

**Simulating fully coupled overland
and variably saturated subsurface flow
using MODFLOW**

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DEDICATION

For Kelley and my parents, Bev and Dick.

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Abstract

Simulating fully coupled overland and variably saturated subsurface flow using MODFLOW

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The three-dimensional (3-D), modular finite-difference ground water model MODFLOW has been modified to simulate three-dimensional (3-D) variably saturated flow (using Richard's equation) and two-dimensional (2-D) overland flow (using the kinematic wave approximation). Surface and subsurface flow are coupled at the iteration level and both are contained within the MODFLOW finite difference grid. The resulting modifications retain the modular structure of the MODFLOW code and preserve the model's existing capabilities as well as its compatibility with existing transport models and commercial pre/post processors.

Model performance is evaluated with an analytical solution for 1-dimensional constant head infiltration (Dirichlet boundary condition), results from a field experiment of 1-dimensional constant rainfall infiltration (Neumann boundary condition) and results from a 2-dimensional conjunctive surface-subsurface flow soil flume experiment. An investigation into the relative influence of model grid size and soil characteristics on model performance is also undertaken and it is determined that non-linear soils require fine spatial discretization for acceptable solution convergence. The overall success of the model in simulating conjunctive surface/subsurface flow, mixed boundary conditions and variable soil types demonstrates its utility for future hydrologic investigations.

Chapter 1

Introduction

1.1 Hydrologic Modeling: An Overview

Over the past century, hydrologic science has established itself as an increasingly pertinent field of study that integrates a wide range of scientific disciplines (from physics and mathematics to chemistry, geology and statistics) in order to address a broad spectrum of applications. There have been numerous advances in the understanding of groundwater and stream hydraulics, runoff processes, and quantitative geomorphology as well as improvements in data collection techniques, statistical applications to hydrologic data, and numerical methods used for modeling hydrologic processes. This knowledge base is providing the impetus for scientific development in physical hydrology as the twenty-first century begins. Central to current research efforts are; a) the ability to understand and model hydrologic processes at various scales (e.g. hillslope, basin, continental, global), and b) the need for a more detailed empirical knowledge of the mechanisms involved in aquifer-stream interactions. (*Dingman, 2002*)

Simulation modeling has become an increasingly efficient and effective method of investigating hydrologic processes due to the recent technological advances in data collection, storage and processing. Dooge (1986) defines a simulation model as a representation of the physical world “which is simpler than the prototype system and which can reproduce some but not all of the characteristics thereof”. In the context of this study, the term ‘hydrologic model’ refers to a mathematical tool that allows the user

to simulate one or more of the following hydrologic processes within a watershed (illustrated in **figure 1.1**): overland flow (runoff), stream (channel) flow, saturated ground water flow, infiltration (unsaturated ground water flow), snowmelt, evaporation, transpiration, recharge, and surface-subsurface interactions (e.g. seepage faces). The processes relevant to this work will be discussed in greater detail in **section 1.2**.

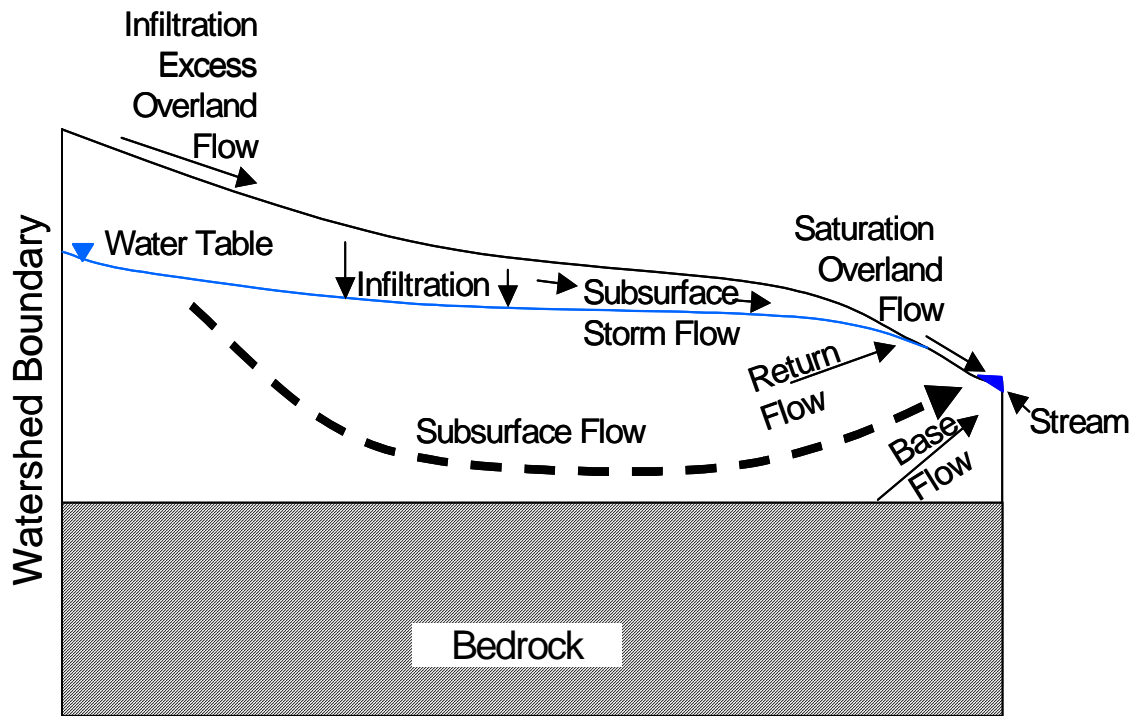


Figure 1.1: Flow mechanisms that control the hydrologic processes of a watershed

The basis of a hydrologic model is, in general empirical, compartmental, or physical. Empirical approaches use relationships developed from observational data to model the hydrologic process being studied based on factors such as soil type and basin topography (e.g. SCS curve number method; *Soil Conservation Service*, 1973). Compartmental models generally represent a system as an interconnected network of “black boxes” that represent separate physical domains with uniform hydrologic characteristics (e.g. vadose zone, flood plain, river). These compartments are usually linked through a set of (usually linear) transfer functions to simulate the storage-discharge relationships between the continua (e.g. infiltration). Physical relationships are used together with semi-empirical ones to represent the characteristics of each box and

their interactions in the network, often requiring calibration of parameters that have no physical meaning (and thus are not measurable). Examples of this type of model include the Stanford Model IV (*Crawford and Linsley, 1966*), the Sacramento model (*Burnash et al., 1973*), and the SWAT model (*Arnold, 1993*). There are also semi-distributed ‘statistical-dynamical’ methods such as TOPMODEL (*Beven and Kirkby, 1979*) and ARNO (*Todini, 1996*) in which basin response is driven by a statistically representative set of grid cells determined by a topographical index through similarity arguments. Physically based models use relationships derived from the basic concepts of physics such as conservation of mass, energy or momentum, diffusion and force balance to simulate flows and storage. Due to the nature of these relationships, physically-based models are ‘distributed’; the spatial domain is discretized into cells (representative elementary volumes, REVs) or elements in order to assign hydrologic parameters (valid for the entire cell or element) that can be observed or estimated from reality. For clarification, the terms ‘physically based model’ and ‘distributed model’ will be used interchangeably in this work (following *Refsgaard, 1996*).

There are two fundamental purposes of a hydrologic model: 1) scientific inquiry, and 2) resource management. As a tool of scientific inquiry, the hydrologic model can be used to test hypotheses concerning specific hydrologic processes (*Beven, 1989*). In the context of resource management, the hydrologic model is used as a tool to guide decision-making. For example, surface water models have been used in flood prediction, erosion control, and the design of storm water control systems; ground water models have been used in the prediction of aquifer yield (water supply) and base flow contributions to streams; both types of models have been used to predict the fate and transport of various contaminants.

Applications in both scientific inquiry and resource management require either a *prediction*: an estimate of the magnitude of some hydrologic quantity in response to a certain hypothetical event or stressor (e.g. estimating aquifer yield from average annual rainfall for water supply design); a *forecast*: an estimate of the hydrologic response to an anticipated event (e.g. estimating river flooding from a recent storm); or a *hindcast*: an estimate of an unmeasured hydrologic response to a previous event (e.g. estimating river

stages in years prior to dam construction) (*Dingman, 2002*). The majority of models are designed for (and thus restricted to) a limited set of applications due to the basic assumptions that each model must make in order to represent the spatial and temporal scale of interest. For example, a flood prediction model that provides an estimate of a river's stage height given certain precipitation level (hourly/daily time scale) is generally not able accurately to estimate seasonal ground water contributions to the stream (baseflow) for the same watershed (monthly/yearly time scale). This issue of scaling in hydrologic models is an ongoing debate in the literature (*Beven, 1989; Grayson et al., 1992b; Beven, 1996a; Beven, 1996b; Refsgaard et al., 1996*) that will not be addressed in this work. However, the behavior of the variably saturated subsurface flow model across a range of spatial grid scales is investigated in **Section 3.1.3** and the implications this behavior has on future model applications is examined.

