*R*ASIN(X/R))
2 - 0.5*((X - D/2.)*SQRT(X*D - X*X) + D*D/4.*(ASIN(2.*X/D - 1.0) -
3 ASIN(-1.0)))
GO TO 39
20 K = KG
X = X2
C*****

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WRITE(61,107) K,X,R,D
107 FORMAT(1H,11HDEBUG CARD7,4E20.8)
S = 37.278338/(D*D)*(K*X - 0.5*(X*SQRT(R*R - X*X) + R*R*ASIN(X/R))
2 - 0.5*((X - D/2.)*SQRT(X*D - X*X) + D*D/4.*(ASIN(2.*X/D - 1.0) -
3 ASIN(-1.0)))
C*****
WRITE(61,104) K,X,S
104 FORMAT(1H,11HDEBUG CARD4,3E15.8)
IF(S - S1) 21,22,23
39 A = 3.1415927/D + 8./(D*D)*(R* ASIN(X/R) - D/2.*(ASIN(2.*X/D - 1.)
2 - ASIN(-1.)))
GO TO 41
40 A = 8.0*R/(D*D)*(ASIN(X1/R) - ASIN(0.0))
41 DIM = (D/2.0)/R
C
C PRINT OUT RESULTS AND CONTINUE DO 11.
C
WRITE(61,55)Y,S,A,S1,DIM
55 FORMAT(1H,F9.5,5X,F7.4,11X,E14.6,12X,E14.6,8X,E14.6)
11 CONTINUE
END
AREA3181
AREA3182
AREA3183
AREA3184
AREA3185
AREA3186
AREA3187
AREA3188
AREA3189
AREA3190
AREA3191
AREA3192
AREA3193
AREA3194
AREA3195
AREA3196
AREA3197
AREA3198
AREA3199
AREA3200
AREA3201

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C      SUBROUTINE NEWTON(KODE,KODE2,CHECK,R,D,S1,X2,Y,X)
C      L.T. NOVAK      31 JAN 72
C
C      SUBROUTINE NEWTON DETERMINES THE INTERSECTION OF THE LIQUID
C      INTERFACE WITH VARIOUS CURVES.  FOR KODE = 1, THE CURVE IS THE
C      CURVE  $Y = -(X - D/2)$ .  FOR KODE = 2, THE CURVE IS THE CIRCULAR
C      CROSS-SECTION OF THE CYLINDER,  $(X-D/2)^2 + Y^2 = D^2/4$ .*****
C      ITERATION CONTINUES UNTIL THE NEW VALUE OF SATURATION (S) IS
C      CLOSE ENOUGH (CHECK) TO THE SPECIFIED VALUE (S1).
C
C      MAKE AN INITIAL GUESSE FOR X SUCH THAT NEGATIVE ARGUMENTS IN
C      SQRT DO NOT OCCUR.
C
C      X = X2/2.0
C      I = 0
C      IF(X.LT.R) GO TO 99
C      X = 0.0
C
C      99 IF(KODE.GT.1) GO TO 20
C      21 A = SQRT(R*R - X*X)
C      F = X*(-X + D/2. + A) - 0.5*(X*A + R*R*ASIN(X/R)) - 0.5*(X2*X2 -
C      2 X*X - D*(X2 - X)) - 0.5*((X2 - D/2.)*SQRT(D*X2 - X2*X2) + D*D/4.
C      3 *(ASIN(2.*X2/D - 1.) - ASIN(-1.))) - S1*D*D/37.278338
C      DF = 0.5*(A - (X*X + R*R)/A) - X
C      GO TO 12
C
C      20 A = SQRT(R*R - X*X)
C      F = 0.5*X*A + SQRT(D*X - X*X)*(0.5*X + D/4.) - 0.5*R*R*ASIN(X/R)
C      2 - 0.5*D*D/4.*(ASIN(2.*X/D - 1.) - ASIN(-1.)) - S1*D*D/37.278338
C      DF = 0.5*(A - (X*X - R*R)/A + SQRT(D*X - X*X) - (D/2.))/
C      2 SQRT(1. - (2.*X/D - 1.)*2) + (0.5*X + D/4.)*(D - 2.*X)/(2.*
C      3 SQRT(D*X - X*X))
C      GO TO 12
C
C      12 I = I + 1
C      E = F/DF
C      XN = X - E
C      IF(KODE2.EQ.0) GO TO 40
C      WRITE(61,50) I,XN,KODE

```

1 NEWTN
 2 NEWTN
 3 NEWTN
 4 NEWTN
 5 NEWTN
 6 NEWTN
 7 NEWTN
 8 NEWTN
 9 NEWTN
 10 NEWTN
 11 NEWTN
 12 NEWTN
 13 NEWTN
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 16 NEWTN
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 28 NEWTN
 29 NEWTN
 30 NEWTN
 31 NEWTN
 32 NEWTN
 33 NEWTN
 34 NEWTN
 35 NEWTN
 36 NEWTN

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50 FORMAT(1H ,26HSUB. NEWTON,  ITERATION = ,I3,10X,22HCURRENT VALUE ONEWTN 37
2F XN = ,E20.10,10X,7HKODE = ,I3) NEWTN 38
40 X = XN NEWTN 39
    IF(I.GT.50) GO TO 10 NEWTN 40
    IF(X.LT.R) GO TO 24 NEWTN 41
    X = 0.0 NEWTN 42
24 IF(KODE.GT.1) GO TO 23 NEWTN 43
    S = F*37.278338/(D*D) + S1 NEWTN 44
    Y = ABS(S - S1) NEWTN 45
    WRITE(61,100) S,S1,Y,X,F,DF NEWTN 46
100 FORMAT(1H ,11HDEBUG NEWT1,6E17.8) NEWTN 47
    IF(Y.GT.CHECK) GO TO 21 NEWTN 48
    GO TO 11 NEWTN 49
23 S = F*37.278338/(D*D) + S1 NEWTN 50
    Y = ABS(S - S1) NEWTN 51
    WRITE(61,101) S,S1,Y,X,F,DF NEWTN 52
101 FORMAT(1H ,11HDEBUG NEWT2,6E17.8) NEWTN 53
    IF(Y.GT.CHECK) GO TO 20 NEWTN 54
    GO TO 11 NEWTN 55
10 WRITE(61,51) X,Y,KODE,S NEWTN 56
51 FORMAT(1H0,67HHAVE COMPLETED 50 ITERATIONS AND HAVE NOT CONVERGED NEWTN 57
    2TO ANSWER, X = ,E15.8,2X,8HERROR = ,E15.8,2X,7HKODE = ,I3,/,1H , NEWTN 58
    34HS = ,E20.8) NEWTN 59
11 WRITE(61,52) X,Y,KODE,I,S NEWTN 60
52 FORMAT(1H0,59HLEAVING SUBROUTINE NEWTON, THE ROOT OF THE EQUATION NEWTN 61
    2IS X = ,E15.8,2X,34HERROR IS LESS THAN OR EQUAL TO ,E15.8,/,1H NEWTN 62
    3 ,7HKODE = ,I3,10X,I3,3X,26HITERATIONS WERE COMPLETED.,5X,4HS = , NEWTN 63
    4E20.8,////) NEWTN 64
    RETURN NEWTN 65
    END NEWTN 66

```

APPENDIX F

COMPUTER PROGRAM SUBROUTINES CONTAINING

PHYSICAL PROPERTY DATA

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SUBROUTINE CAPPY(N,S,T,SI)
DIMENSION S(100),T(100),SI(100)
L.T. NOVAK      05 MAY 72  SUBROUTINE CAPPY

SUBROUTINE CAPPY(N,S,T,SI)  CALCULATES AND RETURNS THE CAPILLARY
POTENTIAL SI IN CM. OF WATER FOR A GIVEN VALUE OF SATURATION S AND
TEMPERATURE T.  THE RANGE ON T IS 20. TO 60. DEG.C.
THE DATA OF HANKS ET.AL. SOIL SCI. PROC.,31(593)1967 WAS CURVE
FITTED.  THE CAPILLARY POTENTIAL DATA IS FOR DRYING OF VALENTINE
SAND.  PROFILE AT T=0 WAS USED TO GET CAP. POT. BETWEEN 0.41-1.0

DO 10 I = 1,N
IF(S(I).GE.0.0) GO TO 11
WRITE(61,50) S(I)
50 FORMAT(1H ,13HSATURATION = ,E20.12,3X,37HIN CAPPY  SHOULD STOP THECAPPY 16
2 PROGRAM NOW)
GO TO 12
11 IF(S(I).LE.0.4000) GO TO 12
IF(S(I).GE.0.8000) GO TO 13
SI(I) = -EXP(-.5601216342*S(I) + 4.148781781)
GO TO 20
13 IF(S(I).LT.0.990) GO TO 12
IF(S(I).LT.1.00001) GO TO 14
S(I) = 1.0000
14 SI(I) = -EXP(-275.467338*(S(I) - 1.00000))
GO TO 20
12 SI(I) = -EXP(16.4606 - 146.652*S(I) + 703.828*S(I)*S(I) - 1742.45*CAPPY 28
2S(I)*S(I)*S(I) + 2319.14*S(I)*S(I)*S(I)*S(I) - 1569.01*S(I)*S(I)* 29
3S(I)*S(I)*S(I) + 421.370*S(I)*S(I)*S(I)*S(I)*S(I)*S(I)) 30
20 IF(ABS(T (I) - 25.0).LE.5.0) GO TO 10
X = (76.0292 - 0.162316*T (I))/71.970
SI(I) = SI(I)*(1.0 + 0.081158*ALOG(X))/(1.0 - 0.081158*ALOG(X))
10 CONTINUE
RETURN
END
CAPPY 1
CAPPY 2
CAPPY 3
CAPPY 4
CAPPY 5
CAPPY 6
CAPPY 7
CAPPY 8
CAPPY 9
CAPPY 10
CAPPY 11
CAPPY 12
CAPPY 13
CAPPY 14
CAPPY 15
CAPPY 16
CAPPY 17
CAPPY 18
CAPPY 19
CAPPY 20
CAPPY 21
CAPPY 22
CAPPY 23
CAPPY 24
CAPPY 25
CAPPY 26
CAPPY 27
CAPPY 28
CAPPY 29
CAPPY 30
CAPPY 31
CAPPY 32
CAPPY 33
CAPPY 34
CAPPY 35
CAPPY 36

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```

SUBROUTINE CAPPY(N,S,T,SI)
DIMENSION S(100),T(100),SI(100)
L.T. NOVAK      30 FEB 72  SUBROUTINE CAPPY

SUBROUTINE CAPPY(N,S,T,SI)  CALCULATES AND RETURNS THE CAPILLARY
POTENTIAL SI IN CM. OF WATER FOR A GIVEN VALUE OF SATURATION S AND
TEMPERATURE T.  THE RANGE ON T IS 20. TO 60. DEG.C.
THE DATA OF W.J. STAPLE, SOIL SCI. PROC.,33(840)1969 WAS CURVE
FITTED.  THE CAPILLARY POTENTIAL DATA IS FOR DRYING OF UPLANDS
SAND (78 PERCENT 30 - 100 MESH).

DO 10 I = 1,N
IF(S(I).GE.0.0) GO TO 11
WRITE(61,50) S(I)
50 FORMAT(1H ,13HSATURATION = ,E20.12,3X,37HIN CAPPY  SHOULD STOP  THE
2 PROGRAM NOW)
GO TO 12
11 IF(S(I).LT.1.00001) GO TO 12
S(I) = 1.0000
12 SI(I) = -EXP(16.1309 - 50.6683*S (I) + 72.8620*S (I)**2
2 - 36.0635*S (I)**3)
IF(ABS(T (I) - 25.0).LE.5.0) GO TO 10
X = (76.0292 - 0.162316*T (I))/71.970
SI(I) = SI(I)*(1.0 + 0.081158*ALOG(X))/(1.0 - 0.081158*ALOG(X))
10 CONTINUE
RETURN
END

```

```

SUBROUTINE CAPPR(N,S,SI)
DIMENSION S( 50),SI( 50)
C-----L.T. NOVAK 05 MAY 72
C-----SUBROUTINE CAPPR(N,S,SI)
C-----POTENTIAL SI IN CM. OF WATER FOR A GIVEN VALUE OF SATURATION S.
C-----THE DATA OF HANKS ET.AL.,SOIL SCI.PROC.,31(593)1967 WAS CURVE
C-----FITTED. THE CAPILLARY POTENTIAL DATA IS FOR DRYING OF VALENTINE
C-----SAND
DO 20 I = 1,N
IF(S(I).GE.0.015) GO TO 11
S(I) = 0.015
GO TO 12
11 IF(S(I).LE.0.4000) GO TO 12
IF(S(I).GE.0.8000) GO TO 13
SI(I) = -EXP(-.5601216342*S(I) + 4.148781781)
GO TO 20
13 IF(S(I).LT.0.990) GO TO 12
IF(S(I).LT.1.00001) GO TO 14
S(I) = 1.0000
14 SI(I) = -EXP(-275.467338*(S(I) - 1.00000))
GO TO 20
12 SI(I) = -EXP(16.4606 - 146.652*S(I) + 703.828*S(I)*S(I) - 1742.45*
2S(I)*S(I)*S(I) + 2319.14*S(I)*S(I)*S(I) - 1569.01*S(I)*S(I)*
3S(I)*S(I)*S(I) + 421.370*S(I)*S(I)*S(I)*S(I)*S(I))
20 CONTINUE
RETURN
END
CAPPR 1
CAPPR 2
CAPPR 3
CAPPR 4
CAPPR 5
CAPPR 6
CAPPR 7
CAPPR 8
CAPPR 9
CAPPR 10
CAPPR 11
CAPPR 12
CAPPR 13
CAPPR 14
CAPPR 15
CAPPR 16
CAPPR 17
CAPPR 18
CAPPR 19
CAPPR 20
CAPPR 21
CAPPR 22
CAPPR 23
CAPPR 24
CAPPR 25
CAPPR 26
CAPPR 27