1.2 Research Survey

1.2.1 Field observations

The major surface and subsurface response mechanisms for watersheds have been identified and characterized as a result of the extensive field studies dating back to Horton's pioneering work in the 1930s. These mechanisms (**figure 1.1**) are interdependent and any number of them can operate in a given basin or hillslope during a given event (*Anderson and Burt*, 1990). The dominant processes vary with each event and even within the event itself, depending on factors such as antecedent soil moisture, rainfall intensity, and soil permeability (*Whipkey and Kirkby*, 1978). There are several excellent summaries of this field research in the literature including: *Dunne*, 1978; *Anderson and Burt*, 1990; *Bonell*, 1993; and *Dingman*, 2002.

With regard to storm-generated stream flow, there are three principal mechanisms (*Dunne*, 1978):

- *Saturation excess overland flow (return flow)*: surface flow generated by rainfall on saturated soil induced by a rising water table.
- *Infiltration excess overland flow (Horton overland flow)*: Surface flow generated by a rainfall event with an intensity that is greater than the maximum (saturated) hydraulic conductivity of the soil and duration longer than the saturation (ponding) time of the soil (*Horton*, 1933).
- *Subsurface storm flow (interflow)*: horizontal subsurface flow caused by rapid saturation of near-surface soil that creates a transient anisotropy in the hydraulic conductivity.

These basic mechanisms partition rainfall during a storm event and therefore control (in varying capacities) the transient runoff response of a hillslope or basin. In general (see **figure 1.2**), infiltration excess overland flow is the dominant runoff mechanism for hot, dry climates with little ground cover, whereas saturated excess overland flow occurs regions near stream channels and lakes (*variable source areas*: transient wetland areas

that contribute to overall storm flow) in humid climates with dense ground cover. Subsurface storm flow generally occurs in steep valleys containing high hydraulic conductivity surface soils overlying an “impeding horizon” (*Dunne*, 1978). Surface runoff occurs in the mixed sheet or rill flow regime, and is neither fully turbulent nor fully laminar (*Moore and Foster*, 1990). The water either infiltrates back into the down slope soil (the “runoff/runon” phenomenon), flows into a stream or channel or is stored in topological depressions. Overland flow velocities are significantly faster than those in the subsurface and therefore the surface runoff response is primarily responsible for the peaks of a stream’s storm hydrograph.

There are multiple factors that influence the interactions between the surface and subsurface flow domains. These include topographic features (e.g. slope concavities), soil hydraulic conductivity variations (e.g. thinning of a high-conductivity surface layer), near-surface aquitard layers (which create a perched water table), high conductivity “flow-tubes” or macropores (e.g. root holes), and subsurface pressure waves (*Whipkey and Kirkby*, 1978). There is also continuous interaction and exchange in the near-stream hyporeic zone between the stream stage and the local ground water flow system. The relative influence of these factors on storm flow is primarily dependant on rainfall intensity and duration (e.g. soil permeability increases non-linearly with saturation).

1.2.2 Physically-based modeling

In 1969, Freeze and Harlan ushered in the modern era of distributed hydrologic modeling. They established the basic structure of a fully-coupled watershed model that, combined with the technological advances in computing over the past few decades, has established modeling as a central focus of hydrology. Their model structure serves as the backbone of the majority of physically-based models currently in use. There are several good summaries of distributed hydrologic concepts and models in the literature, including (but not limited to): *Freeze* [1978], *Anderson and Burt* [1985], *Singh* [1995], *O’Connell and Todini* [1996], *Abbott and Refsgaard* [1996], and *Beven* [2000]. The abundance of modeling research precludes a complete summary in this context; however, several key concepts and modeling studies relevant to this work warrant further elaboration.

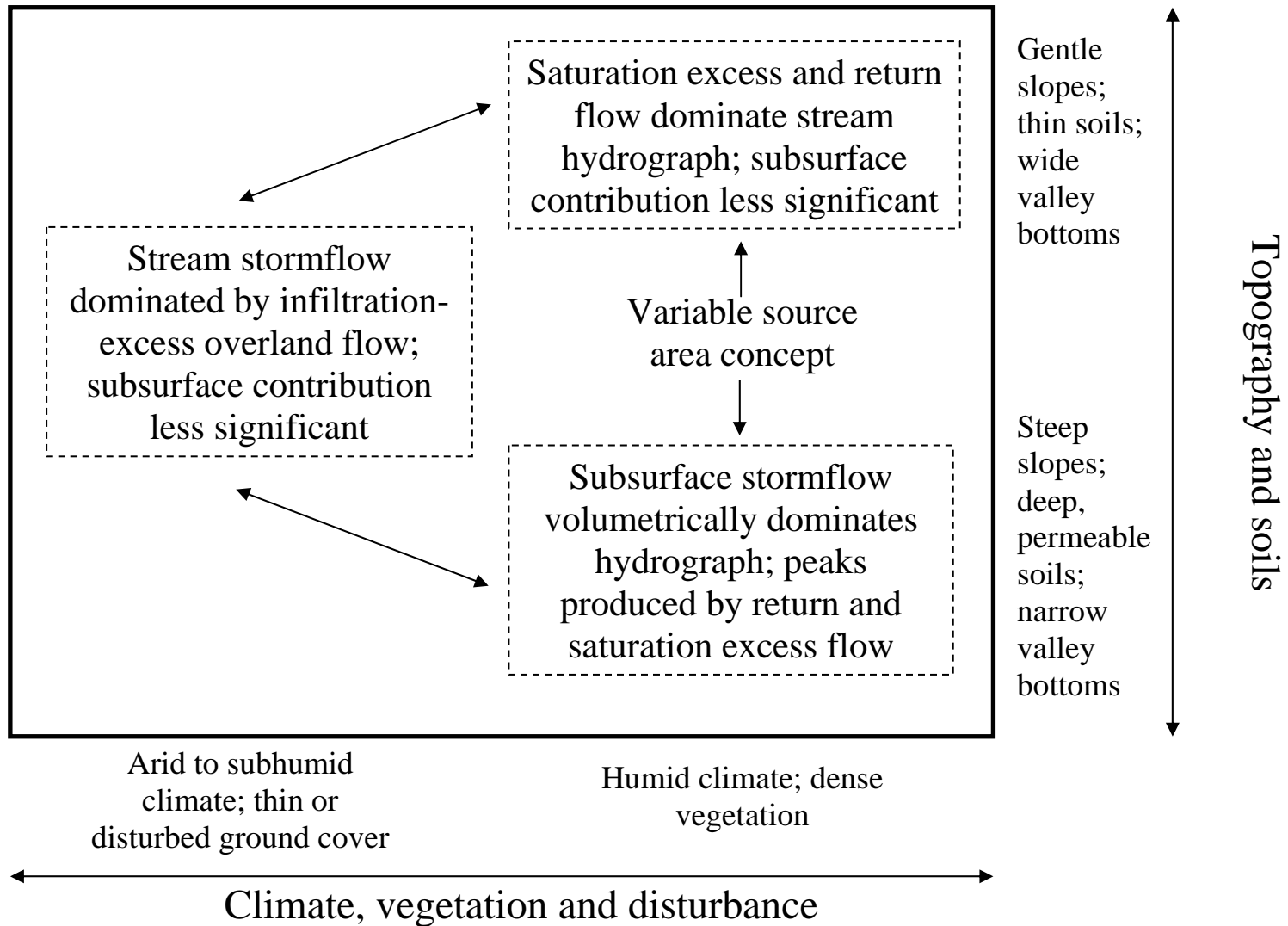


Figure 1.2 The relationship between overland flow mechanisms and their major controlling factors (adapted from *Dunne, 1978*)

There are a number of methods for representing basin response in physically-based hydrologic models. As stated previously (**section 1.1**), these methods are either physically or empirically based. For surface flow, the full Saint Venant equations for shallow water flow offer the most rigorous and complete physical representation but are computationally intensive and difficult to apply to large systems (*Freeze, 1972a*). Most distributed models employ simplifying assumptions to these equations to increase their operational efficiency. The most basic of the resulting simplifications is the kinematic wave approximation. This approximation employs two main assumptions: 1) the flow width is assumed to be much greater than the depth ($\text{depth} \approx \text{hydraulic radius}$), and 2) this depth assumed constant ($\frac{\partial h}{\partial x} \approx 0$), making the water surface parallel to the ground surface. This does not allow for realistic simulation of downstream boundary conditions in overland flow and often results in numerical anomalies (e.g. the ‘kinematic shock’ phenomenon). The approximation is most appropriate for simulating flow over steep, smooth hillslopes (*Vieira, 1983*). Despite its limitations, the kinematic wave approximation continues to be a useful tool in hydrologic modeling (e.g. *Beldring, 2000*).

Many surface water models simulate subsurface flow using an infiltration sink relationship (e.g. *Green and Ampt, 1911*). This increases model efficiency through the assumption that interactions with subsurface have a minimal impact on the transient response associated with rainfall events. Subsurface models generally employ distributed numerical approximations of the saturated-unsaturated flow equation while treating surface interactions as a seepage face sink (*Neuman, 1973*). In most coupled models, surface-subsurface interactions are simulated by matching the boundary conditions at the land surface interface (*Smith and Woolhiser, 1971; Freeze, 1972a & b; Smith and Hebbert, 1983; Abbott et al., 1986; Govindaraju and Kavvas, 1991; Arnold et al., 1993; Wigmosta et al., 1994; Todini, 1996; Perkins and Kousis, 1996; Bronstert and Plate, 1998; Singh and Bhallamudi, 1998; Yu and Schwartz, 1998; Vanderkwaak, 1999; Perkins and Sophocleous, 1999*). The boundary is set at a specified flux until surface ponding occurs after which soil pressure head is constrained to the surface water depth. This has historically created difficulties in algorithm design and computational efficiency. Simulating the interaction across this boundary is difficult due to the

heterogeneous nature of the topography, soil characteristics and hydrologic response of an inherently transient natural system (*Perkins and Kousis, 1996*).