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```

C      SUBROUTINE HYCON(N,S,HCON)
C      DIMENSION S(100),HCON(100)
C
C      L.T. NOVAK      30 FEB 72  SUBROUTINE HYCON
C
C      SUBROUTINE HYCON(N,S,HCON)  CALCULATES AND RETURNS THE HYDRAULIC
C      CONDUCTIVITY IN CM./DAY FOR A GIVEN VALUE OF SATURATION
C      THE DATA OF W.J. STAPLE, SOIL SCI. PROC.,33(840)1969 WAS CURVE
C      FITTED.  THE HYDRAULIC CONDUCTIVITY DATA IS FOR DRYING OF UPLANDS
C      SAND (78 PERCENT 30 - 100 MESH).
C
C      HYDRAULIC CONDUCTIVITY OF STAPLE IS REDUCED 0.1
C
C      DO 20 I = 1,N
C      IF(S(I).GE.0.0) GO TO 10
C      WRITE(61,50) S(I)
C
C      50 FORMAT(1H ,13HSATURATION = ,E20.12,3X,37HIN HYCON  SHOULD STOP THE
C      2 PROGRAM NOW)
C      10 IF(S(I) - 0.410) 8,9,9
C      8 HCON(I) =(EXP(44.2*S (I) - 20.2))*0.1
C      GO TO 20
C      9 IF(S(I) - 0.96) 14,14,15
C      14 HCON(I) =(EXP(-17.1845 + 46.3447*S (I) - 23.9431*S (I)**2))*0.1
C      GO TO 20
C      15 IF(S(I).LT.1.00001) GO TO 16
C      S(I) = 1.0000
C      16 HCON(I) = 18.875522
C      20 CONTINUE
C      RETURN
C      END
HYCON 1
HYCON 2
HYCON 3
HYCON 4
HYCON 5
HYCON 6
HYCON 7
HYCON 8
HYCON 9
HYCON 10
HYCON 11
HYCON 12
HYCON 13
HYCON 14
HYCON 15
HYCON 16
HYCON 17
HYCON 18
HYCON 19
HYCON 20
HYCON 21
HYCON 22
HYCON 23
HYCON 24
HYCON 25
HYCON 26
HYCON 27
HYCON 28
HYCON 29
HYCON 30

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U U U U U U U U U

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SUBROUTINE THCON(N,S,COND)
DIMENSION S(100),COND(100)
C
C L.T. NOVAK      30 FEB 72  SUBROUTINE THCON
C
C SUBROUTINE THCON(N,S,COND)  CALCULATES AND RETURNS THE THERMAL
C-----CONDUCTIVITY IN CAL/CM.DAY.C. FOR A GIVEN VALUE OF SATURATION
C THE DATA OF A.F. MUENCH, PHD THESIS, 69-12533, PP. 74-80, UNIV.
C MICROFILMS WAS CURVE FIT. THE DATA IS FOR A 20-30 MESH OTTAWA
C SAND.
C
DO 16 I = 1,N
IF(S(I).GE.0.0) GO TO 17
WRITE(61,50) S(I)
50 FORMAT(1H ,13HSATURATION = ,E20.12,3X,37HIN THCON  SHOULD STOP THE
2 PROGRAM NOW)
17 IF(S(I) - 0.085) 10,11,11
10 COND(I) = 2842.56*S(I) + 73.44
GO TO 16
11 IF(S(I) - 0.155) 12,12,13
12 COND(I) = 295.488 + 432.00*SQRT(0.205*0.205 - (S(I) - 0.29)**2)
GO TO 16
13 IF(S(I).LT.1.00001) GO TO 14
S(I) = 1.0000
14 COND(I) = 333.504*S(I) + 312.768
16 CONTINUE
RETURN
END
THCON 1
THCON 2
THCON 3
THCON 4
THCON 5
THCON 6
THCON 7
THCON 8
THCON 9
THCON 10
THCON 11
THCON 12
THCON 13
THCON 14
THCON 15
THCON 16
THCON 17
THCON 18
THCON 19
THCON 20
THCON 21
THCON 22
THCON 23
THCON 24
THCON 25
THCON 26
THCON 27
THCON 28

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```

SUBROUTINE HTCAP(N,S,CP)
DIMENSION S(100),CP(100)

L.T. NOVAK      30 FEB 72  SUBROUTINE HTCAP

SUBROUTINE HTCAP(N,S,CP)  CALCULATES AND RETURNS THE HEAT CAPACITY
IN CAL/CM**3DEG.C. FOR A GIVEN VALUE OF SATURATION S.
THE DATA OF A.F. MOENCH, PHD THESIS, 69-12533, PP. 74-80, UNIV.
MICROFILMS WAS CURVE FIT. THE DATA IS FOR A 20-30 MESH OTTAWA
SAND.

DO 12 I = 1,N
IF(S(I).GE.0.0) GO TO 13
WRITE(61,50) S(I)
50 FORMAT(1H,13HSATURATION = ,E20.12,3X,37HIN HTCAP SHOULD STOP THE
2 PROGRAM NOW)
GO TO 10
13 IF(S(I).LT.1.00001) GO TO 10
S(I) = 1.0000
10 CP(I) = 0.309196 + 0.340390*S(I)
12 CONTINUE
RETURN
END

```

```

C      SUBROUTINE EQXW(N,S,T,XWS)
C      DIMENSION S(100),T(100),XWS(100),SI(100)
C
C      L.T. NOVAK      30 FEB 72  SUBROUTINE EQXW
C
C      SUBROUTINE EQXW CALCULATES AND RETURNS THE EQUILIBRIUM MOLE
C      FRACTION OF WATER IN THE GAS PHASE.  THE EQUILIBRIUM MOLE FRACTION
C      IS A FUNCTION OF SATURATION AND TEMPERATURE.  VAPOR PRESSURE DATA
C      FROM THE HDBK. OF CHEM. AND PHYSICS, 46TH ED., PAGES E7-E8 WAS
C      CURVE FIT AS  $\ln(P/760) = A + B(1/T) + C(1/T^2)$ .  THIS DATA WAS
C      FIT OVER THE RANGE 20-70 DEG.C.  THE TOTAL PRESSURE IN THE GAS
C      PHASE IS 1 ATM. OR 760 MM. HG.
C
C      THE MODIFIED CLAPEYRON EQUATION.
C
C      DO 20 I = 1,N
C      IF(S(I).GE.0.0) GO TO 12
C      WRITE(61,50) S(I)
C      50 FORMAT(1H,13HSATURATION = ,E20.12,3X,37HIN EQXW  SHOULD STOP THEEQXW
C      2 PROGRAM NOW)
C      GO TO 13
C      12 IF(S(I).LT.1.00001) GO TO 13
C      S(I) = 1.0000
C      13 IF(5.416580111E-08.GT.5.499032E-06*(1./(273.15+T(I)))) GO TO 11
C      WRITE(61,52) S(I),T(I)
C      52 FORMAT(1H0,54HIN SUBROUTINE EQXW, NEGATIVE ARGUMENT IN SQRT, S, T
C      2= ,2E15.8)
C      GO TO 20
C      11 XWS(I) = EXP(-72.20849051 + (SQRT(5.416580111E-08 - 5.499032E-06*
C      2 (1./(273.15 + T(I)))))/2.749516E-06)
C
C      THE POYNTING EQUATION - FOR CORRECTING FOR BOUND WATER.
C
C      CALL CAPPY(N,S,T,SI)
C      XWS(I) = XWS(I)*EXP(2.14397578E-04*SI(I)/(273.15 + T(I)))
C      20 CONTINUE

```

RETURN
END

EQXW 37
EQXW 38

U U U U U U U U

APPENDIX G
COMPUTER PROGRAM FOR NUMERICAL SOLUTION
TO THE GENERAL MODEL


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C SUBROUTINE HTCAP(N,S,CP) GRIND 37
C SUBROUTINE THCON(N,S,COND) GRIND 38
C SUBROUTINE DELVP(N,T,DELV) GRIND 39
C GRIND 40
C ***** GRIND 41
C INPUT INFORMATION GRIND 42
C GRIND 43
C GRIND 44
C THE FIRST READ STATEMENT ENABLES THE USER TO READ IN VERBAL GRIND 45
C INFORMATION IN THE 20A4 FORMAT. THE VARIABLE MTINF(20) IS USED TOGRIND 46
C PRINT OUT THIS INFORMATION. THE SECOND READ STATEMENT IS USED TO GRIND 47
C INPUT THE VARIABLE FORMAT INFORMATION. THE VARIABLE FORMATS ARE GRIND 48
C MT11, MT12, MT13, MT14. THE VARIABLE FORMATS ARE USED TO ENABLE GRIND 49
C THE USER TO SPECIFY THE FORMATS USED FOR READING IN THE PHYSICAL GRIND 50
C PARAMETERS, BOUNDARY CONDITIONS, NUMERICAL INFORMATION, AND GRIND 51
C INITIAL CONDITIONS. IF IT IS DESIRED TO SPECIFY THE RATIO OF GRIND 52
C DELT TO DELZ, READ IN KODE1 AS 0. GRIND 53
C KODE2 SPECIFIES HOW OFTEN THE PROFILES ARE TO BE PRINTED OUT. FORGRIND 54
C EXAMPLE, IF KODE2 = 5, THE PROFILES WILL BE PRINTED OUT EVERY FIVEGRIND 55
C TIME ITERATIONS. GRIND 56
C NSTOP SPECIFIES THE ITERATION NUMBER AT WHICH THE ITERATION ON GRIND 57
C TIME WILL STOP. GRIND 58
C GRIND 59
C ***** GRIND 60
C DEFINITIONS OF COMPUTER VARIABLES GRIND 61
C ----- GRIND 62
C GRIND 63
C GRIND 64
C GRIND 65
C GRIND 66
C GRIND 67
C GRIND 68
C GRIND 69
C GRIND 70
C GRIND 71
C GRIND 72

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C-----A(I) INTERFACIAL AREA BETWEEN GAS AND LIQUID PHASES (1/CM)
 C-----C(I) CONCENTRATION DIVIDED BY P/R = $XW(I)*(1 - S(I))/T(I)$
 C-----COND(I) EFFECTIVE THERMAL CONDUCTIVITY OF THE POROUS MEDIA
 (CAL/CM-DAY-DEG.C.)
 C-----CL COLUMN LENGTH (CM)

C-----DELT	TIME INCREMENT SIZE (DAYS)	GRIND 73
C-----DELV(I)	HEAT OF VAPORIZATION OF WATER (CAL/GM)	GRIND 74
C-----DELZ	SPACE INCREMENT SIZE (CM)	GRIND 75
C-----DI	INSIDE COLUMN DIAMETER (CM)	GRIND 76
C-----DO	OUTSIDE COLUMN DIAMETER (CM)	GRIND 77
C-----DOR	ORDINARY DIFFUSION COEFFICIENT FOR WATER IN AIR AT 0 CENT	GRIND 78
C	(CM**2/DAY)	GRIND 79
C-----DORD	ORDINARY DIFFUSION COEFFICIENT FOR WATER IN AIR AS A	GRIND 80
C	FUNCTION OF TEMPERATURE (CM**2/DAY)	GRIND 81
C-----EPS	POROSITY OF POROUS MEDIA (DIM)	GRIND 82
C-----EVAPO	EVAPORATION DRIVING FORCE (XWS(I) - XW(I))	GRIND 83
C-----FILMH	FILM HEAT TRANSFER COEFFICIENT AT THE INTERFACE BETWEEN	GRIND 84
C	THE ATMOSPHERE AND POROUS MEDIA (CAL/CM**2-DAY-DEG.C)	GRIND 85
C-----FILMK	FILM MASS TRANSFER COEFFICIENT AT THE INTERFACE BETWEEN	GRIND 86
C	THE ATMOSPHERE AND POROUS MEDIA (CM/DAY)	GRIND 87
C-----HCON(I)	HYDRAULIC CONDUCTIVITY (CM/DAY)	GRIND 88
C-----I	DO LOOP INTEGER REPRESENTING THE SPACE INCREMENT NUMBER	GRIND 89
C-----J	DO LOOP INTEGER REPRESENTING THE TIME INCREMENT NUMBER	GRIND 90
C-----KOVE	OVER ALL MASS TRANSFER COEFFICIENT BETWEEN THE GAS AND	GRIND 91
C	LIQUID PHASES IN THE POROUS MEDIA AT 25 C. (CM/DAY)	GRIND 92
C-----KOVER	OVER ALL MASS TRANSFER COEFFICIENT BETWEEN THE GAS AND	GRIND 93
C	LIQUID PHASES IN THE POROUS MEDIA AS A FUNCTION OF	GRIND 94
C	TEMPERATURE (CM/DAY)	GRIND 95
C-----M	THE MAXIMUM NUMBER OF TIME INCREMENTS	GRIND 96
C-----MWT	MOLECULAR WEIGHT OF WATER (GM/GM-MOLES)	GRIND 97
C-----N	NUMBER OF SPACE INCREMENTS	GRIND 98
C-----NG(I)	WATER FLUX IN GAS PHASE DIVIDED BY P/R	GRIND 99
C-----NW	WATER FLUX IN GAS PHASE (GM/CM**2-DAY)	GRIND 100
C-----P	PRESSURE IN GAS PHASE (ATM)	GRIND 101
C-----Q(I)	CONDUCTIVE ENERGY FLUX IN POROUS MEDIA (OR SOIL)	GRIND 102
C-----QR	RADIATIVE ENERGY FLUX (CAL/CM**2-DAY)	GRIND 103
C-----R	GAS LAW CONSTANT (ATM-CM**3/GM-MOLE-DEG.K.)	GRIND 104
C-----RATIO	RATIO = DELT/DELZ (DIM)	GRIND 105
C-----S(I)	SATURATION OF POROUS MEDIA (OR SOIL)	GRIND 106
C-----SI(I)	CAPILLARY POTENTIAL (CM)	GRIND 107
C-----ST	MAXIMUM SIMULATION TIME (DAYS)	GRIND 108

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C-----TA      AMBIENT TEMPERATURE (DEG.C.)
C-----T(I)     TEMPERATURE OF POROUS MEDIA (OR SOIL)
C-----UOVER    OVER ALL HEAT TRANSFER COEFFICIENT AT THE COLUMN WALL
C              (CAL/CM**2-DAY-DEG.C.)
C-----V(I)     VOLUMETRIC FLUX OF LIQUID WATER IN POROUS MEDIA (OR SOIL)GRINDI109
C-----VSEPS    LIQUID WATER FLUX IN POROUS MEDIA (GM/CM**2-DAY)GRINDI110
C-----XWA      AMBIENT MOLE FRACTION OF WATER (DIM)GRINDI111
C-----XW(I)     MOLE FRACTION OF WATER IN THE GAS PHASE OF POROUS MEDIA (GRINDI112
C-----XWS(I)    EQUILIBRIUM MOLE FRACTION OF WATER IN THE GAS PHASE OF GRINDI113
C               POROUS MEDIA (DIM)GRINDI114
C-----Z        SPACE VARIABLE (CM)GRINDI115
C             C*****GRINDI116
C*****GRINDI117
C*****GRINDI118
C*****GRINDI119
C*****GRINDI120
C*****GRINDI121
C*****GRINDI122
C*****GRINDI123
C*****GRINDI124
C          REAL KOVE,KOVER,MWT,NG,NW
C          DIMENSION A( 50),C( 50),COND( 50),DELV( 50),HCON( 50),NG( 50),
C            Q( 50),S( 50),SI( 50),T( 50),V( 50),XW(50),XWS( 50),CP( 50)
C            DIMENSION MTI1(20),MTI2(20),MTI3(20),MTI4(20),MTINF(20)
C            EXTERNAL SQRT,EXP,ALOG,ABS
C
C-----READ IN AND PRINT GENERAL INFORMATION
C
C       DO 29 JIN = 1,7
C         READ(60,1001) MTINF
C           29 WRITE(61,1001) MTINF
C             1001 FORMAT(20A4)
C
C-----READ IN AND PRINT VARIABLE FORMAT INFORMATION
C
C       READ(60,1002) MTI1,MTI2,MTI3,MTI4
C         1002 FORMAT(20A4)
C         WRITE(61,1009) MTI1,MTI2,MTI3,MTI4
C         1009 FORMAT('HO,53THE FOLLOWING IS THE VARIABLE FORMAT INFORMATION REAGRNDI144
```

```

2D,/1H0,7HMT11 = ,20A4,/1H0,7HMT12 = ,20A4,/1H0,7HMT13 = ,20A4,
3 /1H0,7HMT14 = ,20A4)
C
C-----READ IN AND PRINT PHYSICAL PARAMETERS FOR SYSTEM
C
      READ(60,MT11) CL,DO,DI,EPS,DOR,KOVE,P,MWT,R
      WRITE(61,1003) CL,DO,DI,EPS,DOR,KOVE,P,MWT,R
1003 FORMAT(1H1,62H THE FOLLOWING IS A LIST OF PHYSICAL PARAMETERS FOR TGRIND152
2HE SYSTEM.,//1H0,19HCOLUMN LENGTH (CM.),28X,E15.8,/1H0,15HCOLUMN OGRIND153
3D (CM.),32X,E15.8,/1H0,15HCOLUMN ID (CM.),32X,E15.8,/1H0,15HPOROSIGRIND154
4TY (DIM.),32X,E15.8,/1H0,46HORDINARY DIFFUSION COEF. AIR-WATER (CMGRIND155
5**2/DAY),E16.8,/1H0,35H OVER ALL MASS TRANSFER COEF.(1/DAY),E27.8,/GRIND156
61H0,15HPRESSURE (ATM.),E47.8,/1H0,22HMOLECULAR WT. OF WATER,E40.8,GRIND157
7/1H0,37HGAS CONSTANT (CC.-ATM/GM.MOLE-DEG.K.),E25.8,////////)
      WRITE(61,1000)
GRIND158
GRIND159
GRIND160
GRIND161
GRIND162
GRIND163
GRIND164
1004 FORMAT(1H0,46H THE FOLLOWING IS A LIST OF BOUNDARY CONDITIONS,//1H0GRIND165
2,28H AMBIENT TEMPERATURE (DEG.C.),E45.8,/1H0,43H AMBIENT MOLE FRACTIGRIND166
3ON OF WATER VAPOR (DIM.),E30.8,/1H0,30H RADIATION FLUX (CAL/CM**2-DGRIND167
4AY),E43.8,/1H0,56H WALL OVER ALL HEAT TRANSFER COEF. (CAL/CM**2-DAYGRIND168
5-DEG.C.),E17.8,/1H0,28H FILMH (CAL./CM.**2-DAY-DEG.),E45.8)
      WRITE(61,1000)
GRIND169
GRIND170
1000 FORMAT (1H0,120H*****GRIND171
2*****GRIND172
3***,/)
GRIND173
GRIND174
GRIND175
GRIND176
GRIND177
GRIND178
GRIND179
GRIND180
C
C-----READ IN AND PRINT NUMERICAL INFORMATION
C
      READ(60,1011) NSTOP
1011 FORMAT(I9)
      READ(60,MT13) KODE1,KODE2,RATIO,N,M,ST
      IF(KODE1.EQ.0) GO TO 10

```

```

XN = N
XM = M
DELZ = CL/XN
DELT = ST/XM
RATIO = DELT/DELZ
GO TO 11
10 XN = N
DELZ = CL/XN
DELT = DELZ*RATIO
XM = ST/DELT
M = XM
11 WRITE(61,1007) ST,DELT,M,CL,DELZ,N,RATIO
1007 FORMAT(1H1,21HNUMERICAL INFORMATION,//1H0,30HMAXIMUM SIMULATION TIGRIND192
2ME (DAYS),E20.8,/1H0,29HSIZE OF TIME INCREMENT (DAYS),E21.8,/1H0,2GRIND193
39HTHE NUMBER OF TIME INCREMENTS,I21,/1H0,19HCOLUMN LENGTH (CM.),E3GRIND194
41.8,/1H0,29HSIZE OF SPACE INCREMENT (CM.),E21.8,/1H0,26HNUMBER OF GRIND196
5SPACE INCREMENTS,I24,/1H0,21HRAIO OF DELT TO DELZ,E29.8)
WRITE(61,1000)
C
C-----READ IN AND PRINT OUT INITIAL CONDITIONS
C
READ(60,MT14) (S(I),I=1,N),(T(I),I=1,N),(XW(I),I=1,N)
WRITE(61,1005)
1005 FORMAT(1H1,52HTHE FOLLOWING IS A LISTING OF THE INITIAL CONDITIONSGRIND204
2,/1H,52H*** ***** ** * ***** ** *** ***** //1HGRIND205
30,9HINCREMENT,11X,8HPOSITION,12X,10HSATURATION,10X,11HTEMPERATURE,GRIND206
49X,28HMOLE FRACTION OF WATER VAPOR,/1H,28X,5H(CM.),14X,6H(DIM.), GRIND207
511X,8H(DEG.C.),15X,6H(DIM.))
WRITE(61,1000)
DO 20 ID = 1,N
C(ID) = XW(ID)*(1.0000 - S(ID))/(273.15 + T(ID))
Z = ID - 1
Z = DELZ*Z
20 WRITE(61,1006) ID,Z,S(ID),T(ID),XW(ID)
1006 FORMAT(10,6X,E20.13,4X,3E23.13)
C
GRIND181
GRIND182
GRIND183
GRIND184
GRIND185
GRIND186
GRIND187
GRIND188
GRIND189
GRIND190
GRIND191
GRIND192
GRIND193
GRIND194
GRIND195
GRIND196
GRIND197
GRIND198
GRIND199
GRIND200
GRIND201
GRIND202
GRIND203
GRIND204
GRIND205
GRIND206
GRIND207
GRIND208
GRIND209
GRIND210
GRIND211
GRIND212
GRIND213
GRIND214
GRIND215
GRIND216

```

```

C-----PRINT OUT TITLE PAGE FOR FINITE DIFFERENCE CALCULATIONS
C
      WRITE(61,1008)
      1008 FORMAT(1H1,5HTIME ,5X,8HPOSITION,6X,10HSATURATION,4X,11HTEMPERATURE,GRIND217
      2E,2X,12HMOLE FRAC OF,2X,14HEQLB MOLE FRAC,3X,11HLIQUID FLUX,4X,10HGRIND218
      3VAPOR FLUX,5X,11HENERGY FLUX,/1H ,6HINCRT,45X,11HWATER VAPOR,/1H ,GRIND219
      412X,4H(CM),10X,5H(DIM),8X,8H(DEG.C.),9X,5H(DIM),10X,5H(DIM),3X,14HGRIND220
      5(GM/CM**2-DAY),3X,14H(GM/CM**2-DAY),2X,15H(CAL/CM**2-DAY),//) GRIND221
      GRIND222
      GRIND223
      GRIND224
      GRIND225
      GRIND226
      GRIND227
      GRIND228
      GRIND229
      GRIND230
      GRIND231
      GRIND232
      GRIND233
      GRIND234
      GRIND235
      GRIND236
      GRIND237
      GRIND238
      GRIND239
      GRIND240
      GRIND241
      GRIND242
      GRIND243
      GRIND244
      GRIND245
      GRIND246
      GRIND247
      GRIND248
      GRIND249
      GRIND250
      GRIND251
      GRIND252

      A11 = KOVE*P*MWT/(EPS*R)
      A2 = P*EPS/R*18.0
      A33 = KOVE/EPS
      A4 = 4.0*DO*UOVER/(DI*DI)

      C-----BEGIN FINITE DIFFERENCE CALCULATIONS USING FIRST ORDER FORWARD
      C-----DIFFERENCE FORMULA ON TIME
      C
      CODE3 = CODE2
      DO 28 J = 1,M
      IF(J.GT.NSTOP) GO TO 6969
      CALL CAPPY (N,S,T,SI)
      CALL HYCON (N,S,HCON)
      CALL EQXW (N,S,T,XWS)
      CALL AREA (N,S,A)
      CALL HTCAP (N,S,CP)
      CALL THCON (N,S,COND)
      CALL DELVP (N,T,DELV)

      C-----BEGIN SPACE ITERATIONS.
      C
      DO 12 I = 1,N
      IF(I.NE.1) GO TO 13