Several of these coupled models merit further discussion. In his pioneering 1972 work, Freeze coupled a three-dimensional (3-D) groundwater model with a one-dimensional (1-D) channel flow model to investigate the influence of the subsurface flow on surface runoff. This model solved the full shallow water equations in one dimension for simulating channel flow. A linear time-delay algorithm was used to route groundwater seepage to the channel. His simulations revealed that surface flow is dependant on subsurface hydrogeologic configuration, soil hydraulic properties, event characteristics (rainfall intensity, duration and distribution) and confirmed the findings of *Ragan [1968]* and *Dunne [1970]* that infiltration excess (Hortonian) overland flow is a rare occurrence in humid/subhumid regions.

The *Système Hydrologique Européen* or “SHE” was developed in 1986 by a consortium of European scientists and engineers as the most complex and physically rigorous hydrologic modeling system of its time (*Abbott et al., 1986*). Surface flow (2-D overland flow and 1-D channel flow) and subsurface flow (1-D unsaturated and 2-D saturated flow) are modeled separately using independent time steps and a mixture of implicit and explicit numerical techniques. The processes are coupled via an interface module that matches the boundary conditions and synchronizes the time steps. The original system included extensive source/sink modules for snowmelt, evaporation/transpiration, and canopy interception. SHE has been continuously enhanced and modified since its inception, with the latest versions, MIKE SHE (*Refsgaard and Storm, 1995*) and SHE/SHEsOD (*Bathurst et al., 1996*) adding improved numerical methods and modules for solute and sediment transport, geochemical processes, erosion, dual subsurface porosity and 3-D saturated subsurface flow.

More recently, *Brown [1995]* coupled subsurface flow with surface flow internally by redefining the capacitance and permeability in the top model layer the TRUST model (*Narasimhan et al., 1978*). This is a unique coupling approach, as it

eliminates the need to match boundary conditions while synchronizing the time steps of the respective flow domains. Modified soil characteristic curves were used to approximate dual porosity flow by inducing high permeability near saturation. Brown's simulations showed that macropore flow exerts a large influence on the subsurface contribution to stream flow and confirmed that channel geometry and structural heterogeneity were critical factors in determining the relative contributions of surface and subsurface flow.

An equally unique modeling approach has been taken by a group of scientists at the Kansas Geological Survey (*Sophocleous et al.*, 1998; *Perkins and Sophocleous*, 1999; *Sophocleous et al.*, 1999; *Sophocleous and Perkins*, 2000). This group has developed an interface module that allows the well-known and widely used 3-D saturated subsurface model MODFLOW (*McDonald and Harbaugh*, 1988) to be coupled to a user-specified surface runoff model. The lumped-parameter watershed model SWAT (*Arnold*, 1993) was used in their main studies (*Perkins and Sophocleous*, 1999; *Sophocleous et al.*, 1999) and an equivalent, yet simpler code, POTYLDL (*Koelliker*, 1994) for studying the Wet Walnut Creek basin (*Sophocleous et al.*, 1998). The interface module links the two models by taking a spatially weighted average of the surface response at each time step and distributing the resulting interface fluxes to the corresponding spatial and temporal location in the aquifer model. The resulting "integrated" model has significantly lower input data requirements than other fully distributed watershed models (e.g. SHE, *Abbott et al.*, 1986) while enhancing the ability to examine stream-aquifer interactions, distributed well withdrawals and land use impacts. These studies show that the versatile applicability and medium complexity of this approach facilitate its use in resource management applications.

VanderKwaak demonstrated the applicability of a fully-coupled comprehensive physics-based modeling approach across multiple spatial scales with the Integrated Hydrology Model (InHM) (*VanderKwaak*, 1999). InHM is a 2-D land surface and 3-D dual-continua subsurface finite element model that simultaneously solves for flow and transport of multiple solutes. Domain interactions are controlled either by continuity

equations or through physically-based first order flux relationships. Several discretization and matrix solution techniques are incorporated into the model for efficiency and robustness. InHM has been used to simulate several controlled field experiments of solute flow and transport (*VanderKwaak, 1999; VanderKwaak and Sudicky, 2000*) and to examine the relative influence of streamflow generation mechanisms in the well-documented R-5 catchment (*VanderKwaak and Loague, 2001, Loague and VanderKwaak, 2002*). On a larger scale, InHM is being used to investigate seasonal water-table behavior and contaminant transport within a well-characterized 75 km² watershed (*Sudicky et al., 2000*). With the relative success of these initial studies, InHM has demonstrated the effectiveness of a comprehensive physics-based approach in representing flow and transport of contaminants.

1.3 Thesis Objectives

“Recent experience with resolution of difficult water-management and allocation problems has shown that a capability to simulate the characteristics of the hydrologic system, at watershed scale, is critical.”

”We must improve tools for simulating interactions between ground water and surface water to quantify the effects of human activity”

Source: “Ground water and Surface water: A single resource,” Winter et al., USGS, 1998

There currently exists a need for a versatile, medium-complexity, physically-based model that is capable of simulating the ground water–surface water interactions throughout a watershed. More specifically, this modeling tool needs to be able to; simulate the mechanisms controlling overland flow and the “runoff/runon” phenomenon; simulate flow through the vadose zone; simulate seepage faces and variable source areas; estimate base flow to a stream or river; and allow the user to define initial and boundary conditions that realistically represent a system’s topography, soil heterogeneity, sources and sinks such as wells or drains, evapotranspiration and precipitation. The model should be designed to represent daily and seasonal behavior (e.g. water table fluctuations and baseflow contributions) rather than event behavior (e.g. flood prediction). For the model to be immediately useful to operational hydrologists and scientists, the approach needs to be somewhat less comprehensive, and thus requiring fewer model parameters to be calibrated, than a system such as MIKE-SHE (*Refsgaard and Storm, 1995*) or InHM (*Vanderkwaak, 1999*). However, in order to investigate surface-subsurface interactions within the vadose zone, this approach should include the capability to simulate unsaturated soil flow (unlike *Sophocleous et al., 1998*).

The primary goal of this study is to present several new capabilities for MODFLOW (*McDonald and Harbaugh, 1988*) that allow the user to simulate overland flow and variably-saturated flow in a distributed, fully-coupled fashion while retaining all of the existing features that are responsible for its widespread usage. The fundamental objectives required to meet this goal are:

- 1) Determine the appropriate mathematical methods that will fulfill the aforementioned needs,
- 2) Use these methods to develop new features within MODFLOW in a way that will retain the model code's modular structure, its multitude of existing features and its compatibility with transport models, commercial graphical interfaces and other software packages;
- 3) Test these features against an analytical solution and empirical results in order to verify the model's utility as a hydrologic tool.

The first two objectives are addressed in **Chapter 2: Model Description** and further detailed in **Appendices A through E**. The final objective is covered in **Chapter 3: Model Verification**. A discussion of the results and implications for future research studies is presented in **Chapter 4: Conclusions and Future Considerations**.

Chapter 2

Model Description

The hydrologic processes of overland flow and variably saturated porous media flow are essential components of a holistic watershed model. The ability to simulate the various mechanisms that control these processes (**figure 1.1**) provides the model-user important insight into watershed systems. Several features were developed and incorporated as ‘packages’ into the three-dimensional (3-D), modular finite-difference model MODFLOW (*McDonald and Harbaugh*, 1988) to simulate these processes in a fully coupled fashion. The model’s modular structure remains intact, retaining all of the present capabilities while providing additional features that allow the user to simulate the hydrologic cycle of a watershed more completely. The governing equations and a basic description of each feature follows.

2.1 Variably Saturated Groundwater Flow

2.1.1 Governing Equations

Three-dimensional, variably saturated isothermal fluid flow in a heterogeneous porous medium is described by an equation that is derived from the incorporation of Darcy's law into the conservation of mass equation for liquid phase flow (*Freeze, 1978*). Darcy's law can be expressed as:

$$v_i = k_r(\psi) \frac{k_i}{n_e} \frac{\rho g}{\mu} \frac{\partial h}{\partial x_i} = K_i(\psi) \frac{\partial h}{\partial x_i} \quad (2.1)$$

where

- i = coordinate indices ($i = 1, 2, 3$)
- v = pore velocity of the fluid [L/T]
- h = total hydraulic head (equal to the sum of the soil water pressure head, ψ , and the elevation head, z) [L]
- ψ = soil pore pressure head ($\psi = h - z$) [L]
- $k_r(\psi)$ = relative permeability of a particular medium (soil type) as a function of pressure head, ψ [-]
- k_i = intrinsic permeability of the medium [L]
- n_e = effective porosity of the medium (drainable void volume / total bulk volume) [-]
- ρ = density of the active fluid (i.e. water) [M/L³]
- g = gravitational acceleration [L²/T²]
- μ = dynamic viscosity of water [M/LT]
- x_i = spatial coordinate [L]
- $K_i(\psi)$ = hydraulic conductivity as a function of soil pressure head [L]