```

```

C-----SPECIFY BOUNDARY CONDITION AT SURFACE
C
FILMK = 4.1000E+03*FILMH
DORD = DOR*((2.7315E+02 + T(I+1))/2.7315E+02)*1.75E+00
V(I) = 0.0000E+00
NG(I) = FILMK/(EPS*(2.7315E+02 + T(I)))*(XWA - XW(I))
Q(I) = QR + FILMH*(TA - T(I))
IF(S(I+1).LT.1.0000) GO TO 30
V(I+1) = 0.0000E+00
GO TO 31
30 V(I+1) = -HCON(I+1)/EPS*((SI(I+1) - SI(I))/DELZ - 1.000E+00)
31 NG(I+1) = -DORD*(1.000E+00 - S(I+1))/((2.7315E+02 + T(I+1))*(1.000E+00
  2 E+00 - XW(I+1)))*(XW(I+1) - XW(I))/DELZ
  Q(I+1) = -COND(I+1)*(T(I+1) - T(I))/DELZ
  GO TO 15
13 IF(I.NE.N) GO TO 14
C-----SPECIFY BOUNDARY CONDITIONS AT BOTTOM OF COLUMN
C
V(I+1) = 0.0000E+00
NG(I+1) = 0.0000E+00
Q(I+1) = 0.0000E+00
GO TO 15
16 IF(S(I).LT.1.0000E+00) GO TO 34
V(I) = 0.0000E+00
GO TO 35
34 V(I) = -HCON(I)/EPS*((SI(I) - SI(I-1))/DELZ - 1.000E+00)
35 DORD = DOR*((2.7315E+02 + T(I))/2.7315E+02)*1.75E+00
NG(I) = -DORD*(1.000E+00 - S(I))/((2.7315E+02 + T(I))*(1.000E+00
  2 - XW(I)))*(XW(I) - XW(I-1))/DELZ
  Q(I) = -COND(I)*(T(I) - T(I-1))/DELZ
  GO TO 15
14 IF(S(I+1).LT.1.0000E+00) GO TO 32
V(I+1) = 0.0000E+00
GO TO 33
GRIND253
GRIND254
GRIND255
GRIND256
GRIND257
GRIND258
GRIND259
GRIND260
GRIND261
GRIND262
GRIND263
GRIND264
GRIND265
GRIND266
GRIND267
GRIND268
GRIND269
GRIND270
GRIND271
GRIND272
GRIND273
GRIND274
GRIND275
GRIND276
GRIND277
GRIND278
GRIND279
GRIND280
GRIND281
GRIND282
GRIND283
GRIND284
GRIND285
GRIND286
GRIND287
GRIND288

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32 V(I+1) = -HCON(I+1)/EPS*((SI(I+1) - SI(I))/DELZ - 1.0000E+00) GRIND289
33 DORD = DOR*((2.7315E+02 + T(I+1))/2.7315E+02)*1.75E+00 GRIND290
    NG(I+1) = -DORD*(1.0000E+00 - S(I+1))/((2.7315E+02 + T(I+1))*(1.00 GRIND291
200E+00 - XW(I+1))*(XW(I+1) - XW(I))/DELZ GRIND292
    Q(I+1) = -COND(I+1)*(T(I+1) - T(I))/DELZ GRIND293
C-----CALCULATE VARIABLES AT THE NEXT TIME INCREMENT GRIND294
C GRIND295
C GRIND296
15 EVAPO = XWS(I) - XW(I) GRIND297
    DCALC = ((2.7315E+02 + T(I))/2.7315E+02)*1.75E+00 GRIND298
    A1 = A11*DCALC GRIND299
    A3 = A33*DCALC GRIND300
    A5 = A1*EPS GRIND301
    S(I) = S(I) - DELT*((V(I+1) - V(I))/DELZ + A1*(A(I)/(2.7315E+02 + GRIND302
2 T(I))*EVAPO) GRIND303
    C(I) = C(I) - DELT*((NG(I+1) - NG(I))/DELZ - A3*A(I)/(2.7315E+02 GRIND304
2 + T(I))*EVAPO) GRIND305
    T(I) = T(I) - DELT/CP(I)*((Q(I+1) - Q(I))/DELZ + A4*(T(I) - TA) GRIND306
2 + DELV(I)*A(I)*A5/(2.7315E+02 + T(I))*EVAPO) GRIND307
    IF(S(I).LT.1.0000E+00) GO TO 48 GRIND308
    XW(I) = XWS(I) GRIND309
    GO TO 49 GRIND310
48 XW(I) = C(I)*(2.7315E+02 + T(I))/(1.0000E+00 - S(I)) GRIND311
49 IF(KODE2.EQ.1) GO TO 19 GRIND312
    IF(J - KODE3.NE.0) GO TO 12 GRIND313
    IF(I.NE.N) GO TO 19 GRIND314
    KODE3 = KODE2 + J GRIND315
19 VSEPS = EPS*V(I) GRIND316
    NW = A2*NG(I) GRIND317
    ZS = I - 1 GRIND318
    Z = DELZ*ZS GRIND319
C-----PRINT OUT CALCULATED VALUES GRIND320
C GRIND321
C GRIND322
1010 WRITE(61,1010) J,Z,S(I),T(I),XW(I),XWS(I),VSEPS,NW,Q(I) GRIND323
    1010 FORMAT(1H ,19,E15.8,4E24.14,/1H ,24X,3E24.14) GRIND324

```

```
IF(I.NE.N) GO TO 12
WRITE(61,1000)
12 CONTINUE
28 CONTINUE
6969 WRITE(61,1012) J
1012 FORMAT(1H0,25HNORMAL TERMINATION, J = ,I9,11HITERATIONS.)
END
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GRIND325
GRIND326
GRIND327
GRIND328
GRIND329
GRIND330
GRIND331
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APPENDIX H
COMPUTER PROGRAM FOR NUMERICAL SOLUTION
TO THE PHILIP AND DE VRIES MODEL

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PROGRAM PHILP(INPUT,OUTPUT,TAPE60=INPUT,TAPE61=OUTPUT)
C-----L.T. NOVAK 28 MARCH 72
C-----PROGRAM SOLVES THE EQUATIONS OF PHILP AND DE VRIES
C-----PRINT MODIFIED FROM PROGRAM PHILP SEQUENCE NO. 176
C-----FORCED CONVECTION PROBLEM
C-----TIME VARYING BOUNDARY CONDITION PROBLEM..TIME ZERO CORRESPONDS TO 1200 HRS
C
C
C THIS PROGRAM SOLVES THE FOLLOWING MATHEMATICAL PROBLEM BY THE
C METHOD OF FINITE DIFFERENCE.
C
C
C 
$$\frac{\partial S}{\partial t} = -\frac{\partial}{\partial z} \left( \rho_e V^0 + \tilde{N}_w M_w \right)$$

C
C 
$$C \frac{\partial T}{\partial t} = -\frac{\partial q}{\partial z} - \frac{\partial \tilde{N}_w}{\partial z} \Delta H_{vap} M_w - 4 D_0 U_0 \frac{(T-T_a)}{D_i^2}$$

C
C 
$$V^0 = -k \left( \frac{dy}{dz} - 1 \right), \tilde{N}_w = -\frac{D_{aw} Pe(1-S)}{RT(1-\tilde{x}_w)}, q = -k_e \frac{\partial T}{\partial z}$$

C
C
C THE ABOVE EQUATIONS ARE A MATHEMATICAL MODEL FOR TWO PHASE
C MOVEMENT OF WATER IN POROUS MEDIA. THE ACTUAL PROBLEM BEING
C SIMULATED IS THE RADIATION DRYING OF SAND IN A LAB COLUMN.
C
C *****
C
C THE FOLLOWING SUBROUTINES ARE NECESSARY TO RUN PROGRAM. EACH
C SUBROUTINE IS DOCUMENTED.
C
C SUBROUTINE CAPPY(N,S,T,SI)
C SUBROUTINE HYCON(N,S,HCON)
C

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C SUBROUTINE EQXW(N,S,T,XWS) PHILP 36
C SUBROUTINE AREA(N,S,A) PHILP 37
C SUBROUTINE HTCAP(N,S,CP) PHILP 38
C SUBROUTINE THCON(N,S,COND) PHILP 39
C SUBROUTINE DELVP(N,T,DELV) PHILP 40
C ***** PHILP 41
C ***** PHILP 42
C INPUT INFORMATION PHILP 43
C PHILP 44
C PHILP 45
C THE FIRST READ STATEMENT ENABLES THE USER TO READ IN VERBAL PHILP 46
C INFORMATION IN THE 20A4 FORMAT. THE VARIABLE MTINF(20) IS USED TO PHILP 47
C PRINT OUT THIS INFORMATION. THE SECOND READ STATEMENT IS USED TO PHILP 48
C INPUT THE VARIABLE FORMAT INFORMATION. THE VARIABLE FORMATS ARE PHILP 49
C MT11, MT12, MT13, MT14. THE VARIABLE FORMATS ARE USED TO ENABLE PHILP 50
C THE USER TO SPECIFY THE FORMATS USED FOR READING IN THE PHYSICAL PHILP 51
C PARAMETERS, BOUNDARY CONDITIONS, NUMERICAL INFORMATION, AND PHILP 52
C INITIAL CONDITIONS. IF IT IS DESIRED TO SPECIFY THE RATIO OF PHILP 53
C DELT TO DELZ, READ IN KODE1 AS 0. PHILP 54
C KODE2 SPECIFIES HOW OFTEN THE PROFILES ARE TO BE PRINTED OUT. PHILP 55
C EXAMPLE, IF KODE2 = 5, THE PROFILES WILL BE PRINTED OUT EVERY FIVE PHILP 56
C TIME ITERATIONS. PHILP 57
C NSTOP SPECIFIES THE ITERATION NUMBER AT WHICH THE ITERATION ON PHILP 58
C TIME WILL STOP. PHILP 59
C ***** PHILP 60
C ***** PHILP 61
C ***** PHILP 62
C DEFINITIONS OF COMPUTER VARIABLES PHILP 63
C ----- PHILP 64
C PHILP 65
C COMPUTER VARIABLE PHILP 66
C ----- PHILP 67
C PHILP 68
C-----A(I) INTERFACIAL AREA BETWEEN GAS AND LIQUID PHASES (1/CM) PHILP 69
C-----C(I) CONCENTRATION DIVIDED BY P/R = XW(I)*(1 - S(I))/T(I) PHILP 70
C-----COND(I) EFFECTIVE THERMAL CONDUCTIVITY OF THE POROUS MEDIA PHILP 71

```

C	(CAL/CM-DAY-DEG.C.)	PHILP 72
C-----CL	COLUMN LENGTH (CM)	PHILP 73
C-----DELT	TIME INCREMENT SIZE (DAYS)	PHILP 74
C-----DELV(I)	HEAT OF VAPORIZATION OF WATER (CAL/GM)	PHILP 75
C-----DELZ	SPACE INCREMENT SIZE (CM)	PHILP 76
C-----DI	INSIDE COLUMN DIAMETER (CM)	PHILP 77
C-----DO	OUTSIDE COLUMN DIAMETER (CM)	PHILP 78
C-----DOR	ORDINARY DIFFUSION COEFFICIENT FOR WATER IN AIR AT 0 CENT	PHILP 79
C	(CM**2/DAY)	PHILP 80
C-----DORD	ORDINARY DIFFUSION COEFFICIENT FOR WATER IN AIR AS A	PHILP 81
C	FUNCTION OF TEMPERATURE (CM**2/DAY)	PHILP 82
C-----EPS	POROSITY OF POROUS MEDIA (DIM)	PHILP 83
C-----EVAPO	EVAPORATION DRIVING FORCE (XWS(I) - XW(I))	PHILP 84
C-----FILMH	FILM HEAT TRANSFER COEFFICIENT AT THE INTERFACE BETWEEN	PHILP 85
C	THE ATMOSPHERE AND POROUS MEDIA (CAL/CM**2-DAY-DEG.C)	PHILP 86
C-----FILMK	FILM MASS TRANSFER COEFFICIENT AT THE INTERFACE BETWEEN	PHILP 87
C	THE ATMOSPHERE AND POROUS MEDIA (CM/DAY)	PHILP 88
C-----HCON(I)	HYDRAULIC CONDUCTIVITY (CM/DAY)	PHILP 89
C-----I	DO LOOP INTEGER REPRESENTING THE SPACE INCREMENT NUMBER	PHILP 90
C-----J	DO LOOP INTEGER REPRESENTING THE TIME INCREMENT NUMBER	PHILP 91
C-----KOVE	OVER ALL MASS TRANSFER COEFFICIENT BETWEEN THE GAS AND	PHILP 92
C	LIQUID PHASES IN THE POROUS MEDIA AT 25 C. (CM/DAY)	PHILP 93
C-----KOVER	OVER ALL MASS TRANSFER COEFFICIENT BETWEEN THE GAS AND	PHILP 94
C	LIQUID PHASES IN THE POROUS MEDIA AS A FUNCTION OF	PHILP 95
C	TEMPERATURE (CM/DAY)	PHILP 96
C-----M	THE MAXIMUM NUMBER OF TIME INCREMENTS	PHILP 97
C-----MWT	MOLECULAR WEIGHT OF WATER (GM/GM-MOLES)	PHILP 98
C-----N	NUMBER OF SPACE INCREMENTS	PHILP 99
C-----NG(I)	WATER FLUX IN GAS PHASE DIVIDED BY P/R	PHILP100
C-----NW	WATER FLUX IN GAS PHASE (GM/CM**2-DAY)	PHILP101
C-----P	PRESSURE IN GAS PHASE (ATM)	PHILP102
C-----Q(I)	CONDUCTIVE ENERGY FLUX IN POROUS MEDIA (OR SOIL)	PHILP103
C-----QR	RADIATIVE ENERGY FLUX (CAL/CM**2-DAY)	PHILP104
C-----R	GAS LAW CONSTANT (ATM-CM**3/GM-MOLE-DEG.K.)	PHILP105
C-----RATIO	RATIO = DELT/DELZ (DIM)	PHILP106
C-----S(I)	SATURATION OF POROUS MEDIA (OR SOIL)	PHILP107

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C-----SI(I)      CAPILLARY POTENTIAL (CM)      PHILP108
C-----ST      MAXIMUM SIMULATION TIME (DAYS)      PHILP109
C-----TA      AMBIENT TEMPERATURE (DEG.C.)      PHILP110
C-----T(I)      TEMPERATURE OF POROUS MEDIA (OR SOIL)      PHILP111
C-----UOVER      OVER ALL HEAT TRANSFER COEFFICIENT AT THE COLUMN WALL      PHILP112
C      (CAL/CM**2-DAY-DEG.C.)      PHILP113
C-----V(I)      VOLUMETRIC FLUX OF LIQUID WATER IN POROUS MEDIA (OR SOIL)      PHILP114
C-----VSEPS      LIQUID WATER FLUX IN POROUS MEDIA (GM/CM**2-DAY)      PHILP115
C-----XWA      AMBIENT MOLE FRACTION OF WATER (DIM)      PHILP116
C-----XW(I)      MOLE FRACTION OF WATER IN THE GAS PHASE OF POROUS MEDIA      PHILP117
C-----XWS(I)      EQUILIBRIUM MOLE FRACTION OF WATER IN THE GAS PHASE OF      PHILP118
C      POROUS MEDIA (DIM)      PHILP119
C-----Z      SPACE VARIABLE (CM)      PHILP120
C      PHILP121
C*****      PHILP122
C*****      PHILP123
C*****      PHILP124
C      PHILP125
      REAL KOVE,KOVER,MWT,NG,NW      PHILP126
      DIMENSION      C( 50),COND( 50),DELV( 50),HCON( 50),NG( 50),      PHILP127
      2 Q( 50),S( 50),SI( 50),T( 50),V( 50),XW(50),XWS( 50),CP( 50)      PHILP128
      DIMENSION MTI1(20),MTI2(20),MTI3(20),MTI4(20),MTINF(20)      PHILP129
      EXTERNAL SORT,EXP,ALOG,ABS      PHILP130
C      PHILP131
C-----READ IN AND PRINT GENERAL INFORMATION      PHILP132
C      PHILP133
      DO 29 JIN = 1,7      PHILP134
      READ(60,1001) MTINF      PHILP135
      1001 FORMAT(20A4)      PHILP136
      29 WRITE(61,1001) MTINF      PHILP137
C      PHILP138
C-----READ IN AND PRINT VARIABLE FORMAT INFORMATION      PHILP139
C      PHILP140
      READ(60,1002) MTI1,MTI2,MTI3,MTI4      PHILP141
      1002 FORMAT(20A4)      PHILP142
      WRITE(61,1009) MTI1,MTI2,MTI3,MTI4      PHILP143

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1009 FORMAT(1H0,53H THE FOLLOWING IS THE VARIABLE FORMAT INFORMATION REAPHILP144
2D,/1H0,7HMTI1 = ,20A4,/1H0,7HMTI2 = ,20A4,/1H0,7HMTI3 = ,20A4,
3 /1H0,7HMTI4 = ,20A4)
C
C-----READ IN AND PRINT PHYSICAL PARAMETERS FOR SYSTEM
C
      READ(60,MTI1) CL,DO,DI,EPS,DOR,KOVE,P,MWT,R
      WRITE(61,1003) CL,DO,DI,EPS,DOR,KOVE,P,MWT,R
1003 FORMAT(1H1,62H THE FOLLOWING IS A LIST OF PHYSICAL PARAMETERS FOR
2HE SYSTEM.,/1H0,19HCOLUMN LENGTH (CM.),28X,E15.8,/1H0,15HCOLUMN OPHILP153
3D (CM.),32X,E15.8,/1H0,15HCOLUMN ID (CM.),32X,E15.8,/1H0,15HPOROSIPHILP154
4TY (DIM.),32X,E15.8,/1H0,46HORDINARY DIFFUSION COEF. AIR-WATER (CMPHILP155
5**2/DAY),E16.8,/1H0,35HOWER ALL MASS TRANSFER COEF.(1/DAY),E27.8,/PHILP156
61H0,15HPRESSURE (ATM.),E47.8,/1H0,22HMOLECULAR WT. OF WATER,E40.8,PHILP157
7/1H0,37HGAS CONSTANT (CC.-ATM/GM.MOLE-DEG.K.),E25.8,////)
      WRITE(61,1000)
C
C-----READ IN AND PRINT BOUNDARY CONDITIONS
C
      READ(60,MTI2) TA,XWA,QR,UOVER,FILMH
      WRITE(61,1004) TA,XWA,QR,UOVER,FILMH
1004 FORMAT(1H0,46H THE FOLLOWING IS A LIST OF BOUNDARY CONDITIONS, //1HOPHILP165
2,28H AMBIENT TEMPERATURE (DEG.C.),E45.8,/1H0,43H AMBIENT MOLE FRACTIPHILP166
3ON OF WATER VAPOR (DIM.),E30.8,/1H0,30H RADIATION FLUX (CAL/CM**2-DPHILP167
4AY),E43.8,/1H0,56HWALL OVER ALL HEAT TRANSFER COEF. (CAL/CM**2-DAYPHILP168
5-DEG.C.),E17.8,/1H0,28HFILMH (CAL./CM.**2-DAY-DEG.),E45.8)
      WRITE(61,1000)
1000 FORMAT (1H0,120H*****
2*****
3****,/)
C
C-----READ IN AND PRINT NUMERICAL INFORMATION
C
      READ(60,1011) NSTOP
1011 FORMAT(I9)
      READ(60,MTI3) KODE1,KODE2,RATIO,N,M,ST
PHILP144
PHILP145
PHILP146
PHILP147
PHILP148
PHILP149
PHILP150
PHILP151
PHILP152
PHILP153
PHILP154
PHILP155
PHILP156
PHILP157
PHILP158
PHILP159
PHILP160
PHILP161
PHILP162
PHILP163
PHILP164
PHILP165
PHILP166
PHILP167
PHILP168
PHILP169
PHILP170
PHILP171
PHILP172
PHILP173
PHILP174
PHILP175
PHILP176
PHILP177
PHILP178
PHILP179

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```

IF(KODE1.EQ.0) GO TO 10
  XN = N
  XM = M
  DELZ = CL/XN
  DELT = ST/XM
  RATIO = DELT/DELZ
  GO TO 11
10 XN = N
  DELZ = CL/XN
  DELT = DELZ*RATIO
  XM = ST/DELT
  M = XM
11 WRITE(61,1007) ST,DELT,M,CL,DELZ,N,RATIO
1007 FORMAT(1H1,21HNUMERICAL INFORMATION,//1H0,30HMAXIMUM SIMULATION TIPHILP193
2ME (DAYS),E20.8,1H0,29HSIZE OF TIME INCREMENT (DAYS),E21.8,1H0,2PHILP194
39HTHE NUMBER OF TIME INCREMENTS,I21,1H0,19HCOLUMN LENGTH (CM.),E3PHILP195
41.8,1H0,29HSIZE OF SPACE INCREMENT (CM.),E21.8,1H0,26HNUMBER OF PHILP196
5SPACE INCREMENTS,I24,1H0,21HRATIO OF DELT TO DELZ,E29.8)
  WRITE(61,1000)
C-----READ IN AND PRINT OUT INITIAL CONDITIONS
C
  READ(60,MT14) (S(I),I=1,N),(T(I),I=1,N),(XW(I),I=1,N)
  WRITE(61,1005)
1005 FORMAT(1H1,52HTHE FOLLOWING IS A LISTING OF THE INITIAL CONDITIONSPHILP203
2,1H ,52H*** ***** ** * ***** ** *** ***** //1HPHILP204
30,9HINCREMENT,11X,8HPOSITION,12X,10HSATURATION,10X,11HTEMPERATURE,PHILP206
49X,28HMOLE FRACTION OF WATER VAPOR,1H ,28X,5H(CM.),14X,6H(DIM.), PHILP207
511X,8H(DEG.C.),15X,6H(DIM.))
  WRITE(61,1000)
  DO 20 ID = 1,N
    Z = ID - 1
    Z = DELZ*Z
20 WRITE(61,1006) ID,Z,S(ID),T(ID),XW(ID)
1006 FORMAT(1H0,6X,E20.13,4X,3E23.13)
C

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PHILP180
PHILP181
PHILP182
PHILP183
PHILP184
PHILP185
PHILP186
PHILP187
PHILP188
PHILP189
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PHILP191
PHILP192
PHILP193
PHILP194
PHILP195
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PHILP208
PHILP209
PHILP210
PHILP211
PHILP212
PHILP213
PHILP214
PHILP215

[illegible]

```

C
C-----SPECIFY BOUNDARY CONDITION AT SURFACE
C
      IF(I.NE.1) GO TO 13
      FILMK = 4.1000E+03*FILMH
      DORD = DOR*((2.7315E+02 + T(I+1))/2.7315E+02)*#1.75E+00
      V(I) = 0.0000E+00
      NG(I) = FILMK/(EPS*(2.7315E+02 + T(I)))*(XWA - XW(I))
      Q(I) = QR + FILMH*(TA - T(I))
      IF(S(I+1).LT.1.0000) GO TO 30
      V(I+1) = 0.0000E+00
      GO TO 31
30 V(I+1) = -HCON(I+1)/EPS*((SI(I+1) - SI(I))/DELZ - 1.000E+00)
31 NG(I+1) = -DORD*(1.000E+00 - S(I+1))/((2.7315E+02 + T(I+1))*(1.000E+00
2 E+00 - XW(I+1)))*(XW(I+1) - XW(I))/DELZ
      Q(I+1) = -COND(I+1)*(T(I+1) - T(I))/DELZ
      GO TO 15
13 IF(I.NE.N) GO TO 14
C
C-----SPECIFY BOUNDARY CONDITIONS AT BOTTOM OF COLUMN
C
      V(I+1) = 0.0000E+00
      NG(I+1) = 0.0000E+00
      Q(I+1) = 0.0000E+00
      GO TO 15
16 IF(S(I).LT.1.0000E+00) GO TO 34
      V(I) = 0.0000E+00
      GO TO 35
34 V(I) = -HCON(I)/EPS*((SI(I) - SI(I-1))/DELZ - 1.000E+00)
35 DORD = DOR*((2.7315E+02 + T(I))/2.7315E+02)*#1.75E+00
      NG(I) = -DORD*(1.000E+00 - S(I))/((2.7315E+02 + T(I))*(1.000E+00
2 - XW(I)))*(XW(I) - XW(I-1))/DELZ
      Q(I) = -COND(I)*(T(I) - T(I-1))/DELZ
      GO TO 15
14 IF(S(I+1).LT.1.0000E+00) GO TO 32
      V(I+1) = 0.0000E+00

```

PHILP252
 PHILP253
 PHILP254
 PHILP255
 PHILP256
 PHILP257
 PHILP258
 PHILP259
 PHILP260
 PHILP261
 PHILP262
 PHILP263
 PHILP264
 PHILP265
 PHILP266
 PHILP267
 PHILP268
 PHILP269
 PHILP270
 PHILP271
 PHILP272
 PHILP273
 PHILP274
 PHILP275
 PHILP275
 PHILP276
 PHILP277
 PHILP278
 PHILP279
 PHILP280
 PHILP281
 PHILP282
 PHILP283
 PHILP284
 PHILP285
 PHILP286

```

GO TO 33
32 V(I+1) = -HCON(I+1)/EPS*((SI(I+1) - SI(I))/DELZ - 1.0000E+00)
33 DORD = DOR*((2.7315E+02 + T(I+1))/2.7315E+02)*.75E+00
NG(I+1) = -DORD*(1.0000E+00 - S(I+1))/((2.7315E+02 + T(I+1))*(1.00
200E+00 - XW(I+1))*(XW(I+1) - XW(I))/DELZ
Q(I+1) = -COND(I+1)*(T(I+1) - T(I))/DELZ
C
C-----CALCULATE VARIABLES AT THE NEXT TIME INCREMENT
C
15 DELNGZ = (NG(I+1) - NG(I))/DELZ
S(I) = S(I) - DELT*((V(I+1) - V(I))/DELZ + A6*DELNGZ)
T(I) = T(I) - DELT/CP(I)*((Q(I+1) - Q(I))/DELZ + A4*(T(I) - TA)
2 + A2*DELV(I)*DELNGZ)
IF(KODE2.EQ.1) GO TO 19
IF(J - KODE3.NE.0) GO TO 12
IF(I.NE.N) GO TO 19
KODE3 = KODE2 + J
19 VSEPS = EPS*V(I)
NW = A2*NG(I)
ZS = I - 1
Z = DELZ*ZS
C
C-----PRINT OUT CALCULATED VALUES
C
WRITE(61,1010) J,Z,S(I),T(I),XW(I),XWS(I),VSEPS,NW,Q(I)
1010 FORMAT(1H ,19,E15.8,4E24.14,/1H ,24X,3E24.14)
IF(I.NE.N) GO TO 12
WRITE(61,1000)
12 CONTINUE
28 CONTINUE
6969 WRITE(61,1012) J
1012 FORMAT(1H0,25HNORMAL TERMINATION, J = ,19,11HITERATIONS.)
END