The continuity equation represents the conservation of mass during fluid flow through an elemental volume of the porous medium. This equation takes the form (Freeze, 1978):

$$\frac{\partial(n\rho v_x)}{\partial x} + \frac{\partial(n\rho v_y)}{\partial y} + \frac{\partial(n\rho v_z)}{\partial z} = \frac{\partial h}{\partial t} \left[\rho n \frac{\partial \Theta}{\partial h} + \rho \Theta \frac{\partial n}{\partial h} + n \Theta \frac{\partial \rho}{\partial h} \right] \quad (2.2)$$

where

$$\begin{aligned} \Theta &= \text{saturation of the soil (water volume / drainable void volume) [-]} \\ t &= \text{time [T]} \end{aligned}$$

The bracketed terms on the right hand side of equation (2.2) describe the storage properties of the medium. These account for changes in liquid stored in the elementary volume due to changes in soil saturation Θ , changes in the soil pore space n , and compression or expansion of the liquid (changes in the fluid density, ρ). For a given soil type or geologic formation, the porosity, density and soil moisture content are assumed to be solely dependant on the soil pressure head ψ . Several terms can be defined to simplify the right hand side of equation 2.2 (Lappala *et al.*, 1993):

$$\begin{aligned} \text{Specific moisture capacity [L}^{-1}\text{]:} \quad C &= \frac{\partial \theta}{\partial \psi} \\ \text{Matrix compressibility [T}^2\text{L/M]:} \quad \alpha_c &= \frac{\partial n}{\partial \bar{\psi}} \\ \text{Fluid compressibility [LT}^2\text{/M]:} \quad \beta_c &= \frac{1}{\rho} \frac{\partial \rho}{\partial \bar{\psi}} \\ \text{Specific storage [L}^{-1}\text{]:} \quad S_s &= \rho g (n\beta_c + \alpha_c) \end{aligned}$$

where

$$\begin{aligned} \theta &= \text{volumetric soil water content } (\Theta \cdot n_e) \text{ (water volume / total bulk volume) [-]} \\ \bar{\psi} &= \text{the average soil pore pressure head in the matrix [L]} \end{aligned}$$

For simplification, the assumption is frequently made that the fluid and soil matrix are only slightly compressible. Therefore the specific storage term, S_s is assumed to be constant for a given soil type or geologic formation. It represents the volume of water per unit aquifer area that a unit volume of soil matrix releases (or takes up) in response to a unit decrease (or increase) in hydraulic head (*Dingman, 2002*). This assumption, combined with equations (2.1) and (2.2), results in what is known as *Richard's equation* for variably saturated flow (*Huyakorn and Pinder, 1983*):

$$\frac{\partial}{\partial x} \left[K_x(\psi) \frac{\partial h}{\partial x} \right] + \frac{\partial}{\partial y} \left[K_y(\psi) \frac{\partial h}{\partial y} \right] + \frac{\partial}{\partial z} \left[K_z(\psi) \frac{\partial h}{\partial z} \right] + W = \frac{\partial h}{\partial t} [\Theta S_s + C(\psi)] \quad (2.3)$$

where:

$$W = \text{volumetric flux per unit volume representing sources and/or sinks [T}^{-1}\text{]}$$

This parabolic equation is highly nonlinear due to the nature of the hydraulic conductivity $K(\psi)$ and specific moisture capacity $C(\psi)$ functions. The ground water flow model, MODFLOW employs several simplifying assumptions in order to simulate saturated flow through porous media. Defining the hydraulic conductivity term as the product of the relative permeability, $k_r(\psi)$ and the saturated hydraulic conductivity, K^s ($K(\psi) = k_r(\psi)K^s$) allows the expression to reduce to the constant value K^s as the relative permeability converges to one for saturated conditions. As the soil pressure head ψ becomes positive and the pores saturate with water, the specific moisture capacity C converges to zero and the soil saturation Θ converges to one. Thus, equation (2.3) converges to the general flow equation used by MODFLOW (equation 1, *Harbaugh et al., 2000*) for saturated subsurface flow:

$$\frac{\partial}{\partial x} \left[K_x^s \frac{\partial h}{\partial x} \right] + \frac{\partial}{\partial y} \left[K_y^s \frac{\partial h}{\partial y} \right] + \frac{\partial}{\partial z} \left[K_z^s \frac{\partial h}{\partial z} \right] + W = S_s \frac{\partial h}{\partial t} \quad (2.4)$$

Equation (2.3) allows MODFLOW to simulate a subsurface domain from the ground surface through the unsaturated (vadose) zone past the water table into the saturated aquifer. Implementing and testing the performance of this new governing equation is detailed in **Section 3.1**.

2.1.2 Soil Characteristic Functions

In order for MODFLOW to simulate variably saturated porous media flow, several relationships must be defined describing the unsaturated flow and storage properties intrinsic to a soil. The soil characteristic functions $K(\psi)$, $\theta(\psi)$, and $C(\psi)$ have been represented in the literature by several different empirical and theoretical methods (Millington and Quirk, 1961; Brooks and Corey, 1964; Mualem, 1976; Haverkamp et al., 1977; van Genuchten, 1980, Broadbridge and White, 1988). The modular design of the MODFLOW model allows for efficient implementation of a variety of different functions within the code. This allows the user to specify the soil characteristic functions most appropriate for a given scenario and resulting in greater flexibility for simulating complex systems. The studies included in this work use the non-hysteretic (singular) van Genuchten-Mualem soil characteristic functions, except where stated otherwise. These functions take the form:

Effective saturation as a function of capillary pressure head (van Genuchten, 1980):

$$\Theta_e(h_c) = \frac{\Theta - \Theta_r}{1 - \Theta_r} = \begin{cases} \frac{1}{[1 + (\alpha h_c)^\beta]^\gamma} & \psi < 0 \\ 1 & \psi \geq 0 \end{cases} \quad (2.5)$$

Specific moisture capacity as a function of effective saturation:

$$C(\Theta_e) = \frac{\partial \theta}{\partial \psi} = -\frac{\gamma \alpha (1 - \Theta_r)}{1 - \gamma} \Theta_e^{1/\gamma} (1 - \Theta_e^{1/\gamma})^\gamma \quad (2.6)$$

Relative permeability as a function of effective saturation (Mualem, 1976):

$$k_r(\Theta_e) = \Theta_e^{1/2} \left[1 - \left(1 - \Theta_e^{1/\gamma} \right)^\gamma \right]^2 \quad (2.7)$$

where:

- h_c = capillary pressure head ($h_c = h_a - \psi$)
- h_a = atmospheric pressure (assumed to be zero) [L]
- Θ_r = residual soil saturation [-]
- β, γ = soil parameters ($\gamma = 1 - 1/\beta$) representing the degree of pore size uniformity (as β increases, uniformity increases) [-]
- α = parameter representing the inverse characteristic length of the soil pores [1/L]

There are numerous methods suggested in the literature for computing the intercell average of the relative permeabilities between grid cells (*Brutsaert, 1971; Warrick, 1991; Zaidel and Russo, 1992; Baker, 1995; Desbarats, 1995*) for block-centered finite difference models. In general, the appropriate method depends on the hydraulic properties of the system and how well the system is characterized. Due to the relatively fine space-time meshes used in this work, an arithmetic mean (or ‘midpoint’ average) is used for all studies presented here.

2.1.3 Modified Picard Iteration Technique

The governing equation of MODFLOW was changed from a “head-based” form to a “mixed” form in order to incorporate the modified Picard iteration technique (*Celia et al., 1990*). This technique was used to minimize the numerical errors resulting from coarse temporal discretization and maintain mass balance for a range of time step sizes. These errors are common in the implicit finite-difference “head-based” formulation of the inherently non-linear Richard’s equation. This ‘modified-Picard’ linearization technique is employed in the backward Euler approximation through the Taylor series expansion of $\theta^{n+1,m+1}$ with respect to total head (h): (*Celia et al., 1990*)

$$\frac{\partial \theta}{\partial t} = C \frac{\partial h}{\partial t} \cong \frac{\theta^{n,m} - \theta^{n-1}}{\Delta t} \quad (2.8)$$

$$\theta^{n,m} = \theta^{n,m-1} + \left. \frac{d\theta}{dh} \right|^{n,m-1} (H^{n,m} - H^{n,m-1}) + O(\partial^2) \quad (2.9)$$

where:

n = time step level

m = iteration level

$H^{n,m}$ = approximate value for h at n^{th} discrete time level ($t = t^n$) and m^{th} iteration

Δt = $t^n - t^{n-1}$

Neglecting all terms higher than linear in (2.9) and combining (2.8) and (2.9) with the storage terms of (2.3) results in the approximation:

$$C \frac{\partial h}{\partial t} + \Theta S_s \frac{\partial h}{\partial t} \cong \frac{\theta^{n,m-1} + C^{n,m-1} (H^{n,m} - H^{n,m-1}) - \theta^{n-1}}{\Delta t} + \Theta^{n-1/2} S_s \frac{H^{n,m} - H^{n-1}}{\Delta t} \quad (2.10)$$

In the MODFLOW model formulation, the finite difference form of equation (2.4) for a grid cell is (Harbaugh *et al.*, 2000, pg 11):

$$\begin{aligned} & CR_{i,j-\frac{1}{2},k} (H_{i,j-1,k}^n - H_{i,j,k}^n) + CR_{i,j+\frac{1}{2},k} (H_{i,j+1,k}^n - H_{i,j,k}^n) \\ & + CC_{i-\frac{1}{2},j,k} (H_{i-1,j,k}^n - H_{i,j,k}^n) + CC_{i+\frac{1}{2},j,k} (H_{i+1,j,k}^n - H_{i,j,k}^n) \\ & + CV_{i,j,k-\frac{1}{2}} (H_{i,j,k-1}^n - H_{i,j,k}^n) + CV_{i,j,k+\frac{1}{2}} (H_{i,j,k+1}^n - H_{i,j,k}^n) \\ & + P_{i,j,k} H_{i,j,k}^n + Q_{i,j,k} = SS_{i,j,k} (DELR_j \times DELC_i \times THICK_{i,j,k}) \frac{H_{i,j,k}^n - H_{i,j,k}^{n-1}}{\Delta t} \end{aligned} \quad (2.11)$$

where:

- $H_{i,j,k}^n$ = total head in cell i,j,k at time step n [L]
- CR, CC, CV = hydraulic conductances between node i,j,k and an adjacent node [L^2/T]
- $P_{i,j,k}$ = sum of head coefficients from source and sink terms [L^2/T]
- $Q_{i,j,k}$ = sum of constants from source and sink terms [L^3/T]
- $SS_{i,j,k}$ = specific storage [L^{-1}]
- $DELR_j$ = cell width of column j in all rows [L]
- $DELC_i$ = cell width of row i in all columns [L]
- $THICK_k$ = vertical thickness of cell i,j,k [L]
- t^n = time at time step n [T]

This is further simplified for solution by computer into:

$$\begin{aligned}
 & CV_{i,j,k-\frac{1}{2}} H_{i,j,k-1}^n + CC_{i-\frac{1}{2},j,k} H_{i-1,j,k}^n + CR_{i,j-\frac{1}{2},k} H_{i,j-1,k}^n \\
 & + \left(-CV_{i,j,k-\frac{1}{2}} - CC_{i-\frac{1}{2},j,k} - CR_{i,j-\frac{1}{2},k} - CV_{i,j,k+\frac{1}{2}} - CC_{i+\frac{1}{2},j,k} - CR_{i,j+\frac{1}{2},k} + HCOF_{i,j,k} \right) H_{i,j,k}^n \\
 & CV_{i,j,k+\frac{1}{2}} H_{i,j,k+1}^n + CC_{i+\frac{1}{2},j,k} H_{i+1,j,k}^n + CR_{i,j+\frac{1}{2},k} H_{i,j+1,k}^n = RHS_{i,j,k}
 \end{aligned} \tag{2.12}$$

where:

$$\begin{aligned}
 RHS_{i,j,k} &= -Q_{i,j,k} - \frac{SS_{i,j,k} (DEL C_i \times DEL R_j \times THICK_k)}{\Delta t} H_{i,j,k}^{n-1} \\
 HCOF_{i,j,k} &= P_{i,j,k} - \frac{SS_{i,j,k} (DEL C_i \times DEL R_j \times THICK_k)}{\Delta t}
 \end{aligned}$$

In order to implement the modified Picard iteration technique into MODFLOW, the RHS and HCOF terms in equation (2.12) are changed to incorporate the unsaturated storage terms:

$$RHS = -Q_{i,j,k} + \left[\frac{\theta^{n,m-1} - \theta^{n-1}}{t^n - t^{n-1}} - \frac{C^{n,m-1} + \Theta^{n-1/2} SS_{i,j,k}}{\Delta t} H_{i,j,k}^{n-1} \right] (DEL C_i \times DEL R_j \times THICK_k) \tag{2.13}$$

$$HCOF = \left[\frac{C^{n,m-1} + \Theta^{n-1/2} SS_{i,j,k}}{\Delta t} \right] (DEL C_i \times DEL R_j \times THICK_k) \tag{2.14}$$

In order to confirm proper implementation of the iteration technique, the simulations of *Celia et al.* (1990) are repeated here. These simulations use the initial and boundary conditions of *Haverkamp et al.* (1977) for constant head infiltration in a sand column (**table 2.1**). Four simulations were performed using the same initial and boundary conditions, varying only the time step (i.e. $\Delta t = 1$ second, 5 seconds, 30 seconds, and 120 seconds). The column profiles for an elapsed time of 360 seconds are shown in **figure 2.1**. These results demonstrate the technique's effectiveness in maintaining a global mass balance across a wide range of time steps. The results presented here match those presented in *Celia et al.* (1990) (not shown here), thereby confirming the correct execution of the technique.

Table 2.1: Model parameters for simulations verifying the Modified-Picard iteration technique (*Celia et al.*, 1990)

Constant head infiltration in sand (<i>Haverkamp et al.</i>, 1977)	
$K_{rel}(h)$	$K_{rel} = \frac{A}{A + h ^\beta}; A=1.175 \text{ E6}, B=4.74$ $K_{sat}=34 \text{ cm/hr}$
$\theta(h)$	$\theta = \frac{\alpha(\theta_s - \theta_r)}{(\alpha + h ^\beta)} + \theta_r; \theta_s=0.287, \theta_r=0.075$ $\alpha=1.611 \text{ E6}, \beta=3.96$
$C(h)$	$C = \alpha\beta \frac{(\theta_s - \theta_r) h ^{\beta-1}}{[\alpha + h ^\beta]^2}$
Initial conditions	$t < 0, z \geq 0, \theta_0 = 0.10 \text{ cm}^3 / \text{cm}^3$
Boundary Conditions	$t \geq 0, z = 0, \theta_1 = 0.267 \text{ cm}^3 / \text{cm}^3$
Discretization	$\Delta x = 1 \text{ cm};$ $\Delta t = 1, 5, 30, \text{ and } 120 \text{ seconds}$

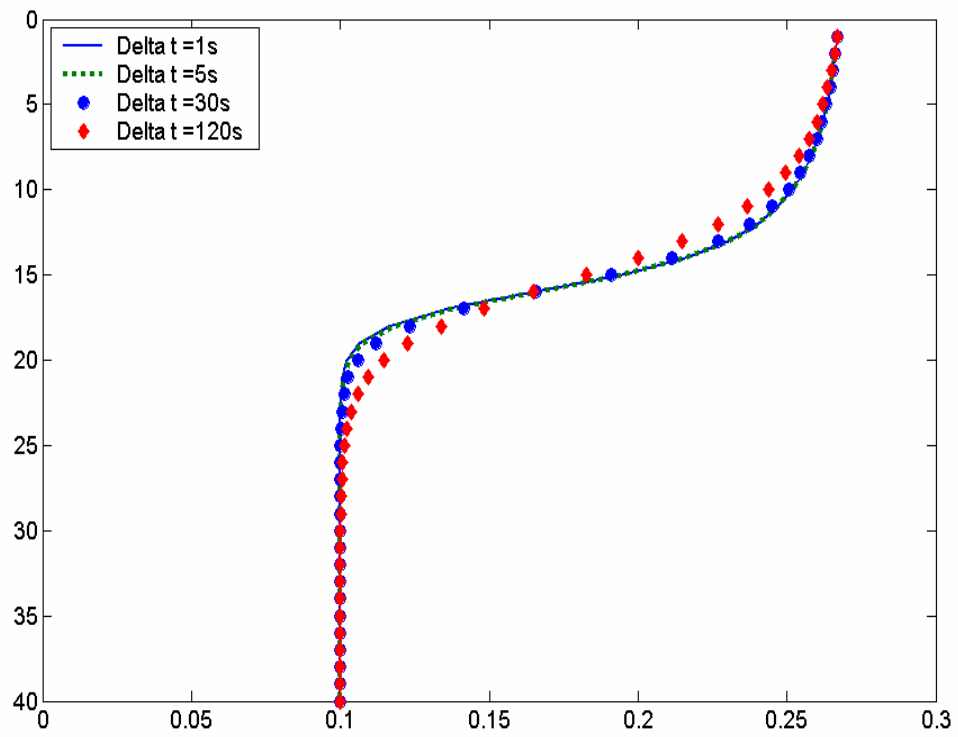


Figure 2.1: Solutions at $T = 360$ seconds for constant head infiltration in a sand column using the Modified Picard linearization technique

2.2 Overland Flow

2.2.1 Implementation in MODFLOW

Several modifications were made in order to adapt MODFLOW for simulating overland flow on the ground surface using the kinematic flow approximation. The overland flow package designates the top of the second grid layer in the model as the ground surface and uses the top layer as an overland flow conductance layer. The cells in this layer are assigned a horizontal conductance value that is computed from the Darcy-Weisbach equation for steady uniform surface flow. The vertical hydraulic conductivity for each overland flow cell is set constant and equal to the saturated conductivity (K^s) of the land surface cell immediately below. The top layer's leakance (intercell vertical hydraulic conductivity divided by the distance between cell nodes) is set equal to K^s divided by the half cell thickness of the second layer. Infiltration is thus controlled by the local head gradient and the soil conditions of the second grid layer. The overland flow layer is treated as a saturated soil layer with no storage properties ($\Theta = 1$, $C = 0$, $S_s = 0$) that only conducts water vertically until the hydraulic head exceeds the ground surface elevation. When this occurs, the effective horizontal conductivity parameters (developed below) are activated and the storage term in equation (2.3) is set equal to one (equivalent to a unit volume of water released per unit decrease in flow height). The top layer's governing equation is thus converted into the kinematic flow approximation for overland flow, allowing the model to perform surface and subsurface computations concurrently in the same time step.