```

PHILP287
 PHILP288
 PHILP289
 PHILP290
 PHILP291
 PHILP292
 PHILP294
 PHILP295
 PHILP296
 PHILP297
 PHILP298
 PHILP299
 PHILP300
 PHILP301
 PHILP302
 PHILP303
 PHILP304
 PHILP305
 PHILP306
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 PHILP311
 PHILP312
 PHILP313
 PHILP314
 PHILP315
 PHILP316
 PHILP317
 PHILP318
 PHILP319
 PHILP320

*****CARDS FOR PHILIP WITH TIME VARYING BOUNDARY CONDITIONS*****

```
TIM = 0.5
TIM = TIM + DELT
IF(TIM.LE.1.00) GO TO 36
TIM = 0.00
36 CALL SOLARA (TIM,QR)
TIM = TIM/24.00
CALL AMBTEM (TIM,TA)
TIM = TIM/24.00
CALL AMBMOL (TIM,XWA)
TIM = TIM/24.00
CALL WINDSP (TIM,WSP)
TIM = TIM/24.00
FILMH = 5.275*WSP
WRITE(61,1013)QR,TA,XWA,WSP
1013 FORMAT(1H0, 26HBOUNDARY CONDITIONS, QR = ,E20.12,2X, 5HTA = ,E20.
212,2X, 6HXWA = ,E20.12,2X, 6HWSP = ,E20.12,/)
PHILP237
PHILP240
PHILP240
PHILP240
PHILP240
PHILP240
PHILP240
PHILP240
PHILP240
PHILP240
PHILP240
PHILP240
PHILP240
PHILP314
PHILP314
PHILP314
```

APPENDIX I
COMPUTER PROGRAM FOR NUMERICAL SOLUTION
TO THE ISOTHERMAL EQUATION

```

C      PROGRAM IWMIPM(INPUT,OUTPUT,TAPE60=INPUT,TAPE61=OUTPUT)
C-----L.T. NOVAK 21 MARCH 72      *****PROGRAM IWMIPM*****
C
C-----THIS PROGRAM SOLVES THE ISOTHERMAL EQUATION OF GARDNER DURING
C-----THE CONSTANT AND FALLING DRYING RATE PERIODS. SOLUTION BY
C-----THE METHOD OF FINITE DIFFERENCE
C-----DURING THE FALLING RATE PERIOD THE SURFACE SATURATION IS CONSTANT
C----- (IRREDUCIBLE SATURATION). THIS IS THE BOUNDARY CONDITION
C-----DURING THE FALLING RATE PERIOD. THE BOUNDARY CONDITION DURING
C-----THE CONSTANT RATE PERIOD MAY BE KNOWN FROM EXPERIMENTS OR BY
C-----SURFACE HEAT AND MASS TRANSFER CALCULATIONS
C
C      THIS PROGRAM SOLVES THE FOLLOWING MATHEMATICAL PROBLEM BY THE
C      METHOD OF FINITE DIFFERENCE

```

$$\frac{\partial S}{\partial t} = - \frac{r_c}{A_e}$$

$$V^o = -K \left(\frac{dx}{dz} - 1 \right)$$

```

C
C      THE ABOVE EQUATION IS A MATHEMATICAL MODEL FOR ONE PHASE WATER
C      MOVEMENT IN POROUS MEDIA. THE ACTUAL PROBLEM BEING SIMULATED
C      IS THE RADIATION DRYING OF SAND IN A LAB COLUMN
C
C-----
C      INPUT INFORMATION
C
C      THE FIRST READ STATEMENT ALLOWS THE USER TO ENTER INFORMATION IN

```

```

C THE 20A4 FORMAT. THE SECOND READ STATEMENT INPUTS THE SOIL DEPTH IWMPM 37
C AND SOIL POROSITY. THE THIRD READ INPUTS THE CONSTANT IWMPM 38
C EVAPORATION RATE, THE FLOW OUT THE BOTTOM OF THE SOIL ELEMENT, AND IWMPM 39
C THE IRREDUCIBLE SATURATION. IWMPM 40
C IWMPM 41
C ***** IWMPM 42
C ***** IWMPM 43
C THE FOLLOWING DOCUMENTED SUBROUTINES ARE NECESSARY TO RUN THE PROG IWMPM 44
C IWMPM 45
C SUBROUTINE CAPPR(N,S,SI) IWMPM 46
C SUBROUTINE HYCON(N,S,HCON) IWMPM 47
C IWMPM 48
C ***** IWMPM 49
C ***** IWMPM 50
C ***** IWMPM 51
C ***** IWMPM 52
C ***** IWMPM 53
C ***** IWMPM 54
C ***** IWMPM 55
C ***** IWMPM 56
C ***** IWMPM 57
C ***** IWMPM 58
C ***** IWMPM 59
C ***** IWMPM 60
C ***** IWMPM 61
C ***** IWMPM 62
C ***** IWMPM 63
C ***** IWMPM 64
C ***** IWMPM 65
C ***** IWMPM 66
C ***** IWMPM 67
C ***** IWMPM 68
C ***** IWMPM 69
C ***** IWMPM 70
C ***** IWMPM 71
C ***** IWMPM 72

```

```

C*****IWMPM 73
C*****IWMPM 74
C*****IWMPM 75
C*****IWMPM 76
C*****IWMPM 77
C*****IWMPM 78
C*****IWMPM 79
C*****IWMPM 80
C*****IWMPM 81
C*****IWMPM 82
C*****IWMPM 83
C*****IWMPM 84
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C*****IWMPM 93
C*****IWMPM 94
C*****IWMPM 95
C*****IWMPM 96
C*****IWMPM 97
C*****IWMPM 98
C*****IWMPM 99
C*****IWMPM100
C*****IWMPM101
C*****IWMPM102
C*****IWMPM103
C*****IWMPM104
C*****IWMPM105
C*****IWMPM106
C*****IWMPM107
C*****IWMPM108

C
C
C      DIMENSION S( 50),V( 50),HCON( 50),SI( 50),MTINF(20)
C
C      EXTERNAL EXP
C
C-----READ IN AND PRINT GENERAL INFORMATION
C
C      DO 100 JIN = 1,6
C      READ(60,1001) MTINF
C
C      1001 FORMAT(20A4)
C      100 WRITE(61,1001) MTINF
C      WRITE(61,1000)
C
C      1000 FORMAT (1H0,120H*****
C      2*****
C      3****,/)
C
C
C-----READ IN AND PRINT PHYSICAL PARAMETERS FOR SYSTEM.
C
C      READ(60,1002) CL,EPS
C      1002 FORMAT(2F20.0)
C      WRITE(61,1003) CL,EPS
C
C      1003 FORMAT(1H0,/,16HCOLUMN LENGTH = ,E20.12,4H CM,/,1H ,11HPOR
C      2OSITY = ,E20.12)
C
C
C-----READ IN AND PRINT BOUNDARY CONDITIONS FOR SYSTEM.
C
C      READ(60,1004) VSURF,VBOTOM,SSURF
C      1004 FORMAT(3F20.0)
C      WRITE(61,1005) VSURF,SSURF,VBOTOM
C
C      1005 FORMAT(1H0,42HDRYING RATE DURING CONSTANT RATE PERIOD = ,E20.12,
C      2 8H CM/DAY,/,1H ,/,
C      31H ,48HSURFACE SATURATION DURING FALLING RATE PERIOD = ,E20.12,/)

```

```

4 1H ,35H DRAINAGE RATE THRU COLUMN BOTTOM = ,E20.12)
WRITE(61,1000)
C
C-----READ IN AND PRINT NUMERICAL INFORMATION.
C-----IF KODE1 IS SET EQUAL TO ZERO, THE RATIO READ IN IS USED.
C-----IF KODE1 IS NOT EQUAL TO ZERO THE VALUES OF N AND M READ
C-----IN ARE USED TO DETERMINE DELZ AND DELT.
C-----KODE2 CONTROLS THE PRINTING OPERATION DURING THE ITERATIVE
C-----CALCULATIONS. KODE2 = 1,2,3,ETC CAUSES AN OUTPUT FOR EVERY 1,2,3
C-----AND ETC ITERATIONS.
C-----NSTOP SPECIFIES THE ITERATION STOPPING POINT
C
      READ(60,1013) NSTOP
      1013 FORMAT(I9)
      READ(60,1006) KODE1,KODE2,RATIO,N,M,ST
      1006 FORMAT(I1,I4,F20.0,2I3,F20.0)
      IF(KODE1.EQ.0) GO TO 10
      XN = N
      XM = M
      DELZ = CL/XN
      DELT = ST/XM
      RATIO = DELT/DELZ
      GO TO 11
      10 XN = N
      DELZ = CL/XN
      DELT = DELZ*RATIO
      XM = ST/DELT
      M = XM
      11 WRITE(61,1007) ST,DELT,M,CL,DELZ,N,RATIO
      1007 FORMAT(1H1,21H NUMERICAL INFORMATION, //1H0,30H MAXIMUM SIMULATION TIME IN
      2ME (DAYS),E20.8, /1H0,29H SIZE OF TIME INCREMENT (DAYS),E21.8, /1H0,2I
      39H THE NUMBER OF TIME INCREMENTS,I21, /1H0,19H COLUMN LENGTH (CM.),E3I
      41.8, /1H0,29H SIZE OF SPACE INCREMENT (CM.),E21.8, /1H0,26H NUMBER OF
      5SPACE INCREMENTS,I24, /1H0,21H RATIO OF DELT TO DELZ,E29.8)
      WRITE(61,1000)
C
IWMPL109
IWMPL110
IWMPL111
IWMPL112
IWMPL113
IWMPL114
IWMPL115
IWMPL116
IWMPL117
IWMPL118
IWMPL119
IWMPL120
IWMPL121
IWMPL122
IWMPL123
IWMPL124
IWMPL125
IWMPL126
IWMPL127
IWMPL128
IWMPL129
IWMPL130
IWMPL131
IWMPL132
IWMPL133
IWMPL134
IWMPL135
IWMPL136
IWMPL137
IWMPL138
IWMPL139
IWMPL140
IWMPL141
IWMPL142
IWMPL143
IWMPL144

```

```

C-----READ IN AND PRINT INITIAL CONDITIONS FOR SYSTEM.
C
      READ(60,1008) (S(I),I=1,N)
      1008 FORMAT(4F20.0)
      WRITE(61,1009) (S(I),I=1,N)
      1009 FORMAT(1H0,/,1H0,30H THE INITIAL CONDITIONS ARE****,/, (5E26.12))
      WRITE(61,1000)
C
C-----PRINT OUT TITLE PAGE
C
      WRITE(61,1011)
      1011 FORMAT(1H1,14H TIME INCREMENT,2X,8H POSITION,10X,10H SATURATION,12X,
      215HV(I+1) (CM/DAY),7X,14HV(I) (CM/DAY),11X,20H CUMULATIVE EVAP.(CM
      3),/,1H ,14H *****,2X,8H *****,10X,10H *****,12X,15H*IWMPM158
      4 *****,7X,14H *****,11X,20H *****)
      CUMVAP = 0.0
      TIMECH = 0.0
      TIME = 100000.0
C
C-----BEGIN FINITE DIFFERENCE CALCULATIONS.
C
      ISTART = 1
      CODE3 = CODE2
      DO 18 JT = 1,M
      IF(JT.GT.NSTOP) GO TO 6969
C
C-----TRANSFER IN THE ARRAYS OF CAPILLARY PRESSURE AND HYDRAULIC CONDUCT
C
      CALL CAPPR(N,S,SI)
      CALL HYCON(N,S,HCON)
      DO 12 I = ISTART,N
      IF(I.NE.1) GO TO 13
C
C-----CHECK TO SEE IF SURFACE SATURATION IS AT THE IRREDUCIBLE LEVEL (SSI
C-----IF SO, START THE FALLING RATE CALCULATION ON THE NEXT TIME INCREME
C

```

```

IF (S(1).GT.SSURF) GO TO 19
ISTART = 2
TIME = JT*DELT
WRITE(61,1012) TIME
1012 FORMAT(1H1, 56HIRREDUCIBLE SATURATION (SSURF) HAS BEEN REACHED, TIIWMPM181
2ME = ,E18.10,3X,5HDAYS.,/1H0, 54HFALLING RATE CALCULATIONS BEGIN OI WMPM182
3N NEXT TIME ITERATION,///) WMPM183
C-----SET SURFACE BOUNDARY CONDITION. WMPM184
C WMPM185
C WMPM186
C WMPM187
C WMPM188
C WMPM189
C WMPM190
C WMPM191
C WMPM192
C WMPM193
C WMPM194
C WMPM195
C WMPM196
C WMPM197
C WMPM198
C WMPM199
C WMPM200
C WMPM201
C WMPM202
C WMPM203
C WMPM204
C WMPM205
C WMPM206
C WMPM207
C WMPM208
C WMPM209
C WMPM210
C WMPM211
C WMPM212
C WMPM213
C WMPM214
C WMPM215
C WMPM216

19 V(I) = VSURF
CUMVAP = CUMVAP + DELT*V(1)
V(I+1) = -HCON(I+1)/EPS*((SI(I+1) - SI(I))/DELZ - 1.0000)
GO TO 16
13 IF(I.NE.N) GO TO 14
C-----SET BOTTOM BOUNDARY CONDITION
C
C WMPM217
C WMPM218
C WMPM219
C WMPM220
C WMPM221
C WMPM222
C WMPM223
C WMPM224
C WMPM225
C WMPM226
C WMPM227
C WMPM228
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C WMPM314
C WMPM315
C WMPM316

V(I+1) = VBOTOM
GO TO 16
14 V(I+1) = -HCON(I+1)/EPS*((SI(I+1) - SI(I))/DELZ - 1.0000)
V(I) = -HCON(I)/EPS*((SI(I) - SI(I-1))/DELZ - 1.0000)
16 S(I) = S(I) - DELT*(V(I+1) - V(I))/DELZ
XI = I - 1
Z = DELZ*XI
TIMECH = JT*DELT
IF(KODE2.EQ.1) GO TO 17
IF(JT - KODE3.NE.0) GO TO 12
IF(I.NE.N) GO TO 17
KODE3 = KODE2 + JT
17 WRITE(61,1010) JT,Z,S(I),V(I+1),V(I),CUMVAP
1010 FORMAT(1H ,I10,5X,F10.6,4X,E20.12,4X,E20.12,4X,E20.12)
IF(I.NE.N) GO TO 12
WRITE(61,1000)
12 CONTINUE
IF(TIMECH.LE.TIME) GO TO 18

```

```
      CUMVAP = CUMVAP + DELT*V(2)
18  CONTINUE
6969 WRITE(61,1014) JT
1014 FORMAT(1H0,25HNORMAL TERMINATION, JT = ,I9,2X,11HITERATIONS.)
      END
```

```
IWMPPM217
IWMPPM218
IWMPPM219
IWMPPM220
IWMPPM221
```

APPENDIX J
OVER ALL WALL HEAT TRANSFER
COEFFICIENT CALCULATION

Radial energy losses from the soil column (see Figure 10) involves heat conduction through the soil, the column wall, and the insulation. An energy balance on the column wall or insulation gives the following equation.

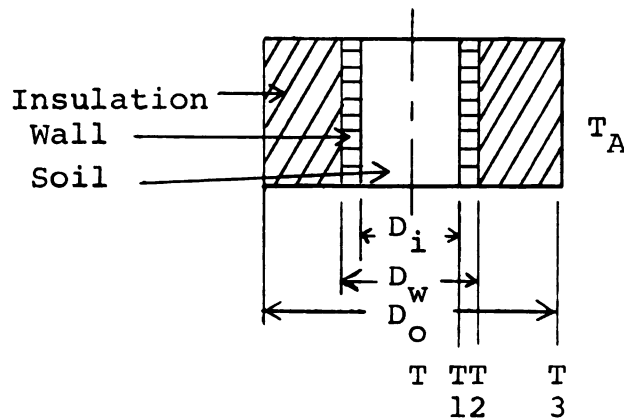
$$(J.1) \quad \rho C_p \frac{\partial T}{\partial t} = \frac{\partial}{\partial z} \left(k \frac{\partial T}{\partial z} \right) + \frac{1}{r} \frac{\partial}{\partial r} \left(r k \frac{\partial T}{\partial r} \right)$$

when Equation (J.1) can be written as Equation (J.2),

$$(J.2) \quad \frac{\partial}{\partial r} \left(r k \frac{\partial T}{\partial r} \right) = 0$$

the over all heat transfer coefficient can be calculated in the following manner. The radial heat flows are:

$$(J.3) \quad q \pi D_o dz = U_o \pi D_o dz (T_A - T) = h \pi D_o dz (T_A - T_3)$$



$$\begin{aligned}
 (J.4) \quad q 2\pi \frac{D_o}{2} dz &= -k_i 2\pi dz \frac{(T_3 - T_2)}{\ln(D_o/D_w)} = -k_w 2\pi dz \frac{(T_2 - T_1)}{\ln(D_w/D_i)} \\
 &= -k_e 2\pi dz \frac{(T_1 - T)}{\ln(D_i/D^*)} = -k_i 2\pi dz \frac{\int \frac{dT}{dr}}{r}
 \end{aligned}$$

Equation (J.3) and (J.4) can be combined to give

$$(J.5) \quad U_o = \frac{1}{\frac{D_o}{2} \left[\frac{\ln(D_i/D^*)}{k_e} + \frac{\ln(D_w/D_i)}{k_w} + \frac{\ln(D_o/D_w)}{k_i} + \frac{2}{hD_o} \right]}$$

The diameters and materials of construction for the soil column in Figure 12 have been given in Table 1. The thermal conductivities for these materials are:

$$k_e = 8.5 \times 10^{-4} \text{ cal/cm-sec-}^{\circ}\text{C (for saturation} = 0, \text{ data of Moench)}$$

$$k_w = 5 \times 10^{-4} \text{ cal/cm-sec-}^{\circ}\text{C (for plexiglass--acrylic resin, data from Polymer Handbook, eds., J. Brandrup, E. Immergut, Interscience, N.Y., 1966).}$$

$$k_i = 8.26 \times 10^{-5} \text{ cal/cm-sec-}^{\circ}\text{C (for styrofoam, data from Principles of Polymer Systems, F. Rodriguez, McGraw Hill, N.Y., 1970).}$$

for $D^* = 9.2 \text{ cm}$ and $h = 1 \text{ btu/hr-ft}^2\text{-}^{\circ}\text{F}$ ($1.355 \times 10^{-4} \text{ cal/cm}^2\text{-sec-}^{\circ}\text{C}$), the over all heat transfer coefficient is

$$U_o = 6.35 \times 10^{-6} \text{ cal/cm-sec-}^{\circ}\text{C} = 0.548 \text{ cal/cm}^2\text{-day-}^{\circ}\text{C}$$

The value of the film coefficient (h) is reasonable for low wind velocities and the over all coefficient is not that sensitive to the film coefficient. The resistance controlling the over all coefficient is the insulation as is shown below.

$$(J.5*) \quad U_o = \frac{1}{\underset{\text{soil}}{.13 \times 10^4} + \underset{\text{wall}}{.257 \times 10^4} + \underset{\text{insulation}}{14.62 \times 10^4} + \underset{\text{film coeff.}}{.74 \times 10^4}} = 6.35 \times 10^{-6}$$

APPENDIX K
SURFACE FILM COEFFICIENTS

The wind velocity at the soil surface has an effect on the surface film mass transfer and heat transfer coefficients. To estimate these coefficients for the soil column in Figure 12, some heat and mass transfer correlations for laminar flow past a flat plate will be used.

$$(K.1) \quad Nu = 0.664 Re_L^{1/2} Pr^{1/3}$$

$$(K.2) \quad Sh = 0.664 Re_L^{1/2} Sc^{1/3}$$

Reference: Bennett, C.O. Myers, J.E., Momentum, Heat, and Mass Transfer, McGraw-Hill, N.Y., 1962, p. 302, 476.

where,

$$(K.3) \quad Sh = \frac{k_{m,s} L}{\mathcal{D}_{aw}}$$

$$(K.4) \quad Nu = \frac{h_s L}{k}$$

$$(K.5) \quad Re_L = \frac{V_g L \rho}{\mu}$$

Using the properties of air at room temperature and a wind velocity of four miles per hour and a dimension of $L = 27$ cm, the surface film heat transfer coefficient is calculated to be $h_s = 1.8 \text{ btu/hr-ft}^2\text{-}^\circ\text{F} = 21.1 \text{ cal/cm}^2\text{-day-}^\circ\text{C}$. By combining Equations (K.1) and (K.2) the surface film mass transfer coefficient can be calculated to be

$$\begin{aligned}
 \text{(K.6)} \quad k_{m,s} &= \text{Nu} \left(\frac{\text{Sc}}{\text{Pr}} \right)^{1/3} = 4100 \cdot h_s \text{ (cm/day)}. \\
 &= 86510 \text{ cm/day}
 \end{aligned}$$

APPENDIX L
CALCULATION OF PART OF THE CAPILLARY
POTENTIAL--SATURATION FUNCTION
FOR VALENTINE SAND

It can be seen from Equation (1.5) that at steady state the volumetric flux of water is constant. Before the actual drying of valentine sand, Hanks, et al. wet the sand covered it, and allowed it to redistribute for a week. The resultant distribution was a saturation profile corresponding to the initial conditions for simulation numbers 3-6 (see Figures 16,17). Assuming that during the week an equilibrium saturation distribution was reached, the capillary potential--saturation function can be calculated over the range of saturations in the initial condition saturation profiles (Figures 16,17).

$$(L.1) \quad v^0 = -K\left(\frac{d\psi}{dz} - 1\right) = 0, \quad \psi = \psi(S)$$

then,

$$(L.2) \quad \psi(S) \Big|_z - \psi(S) \Big|_{z_0} = (z - z_0)$$

The data points in Figure 9 identified as being calculated were calculated from Equation (L.2) and the initial condition data of Hanks et al. The capillary potential at saturation was taken to be

$$(L.3) \quad \psi(S = 1) \Big|_{z_0 = 45} = -1 \text{ cm.}$$

It is not uncommon for air bubbles to cause capillary potentials of this magnitude when the saturation is essentially one.

APPENDIX M
COMPARISON OF CONDUCTIVE ENERGY
FLUX AND CONVECTIVE ENERGY FLUXES

From data obtained from simulation number 5 and contained in Table 7, the conductive energy flux can be compared with the convective energy fluxes which represent the energy transfer by the movement of liquid and vapor water.

When time = 40 days, we have the following:

at $z=0$

$$(M.1) \quad q = +371.04 \text{ cal/cm}^2\text{-day}$$

$$(M.2) \quad q_L = \rho_L C_{p_L} (T - T_{ref}) V^O = 1.0 (48.5 - 25.0) 0 = 0.0 \text{ cal/cm}^2\text{-day}$$

$$(M.3) \quad q_V = \tilde{N}_w M_w C_{p_w} (T - T_{ref}) = -.0360 (48.5 - 25.) = -.845 \text{ cal/cm}^2\text{-day}$$

where, q , q_L , and q_V are the conductive, liquid convective, and vapor convective energy fluxes respectively.

at $z=9$

$$(M.4) \quad q = +248.95$$

$$(M.5) \quad q_L = 1.0 (39.8 - 25.) (-.10892E-02) = -.01615$$

$$(M.6) \quad q_V = -.34923E-01 (39.8 - 25.) = -.516$$

From looking at the fluxes in Table 7 at 40 days it can be seen that the energy fluxes due to convective flow at lower depths are also negligible compared to the conductive energy fluxes.

At $t = 3$ days, the convective flow energy terms in comparison to the conductive energy term seems to be about the largest. This is the start of the falling rate period. at $z=0$

$$(M.7) \quad q = 824.07$$

$$(M.8) \quad q_L = 1.0(26.8-25.)(0) = 0.0$$

$$(M.9) \quad q_V = -.14409E+01(26.8-25.) = -2.45$$

at $z=9$

$$(M.10) \quad q = 45.391$$

$$(M.11) \quad q_L = 1.0(26.0-25.)(-.11182E+01)=-1.1182$$

$$(M.12) \quad q_V = -.13005E-02(26.0-25.)=-.013005$$

comparison between q and q_L and q_V :

$$(M.13) \quad \% = \frac{q_L + q_V}{q} \times 100 = -113.1/45.391 = 2.49$$

At other depths for $t=3$ days, the ratio of convective flow to conductive energy flux will be smaller than 2.49%.

At the beginning of the falling rate period the convective energy fluxes can be as high as $2\frac{1}{2}\%$ of the conductive flux at $z=9$ cm. At other depths this per cent falls to about $\frac{1}{4}\%$. Also after the falling rate period is underway the maximum % convective to conductive flux occurs at $z=9$ cm. and the % is about $\frac{1}{4}$. As an example see Equations (M.1-M.6).