The top boundary condition incorporates a rule-set for partitioning rainfall input based on the soil conditions in the second layer (similar to the rules-set used by *Brown*, 1995). This rule-set operates as a series of logical statements that compares the rainfall rate in each time step to the vertical conductance of the land surface grid cell (2nd layer). Depending on the total hydraulic head in the land surface cell and direction of the head gradient, one of three conditions will exist:

1. The local head gradient is creating exfiltration from the land surface into the overland flow cell. The flux term is applied to the overland flow cell because this gradient prevents downward flow.
2. The rainfall rate is less than the vertical conductance through the land surface cell. The flux term is applied to the land surface cell because the soil has the ability to transmit the water downward.
3. The rainfall rate is greater than the vertical conductance of the land surface cell. The flux term is applied to the overland flow cell because the soil can only partially transmit the flow downward.

Based on this rule set, the only condition in which the rainfall flux is applied to the soil cell is when the cell's conductance exceeds the rainfall rate. However, infiltration from the overland flow layer still occurs as governed by the local head gradient and material properties of the surface cell. This allows the model to simulate the “runoff / run-on” phenomena in which water flowing laterally can infiltrate back into the soil based on local conductance and head gradient conditions.

2.2.2 Governing equations

The kinematic wave approximation's mathematical properties allow it to be incorporated directly into the MODFLOW formulation, i.e. the assumption that the friction slope is equal to the bed slope eliminates the cross derivatives (e.g. $\frac{\partial u_x}{\partial y}$) that require decoupling the surface and subsurface computations. This simplification also eliminates the need for specifying the downstream surface depth boundary condition (Ruan, 1998), making it amenable to MODFLOW's fully implicit formulation. Numerical difficulties associated with this approximation (i.e. “kinematic shock”) can be avoided through simplification of the surface geometry and application of spatially invariant lateral inflow (rainfall) (Beldring, 2000). This fully-integrated approach maintains a mass balance in the partitioning process at the ground surface by including the overland flow cells in the model's formulation of mass conservation (Brown, 1995).

This allows the model to simulate the “runoff/runon” phenomenon, the interaction between surface runoff and infiltration that has important implications on the hillslope scale (*Woolhiser et al.*, 1996). The variability of hydraulic parameters that influence these interactions can easily be incorporated into the conceptual model through the standard MODFLOW input files.

The formulation for horizontal mass conductance in the overland flow cells used in this model is derived from the Darcy-Weisbach equation for steady uniform flow in conduits of constant cross section (*Chin*, 2000):

$$\bar{u}^2 = \frac{8gds}{f} \quad (2.14)$$

where:

$$\begin{aligned} \bar{u}^2 &= \text{vertically averaged mean flow velocity [L/T]} \\ g &= \text{gravitational acceleration [L}^2\text{/T]} \\ d &= \text{mean surface flow depth [L]} \\ s &= \text{local gradient of the water surface [L/L]} \\ f &= \text{dimensionless friction factor} \end{aligned}$$

The assumption of laminar flow is made for all of the model simulations presented in this work (following *Brown*, 1995), setting up a linear relationship between the friction factor and the local flow Reynolds Number $\left(N_R = \bar{u}d\rho/\mu\right)$:

$$f = \frac{k_d}{N_R} \quad (2.15)$$

where:

$$k_d = \text{dimensionless parameter describing the roughness of the hillslope surface (Dunne and Dietrich, 1980)}$$

Combining (2.13) and (2.14) results in an equation that, within this model's formulation, can be directly compared to Darcy's Law (2.1):

$$\bar{u} = 8 \frac{\rho g}{\mu} \frac{d^2}{k_d} \frac{\partial h}{\partial x_i} \quad (2.16)$$

where d is the mean water pressure head (i.e. flow depth = $h - z_{\text{surface}}$) at the ground surface interface. Equating (2.15) and (2.1) yields an effective conductivity (K_{of}) for the overland flow cells:

$$K_{of} = 8 \frac{\rho g}{\mu} \frac{d^2}{k_d} \quad (2.17)$$

This effective conductivity is used within the MODFLOW finite difference formulation for the top layer's grid cells. The strong dependence of this effective conductivity value on the pressure at the ground surface makes it necessary to specify a minimum flow depth (0.1 mm) for the model, below which K_{of} is set to zero. This minimizes the numerical difficulties introduced by this non-linear term. This threshold depth is of the same length-scale order of soil grains, making it difficult to distinguish between surface flow and flow through the porous medium. (*Brown, 1995*)

These modifications convert the horizontal flow formulation of MODFLOW into the two-dimensional (2-D) kinematic wave equation for the model's top grid layer:

$$K_{of}(d) \frac{\partial h}{\partial x} + K_{of}(d) \frac{\partial h}{\partial y} + W = \frac{\partial h}{\partial t} \quad (2.18)$$

where:

$$W = \text{infiltration}, \quad K_z(\psi) \frac{\partial h}{\partial z} \quad [\text{L/T}]$$

Chapter 3

Model Verification

The purpose of this chapter is to test the newly developed features described in **Chapter 2** against analytical solution and empirical data sets in order to verify the model's utility in simulating flow through the vadose zone and across the ground surface. The first section consists of subsurface simulations that compare the model performance against an analytical solution for constant head infiltration in **Section 3.1.1**; against a field study of one-dimensional (1-D) infiltration under constant rainfall conditions in **Section 3.1.2**; and examines the model's performance across a range of spatial grids and soil types in **Section 3.1.3**. The second section (**Section 3.2**) is a simulation of conjunctive 1-D surface and 2-D subsurface flow based on the experiment of *Smith and Woolhiser* (1971). The third section (**Section 3.3**) is a mass balance analysis of a selection of the 1-D simulations from **Section 3.1.3** and of the conjunctive surface-subsurface simulation from **Section 3.2**.

3.1 Subsurface Simulations

3.1.1 One-dimensional analytical solution for unsaturated flow

The strong nonlinearity of Richard's equation precludes a closed form analytical solution of the flow equation except under very restrictive initial and boundary conditions. *Phillip* (1969) presented a quasi-analytical solution for 1-D infiltration in a semi-infinite column under a constant head boundary condition. Philip's solution is used here to verify the accuracy of this model's formulation under unsaturated conditions.

It takes the form of an infinite series (valid for finite values of t):

$$z(\theta, t) = \phi_1 t^{1/2} + \phi_2 t + \phi_3 t^{3/2} + \phi_4 t^2 + \dots \quad (3.1)$$

where

$z(\theta, t)$ = depth [L]

θ = volumetric soil moisture content (decimal fraction)

t = time [T]

ϕ_n = nth order function of θ

This solution is valid for the following initial and boundary conditions:

$$t = 0, \quad z > 0, \quad \theta = \theta_0$$

$$t \geq 0, \quad z = 0, \quad \theta = \theta_1$$

In order to evaluate the performance of the unsaturated flow component of the model presented here, two one-dimensional simulations were performed using the initial and boundary conditions listed above. These simulations represent infiltration in a sand and clay column (respectively) and are based on the work of *Haverkamp et al.* (1977). The initial and boundary conditions as well as the characteristic relationships ($K(h)$, $\theta(h)$, and $C(h)$) used are listed in table 3.1. Model results for both simulations are plotted against Phillip's solution at selected times in **figure 3.1**. In both the sand and the clay cases, the model matches the analytical solution values very closely despite some minor underprediction of the infiltration front for sand (**figure 3.1b**) during the later time ($t = 0.8$ hours).

Table 3.1: Model parameters for constant head infiltration in a soil column

Constant head infiltration in Yolo light clay (<i>Haverkamp et al., 1977</i>)	
$K_{rel}(h_c)$	$K_{rel} = \frac{A}{A + h_c ^\beta}; A=124.6, B=1.77$ $K_{sat}=4.428 \text{ E-2 cm/hr}$
$\theta(h_c)$	$\theta = \frac{\alpha(\theta_s - \theta_r)}{(\alpha + \ln h_c ^\beta)} + \theta_r; \theta_s=0.495, \theta_r=0.124$ $\alpha=739, \beta=4$
$C(h_c)$	$C = \frac{\alpha\beta (\theta_s - \theta_r) h_c ^{\beta-1}}{h_c [\alpha + \ln h_c ^\beta]^2}$
Initial Conditions	$t < 0, z \geq 0, \theta_0 = 0.2376 \text{ cm}^3 / \text{cm}^3$
Boundary Conditions	$t \geq 0, z = 0, \theta_1 = 0.4950 \text{ cm}^3 / \text{cm}^3$
Discretization	$\Delta x = 1 \text{ cm};$ $\Delta t = 40 \text{ seconds (} t < 130 \text{ hours);}$ $\Delta t = 500 \text{ seconds (} t > 130 \text{ hours)}$
Constant head infiltration in sand (<i>Haverkamp et al., 1977</i>)	
$K_{rel}(h_c)$	$K_{rel} = \frac{A}{A + h_c ^\beta}; A=1.175 \text{ E6, B=4.74}$ $K_{sat}=34 \text{ cm/hr}$
$\theta(h_c)$	$\theta = \frac{\alpha(\theta_s - \theta_r)}{(\alpha + h_c ^\beta)} + \theta_r; \theta_s=0.287, \theta_r=0.075$ $\alpha=1.611 \text{ E6, } \beta=3.96$
$C(h_c)$	$C = \alpha\beta \frac{(\theta_s - \theta_r) h_c ^{\beta-1}}{[\alpha + h_c ^\beta]^2}$
Initial Conditions	$t < 0, z \geq 0, \theta_0 = 0.10 \text{ cm}^3 / \text{cm}^3$
Boundary Conditions	$t \geq 0, z = 0, \theta_1 = 0.267 \text{ cm}^3 / \text{cm}^3$
Discretization	$\Delta x = 1 \text{ cm};$ $\Delta t = 5 \text{ seconds}$

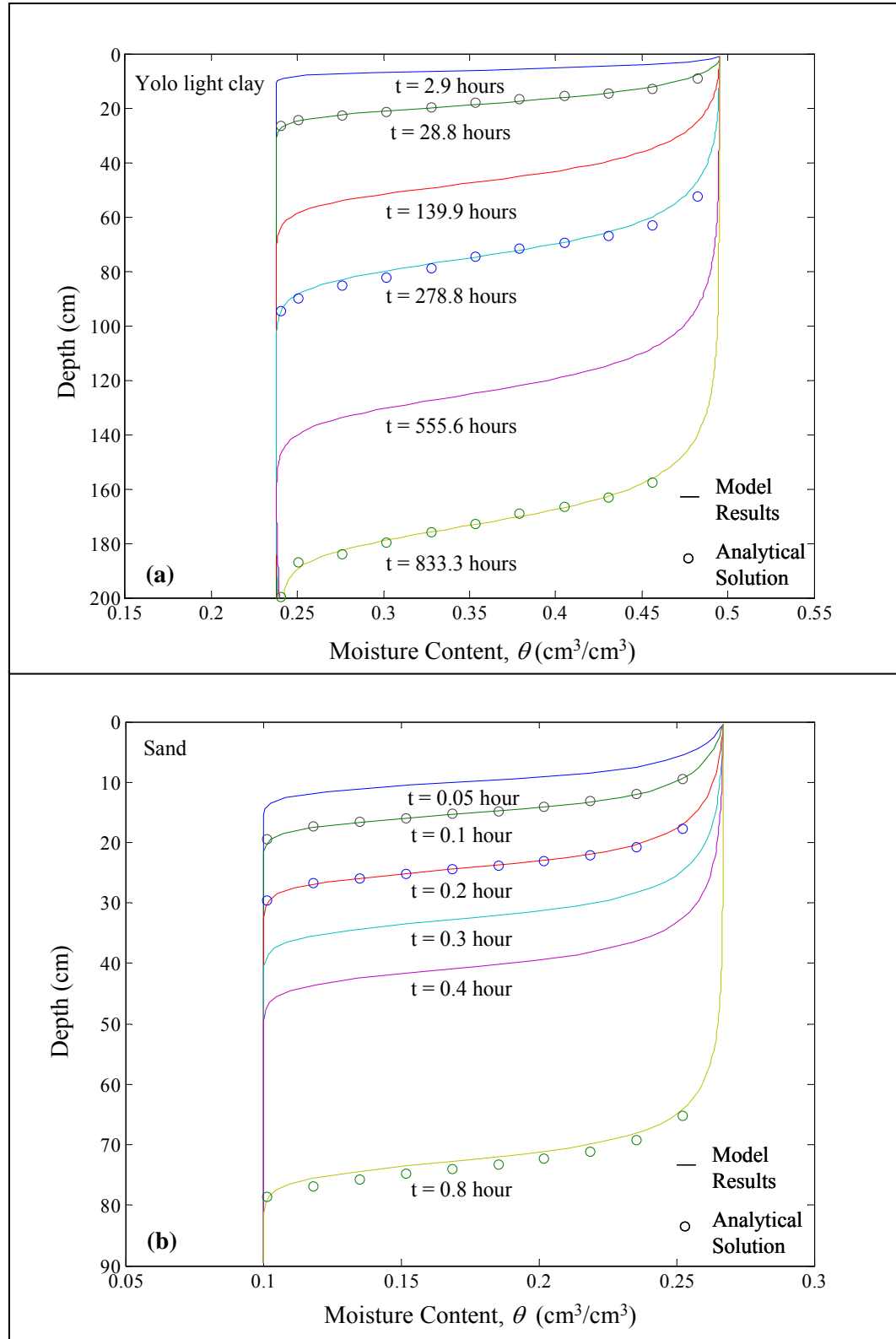


Figure 3.1: Comparison between simulated water content profiles and the Philip's analytical solution obtained at selected times for one-dimensional constant head infiltration in (a) Yolo light clay and (b) sand

3.1.2 One-dimensional field study

To demonstrate its utility in representing physical reality, the model was used to simulate the infiltration study of *Warrick et al.* (1971). This field experiment was performed in a 6.1 meter² soil plot containing tensiometers at 30, 60, 90, 120, 150, 180 cm depths. A conservative tracer solution (0.2 N CaCl₂) was used to track solute transport through the system. Measurements were collected for 17.5 hours during which the soil surface was kept at constant saturation. The tracer solution was applied to the surface for 2.8 hours followed by 15.3 hours of water.

The initial soil moisture profile is approximately linear from $\theta = 0.15 \text{ cm}^3/\text{cm}^3$ at the surface to $\theta = 0.2 \text{ cm}^3/\text{cm}^3$ at $z \leq 60 \text{ cm}$. The soil characteristic functions were fit¹ to the soil hydraulic conductivity and capillary saturation data and are shown in **figures 3.2 and 3.3**, respectively. A summary of the soil parameters and model conditions used for this study as well as the following study (**section 3.1.3**) are listed in **table 3.2**. Results for the flow simulation after 2 hours and 9 hours of infiltration are shown in **figure 3.4** plotted against the experimental data as well as simulation results from the 1-D unsaturated flow finite element model, SUMATRA (*van Genuchten, 1978*). The model represents the experimental results well; there is some over-prediction of the infiltration front at $t=2$ hours that can be attributed to the over-prediction of k_r at low θ in the van Genuchten relationship (**figure 3.3**). The solute transport was also simulated using a modified version of the RT3D transport model (*Clement, 1997*) and the results are presented in **appendix B**.

¹ The experimental data values shown in figure 3.3 and 3.4 was extracted from (*Warrick et al., 1971*) using the “Data Thief” shareware utility. The interpolation utility RETC (*van Genuchten et al., 1997*) was then used to determine the best-fit van Genuchten-Mualem soil parameters for this soil.

Table 3.2: Model parameters for the Warrick et al. (1971) field study (Section 3.1.2) and the soil characteristics and discretization analysis (Section 3.1.3)

Field infiltration study (<i>Warrick et al.</i>, 1971)	
Initial conditions	$t < 0, 0 \leq z \leq 60 \text{ cm},$ $\theta = 0.15 + 0.0008333 * z \text{ (cm}^3 / \text{cm}^3\text{)}$
	$t < 0, z > 60 \text{ cm}, \theta = 0.2 \text{ cm}^3 / \text{cm}^3$
Boundary Conditions	$t > 0, z = 0, \theta_1 = 0.38 \text{ cm}^3 / \text{cm}^3$
Soil Properties (van Genuchten / Mualem parameters, equations 2.5, 2.6, 2.7)	
Medium coarse soil (<i>Warrick et al.</i> , 1971)	$K^s = 38.16 \text{ cm/day}$ $\theta_s = 0.381, \theta_r = 0.15$ $\alpha = 0.016 \text{ cm}^{-1}, \beta = 2.7$
Fine soil	$K^s = 38.16 \text{ cm/day}$ $\theta_s = 0.381, \theta_r = 0.15$ $\alpha = 0.015 \text{ cm}^{-1}, \beta = 1.5$
Coarse soil	$K^s = 38.16 \text{ cm/day}$ $\theta_s = 0.381, \theta_r = 0.15$ $\alpha = 0.2 \text{ cm}^{-1}, \beta = 5.0$