APPENDIX N
COMPUTER PROGRAM SUBROUTINES CONTAINING
NATURAL WEATHER TIME VARYING
BOUNDARY CONDITIONS

		<u>conditions</u>	
	SUBROUTINE SOLARA (TIME,QRAD)		SOLAR 1
C-----	L.T. NOVAK 19 MAY 72*****SUBROUTINE SOLARA*****		SOLAR 2
C-----	THIS SUBROUTINE IS A LINEAR INTERPOLATION OF THE SOLAR RADIATION		SOLAR 3
C-----	DATA TAKEN IN EAST LANSING AT 3 HOUR INTERVALS ON 11 JUNE 71		SOLAR 4
C-----	REFERENCE PROF. KIDDER, AG. ENGR. THE SOLAR RADIATION RATE IS		SOLAR 5
C-----	REPRESENTED BY THE VARIABLE QRAD (CAL/CM**2-DAY). THE TIME UNITS		SOLAR 6
C-----	ARE IN HOURS. THAT IS TIME (HOURS).		SOLAR 7
C-----			SOLAR 8
C-----	READING IN TIME IN DAYS, SO CONVERT TO HOURS.....		SOLAR 9
	TIME = TIME*24.0		SOLAR 10
	IOUT = 3		SOLAR 11
	IF(TIME) 1,2,2		SOLAR 12
	1 WRITE(IOUT,50)		SOLAR 13
	50 FORMAT(1H0, 89H**SUB. SOLARA, TIME LESS THAN ZERO HOURS. CANT		SOLAR 14
	PROCEED. RETURNING TO CALLING PROGRAM.)		SOLAR 15
	RETURN		SOLAR 16
	2 IF(TIME-4.0) 3,3,4		SOLAR 17
	3 QRAD = 0.00		SOLAR 18
	RETURN		SOLAR 19
	4 IF(TIME-5.0) 5,5,6		SOLAR 20
	5 QRAD = 21.6*(TIME-4.0)		SOLAR 21
	RETURN		SOLAR 22
	6 IF(TIME-6.0) 7,7,8		SOLAR 23
	7 QRAD = 235.2*(TIME-5.0) + 21.6		SOLAR 24
	RETURN		SOLAR 25
	8 IF(TIME-10.0) 9,9,10		SOLAR 26
	9 QRAD = 373.8*(TIME-6.0) + 256.8		SOLAR 27
	RETURN		SOLAR 28
	10 IF(TIME-11.0) 11,11,12		SOLAR 29
	11 QRAD = 216.0*(TIME-10.0) + 1752.0		SOLAR 30
	RETURN		SOLAR 31
	12 IF(TIME-12.0) 13,13,14		SOLAR 32
	13 QRAD = 24.0*(TIME-11.0) + 1968.0		SOLAR 33
	RETURN		SOLAR 34
	14 IF(TIME-13.0) 15,15,16		SOLAR 35
			SOLAR 36

```

15 QRA = 40.8*(TIME-12.0) + 1992.0
   RETURN
16 IF(TIME-15.0) 17,17,18
17 QRA = -151.2*(TIME-13.0) + 2032.8
   RETURN
18 IF(TIME-19.0) 19,19,20
19 QRA = -387.6*(TIME-15.0) + 1730.4
   RETURN
20 IF(TIME-20.0) 21,21,22
21 QRA = -153.6*(TIME-19.0) + 180.0
   RETURN
22 IF(TIME-21.0) 23,23,24
23 QRA = -26.4*(TIME-20.0) + 26.4
   RETURN
24 IF(TIME-24.0) 25,25,26
25 QRA = 0.00
   RETURN
26 WRITE(IOUT,51)
51 FORMAT(1H0, 90H**SUB. SOLAR, TIME GREATER THAN 24 HOURS. CANT
2PROCEED. RETURNING TO CALLING PROGRAM.)
   RETURN
   END
SOLAR 37
SOLAR 38
SOLAR 39
SOLAR 40
SOLAR 41
SOLAR 42
SOLAR 43
SOLAR 44
SOLAR 45
SOLAR 46
SOLAR 47
SOLAR 48
SOLAR 49
SOLAR 50
SOLAR 51
SOLAR 52
SOLAR 53
SOLAR 54
SOLAR 55
SOLAR 56
SOLAR 57
SOLAR 58

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SUBROUTINE AMBTEM (TIME,T)
C-----L.T. NOVAK 19 MAY 72*****SUBROUTINE AMBTEM*****
C-----THIS SUBROUTINE IS A LINEAR INTERPOLATION OF THE DRY BULB TEMPER.
C-----DATA TAKEN AT THE LANSING AIRPORT WEATHER STATION AT THREE HOUR
C-----INTERVALS ON 11 JUNE 71. REF. U.S.DEPT. OF COMMERCE LOCAL
C-----CLIMATOLOGICAL DATA FOR JUNE 1971. THE DRY BULB TEMPERATURE OR
C-----AMBIENT TEMPERATURE (T) IS IN UNITS OF DEG. CENTIGRADE, TIME IS
C-----IN UNITS OF HOURS.
C
C-----READING IN TIME IN DAYS, SO CONVERT TO HOURS.....
TIME = TIME*24.0
IOUT = 3
IF(TIME) 1,2,2
1 WRITE(IOUT,50)
50 FORMAT(1H0, 89H**SUB. AMBTEM, TIME LESS THAN ZERO HOURS. CANT
2 PROCEED. RETURNING TO CALLING PROGRAM.)
RETURN
2 IF(TIME-1.0) 3,3,4
3 T = 16.1334 - 2.2334*TIME
RETURN
4 IF(TIME-4.0) 5,5,6
5 T = 13.9 - 3.66667E-01*(TIME-1.0)
RETURN
6 IF(TIME-7.0) 7,7,8
7 T = 12.8 + 5.33334E-01*(TIME-4.0)
RETURN
8 IF(TIME-10.0) 9,9,10
9 T = 14.4 + 2.9667*(TIME-7.0)
RETURN
10 IF(TIME-13.0) 11,11,12
11 T = 23.3 + 9.33334E-01*(TIME-10.0)
RETURN
12 IF(TIME-16.0) 13,13,14
13 T = 26.1
RETURN
AMBTEM 1
AMBTEM 2
AMBTEM 3
AMBTEM 4
AMBTEM 5
AMBTEM 6
AMBTEM 7
AMBTEM 8
AMBTEM 9
AMBTEM 10
AMBTEM 11
AMBTEM 12
AMBTEM 13
AMBTEM 14
AMBTEM 15
AMBTEM 16
AMBTEM 17
AMBTEM 18
AMBTEM 19
AMBTEM 20
AMBTEM 21
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AMBTEM 29
AMBTEM 30
AMBTEM 31
AMBTEM 32
AMBTEM 33
AMBTEM 34
AMBTEM 35
AMBTEM 36

```

```

14 IF(TIME-19.0) 15,15,16
15 T = 26.1 - 3.66667E-01*(TIME-16.0)
   RETURN
16 IF(TIME-22.0) 17,17,18
17 T = 25.0 - 1.466667*(TIME-19.0)
   RETURN
18 IF(TIME-24.0) 19,19,20
19 T = 20.6 - 2.2334*(TIME-22.0)
   RETURN
20 WRITE(IOUT,51)
51 FORMAT(1H0, 90H**SUB. AMBTM, TIME GREATER THAN 24 HOURS. CANT
2PROCEED. RETURNING TO CALLING PROGRAM.)
   RETURN
   END
AMBTM 37
AMBTM 38
AMBTM 39
AMBTM 40
AMBTM 41
AMBTM 42
AMBTM 43
AMBTM 44
AMBTM 45
AMBTM 46
AMBTM 47
AMBTM 48
AMBTM 49
AMBTM 50

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SUBROUTINE AMBMOL(TIME,XWA)
C-----L.T. NOVAK      19 MAY 72*****SUBROUTINE AMBMOL*****
C-----THIS SUBROUTINE IS A LINEAR INTERPOLATION OF THE AMBIENT
C-----MOLE FRACTION OF WATER IN THE ATMOSPHERE AS CALCULATED FROM THE
C-----LANDSLING AIRPORT WEATHER DATA TAKEN AT THREE HOUR INTERVALS ON
C-----11 JUNE 71. REF. U.S.DEPT. OF COMMERCE LOCAL CLIMATOLOGICAL
C-----DATA FOR JUNE 1971 THE AMBIENT MOLE FRACTION (XWA) IS
C-----DIMENSIONLESS, AND TIME IS IN HOURS
C
C-----READING IN TIME IN DAYS, SO CONVERT TO HOURS.....
TIME = TIME*24.0
IOUT = 3
IF(TIME) 1,2,2
1 WRITE(IOUT,50)
50 FORMAT(1H0, 89H**SUB. AMBMOL, TIME LESS THAN ZERO HOURS. CANT P
2ROCEED. RETURNING TO CALLING PROGRAM.)
RETURN
2 IF(TIME-1.0) 3,3,4
3 XWA = -5.364E-03*(TIME) + 0.01508
RETURN
4 IF(TIME-4.0) 5,5,6
5 XWA = 0.009716 + 1.160E-04*(TIME-1.0)
RETURN
6 IF(TIME-7.0) 7,7,8
7 XWA = 0.010064 + 4.2226E-04*(TIME-4.0)
RETURN
8 IF(TIME-10.0) 9,9,10
9 XWA = 0.01133078 + 1.3981367E-03*(TIME-7.0)
RETURN
10 IF(TIME-13.0) 11,11,12
11 XWA = 0.01552519 + 5.743533E-04*(TIME-10.0)
RETURN
12 IF(TIME-16.0) 13,13,14
13 XWA = 0.01724825 + 8.845267E-04*(TIME-13.0)
RETURN

```

AMBMO 1
 AMBMO 2
 AMBMO 3
 AMBMO 4
 AMBMO 5
 AMBMO 6
 AMBMO 7
 AMBMO 8
 AMBMO 9
 AMBMO 10
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 AMBMO 30
 AMBMO 31
 AMBMO 32
 AMBMO 33
 AMBMO 34
 AMBMO 35
 AMBMO 36

```
14 IF(TIME-19.0) 15,15,16
15 XWA = 0.01990183 - 6.97867E-05*(TIME-16.0)
   RETURN
16 IF(TIME-22.0) 17,17,18
17 XWA = 0.01969247 - 1.536038E-03*(TIME-19.0)
   RETURN
18 IF(TIME-24.0) 19,19,20
19 XWA = 0.0150843546 - 1.789435E-03*(TIME-22.0)
   RETURN
20 WRITE(IOUT,51)
51 FORMAT(1H0, 90H**SUB. AMBMOL, TIME GREATER THAN 24 HOURS. CANT
 2PROCEED. RETURNING TO CALLING PROGRAM.)
   RETURN
   END
AMBM0 37
AMBM0 38
AMBM0 39
AMBM0 40
AMBM0 41
AMBM0 42
AMBM0 43
AMBM0 44
AMBM0 45
AMBM0 46
AMBM0 47
AMBM0 48
AMBM0 49
AMBM0 50
```

```

SUBROUTINE WINDSP (TIME,VSP)
C-----L.T. NOVAK 19 MAY 72*****SUBROUTINE WINDSP*****
C-----THIS SUBROUTINE IS A LINEAR INTERPOLATION OF THE WIND SPEED
C-----DATA TAKEN AT THE LANSING AIRPORT WEATHER STATION AT THREE HOUR
C-----INTERVALS ON 11 JUNE 71. REF. U.S.DEPT. OF COMMERCE LOCAL
C-----CLIMATOLOGICAL DATA FOR JUNE 1971. THE WIND SPEED (WSP) HAS
C-----UNITS OF MILES/HOUR, TIME IS IN UNITS OF HOURS
C-----READING IN TIME IN DAYS, SO CONVERT TO HOURS.....
TIME = TIME*24.0
IOUT = 3
IF(TIME) 1,2,2
1 WRITE(IOUT,50)
50 FORMAT(1H0, 89H**SUB. WINDSP, TIME LESS THAN ZERO HOURS. CANT
2 PROCEED. RETURNING TO CALLING PROGRAM.)
RETURN
2 IF(TIME-1.0) 3,3,4
3 VSP = 8.05 + 1.15*(TIME)
RETURN
4 IF(TIME-4.0) 5,5,6
5 VSP = 9.2 + 3.66667E-01*(TIME-1.0)
RETURN
6 IF(TIME-7.0) 7,7,8
7 VSP = 10.3 - 1.133334*(TIME-4.0)
RETURN
8 IF(TIME-10.0) 9,9,10
9 VSP = 6.9 + 1.133334*(TIME-7.0)
RETURN
10 IF(TIME-16.0) 11,11,12
11 VSP = 10.3 + 7.833334E-01*(TIME-10.0)
RETURN
12 IF(TIME-19.0) 13,13,14
13 VSP = 15.0 - 7.833334E-01*(TIME-16.0)
RETURN
14 IF(TIME-22.0) 15,15,16

```

WINDS 1
WINDS 2
WINDS 3
WINDS 4
WINDS 5
WINDS 6
WINDS 7
WINDS 8
WINDS 9
WINDS 10
WINDS 11
WINDS 12
WINDS 13
WINDS 14
PWINDS 15
WINDS 16
WINDS 17
WINDS 18
WINDS 19
WINDS 20
WINDS 21
WINDS 22
WINDS 23
WINDS 24
WINDS 25
WINDS 26
WINDS 27
WINDS 28
WINDS 29
WINDS 30
WINDS 31
WINDS 32
WINDS 33
WINDS 34
WINDS 35
WINDS 36

```
15 VSP = 12.65 - 2.30*(TIME-19.0)
   RETURN
16 IF(TIME-24.0) 17,17,18
17 VSP = 5.75 + 1.1500*(TIME-22.0)
   RETURN
18 WRITE(IOUT,51)
51 FORMAT(1H0, 90H**SUB. WINDSP, TIME GREATER THAN 24 HOURS. CANT
2PROCEED. RETURNING TO CALLING PROGRAM.)
   RETURN
   END
```

WINDS 37
WINDS 38
WINDS 39
WINDS 40
WINDS 41
WINDS 42
WINDS 43
WINDS 44
WINDS 45
WINDS 46

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