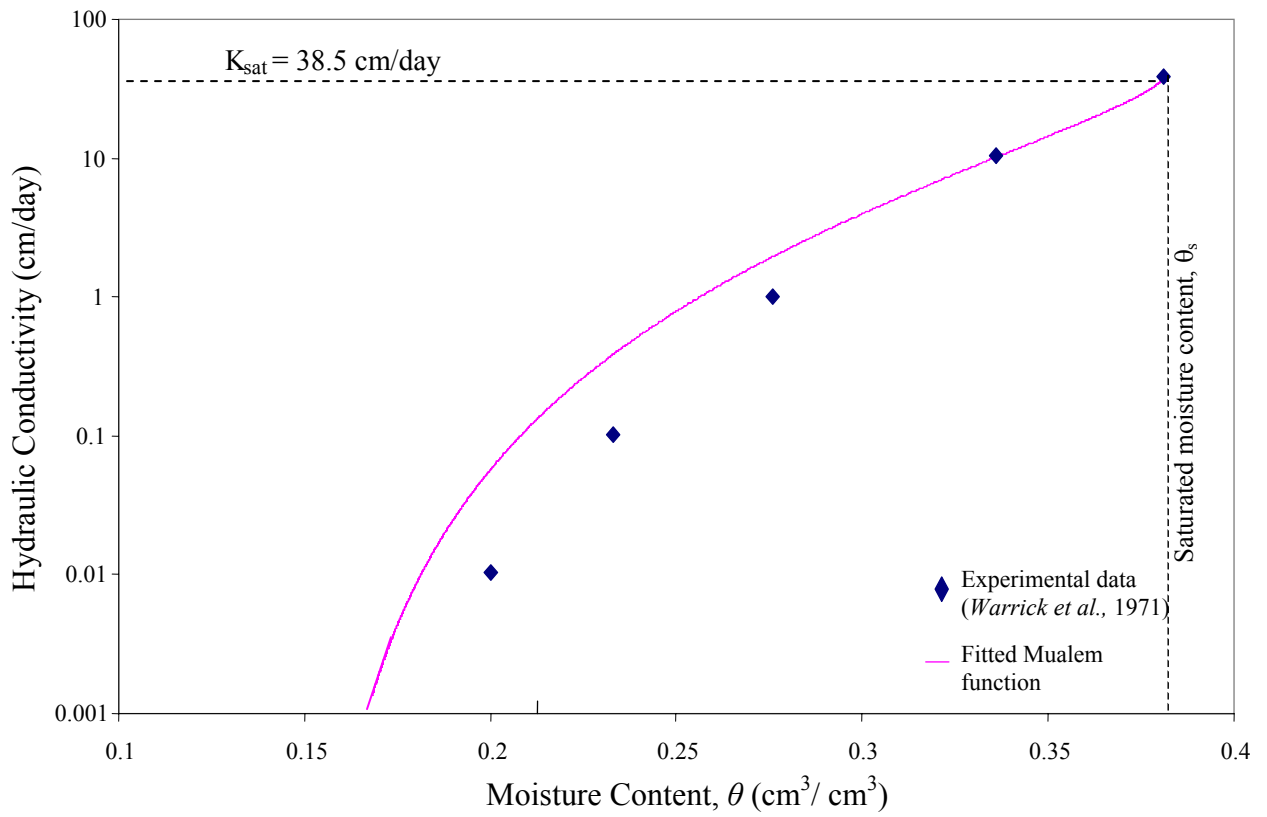


Figure 3.2: Experimental hydraulic conductivity data (Warrick *et al.*, 1971) fitted by the Mualem function for relative permeability (equation 2.7)

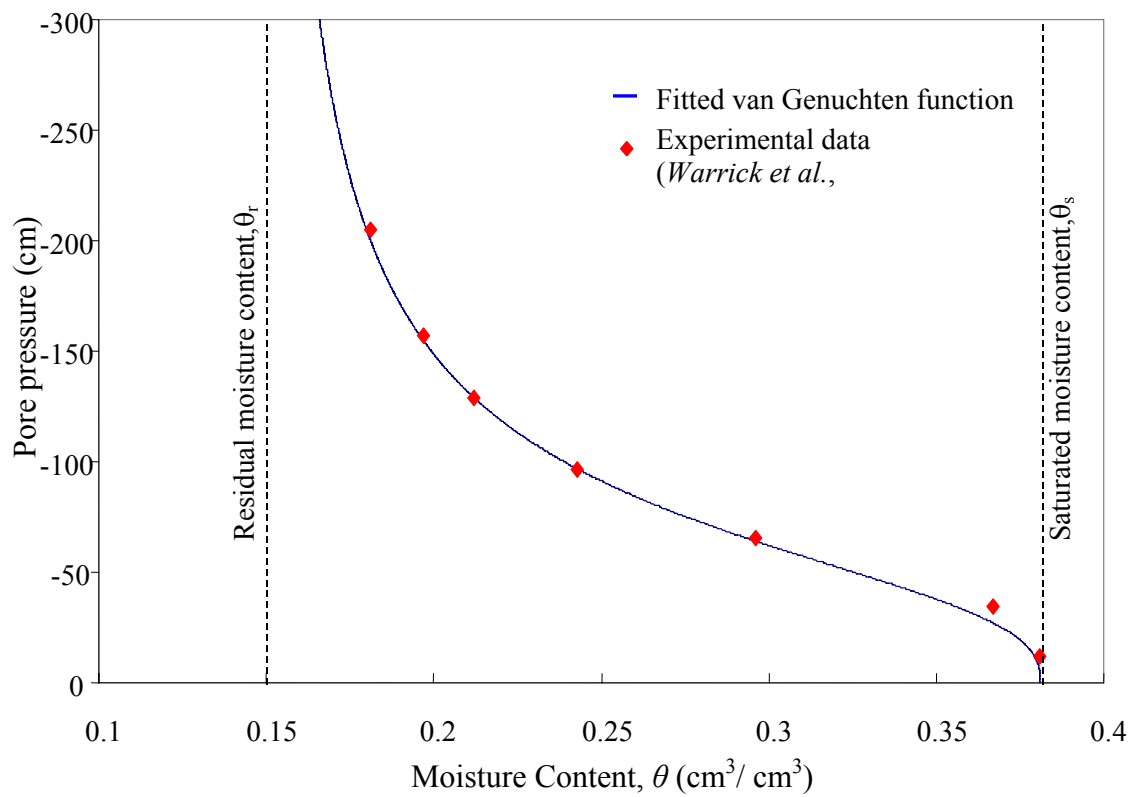


Figure 3.3: Experimental capillary saturation data (Warrick et al., 1971) fitted by the van Genuchten function for soil saturation (equation 2.5)

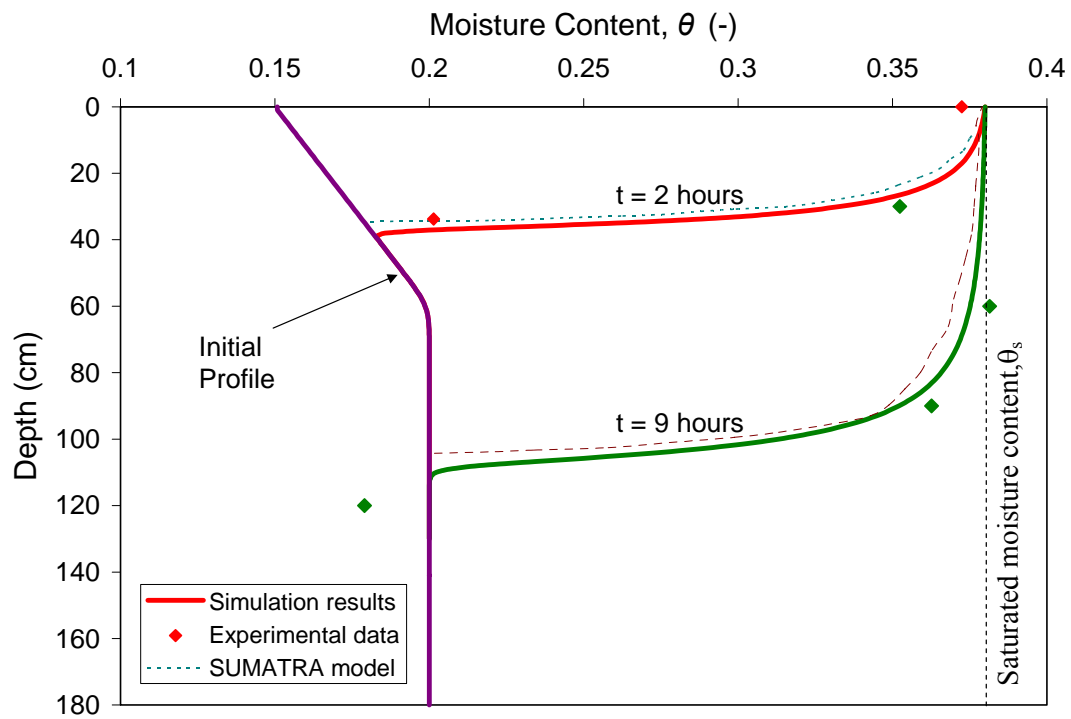


Figure 3.4: Results from the 1-D verification simulation are plotted against experimental data (Warrick *et al.*, 1971) and the results of a comparable model (SUMATRA; van Genuchten, 1978)

3.1.3 Spatial discretization and soil characteristics analysis

The impacts of model grid size and soil characteristics on model performance have been recognized for some time (*Smith, 1970; Short et al., 1995; Miller et al., 1998*). The relative influence of these two factors on a numerical solution is examined here to provide insight regarding vertical grid spacing. Grid spacing becomes a particularly important factor in the multidimensional simulation of heterogeneous systems where computational efficiency is highly dependant on discretization. The initial and boundary conditions of the *Warrick et al. (1971)* field study (**table 3.2**) are used here as the basis for simulating infiltration through several typical soil types (**figure 3.5**). The infiltration is simulated using five different spatial discretizations ($\Delta z = 1 \text{ cm}, 5 \text{ cm}, 10 \text{ cm}, 20 \text{ cm},$ and 30 cm).

The simulation results for all grid spacings at two elapsed times ($T = 2$ and 9 hours) for the coarse, medium coarse and fine soils are shown in **figure 3.6 (a),(b), and (c)**, respectively. The results indicate that the numerical solution's accuracy degrades with increasing grid cell size for all soil types. Increasing the grid size has the greatest impact on the simulations for coarse soil, causing significant over-estimation of the infiltration front.

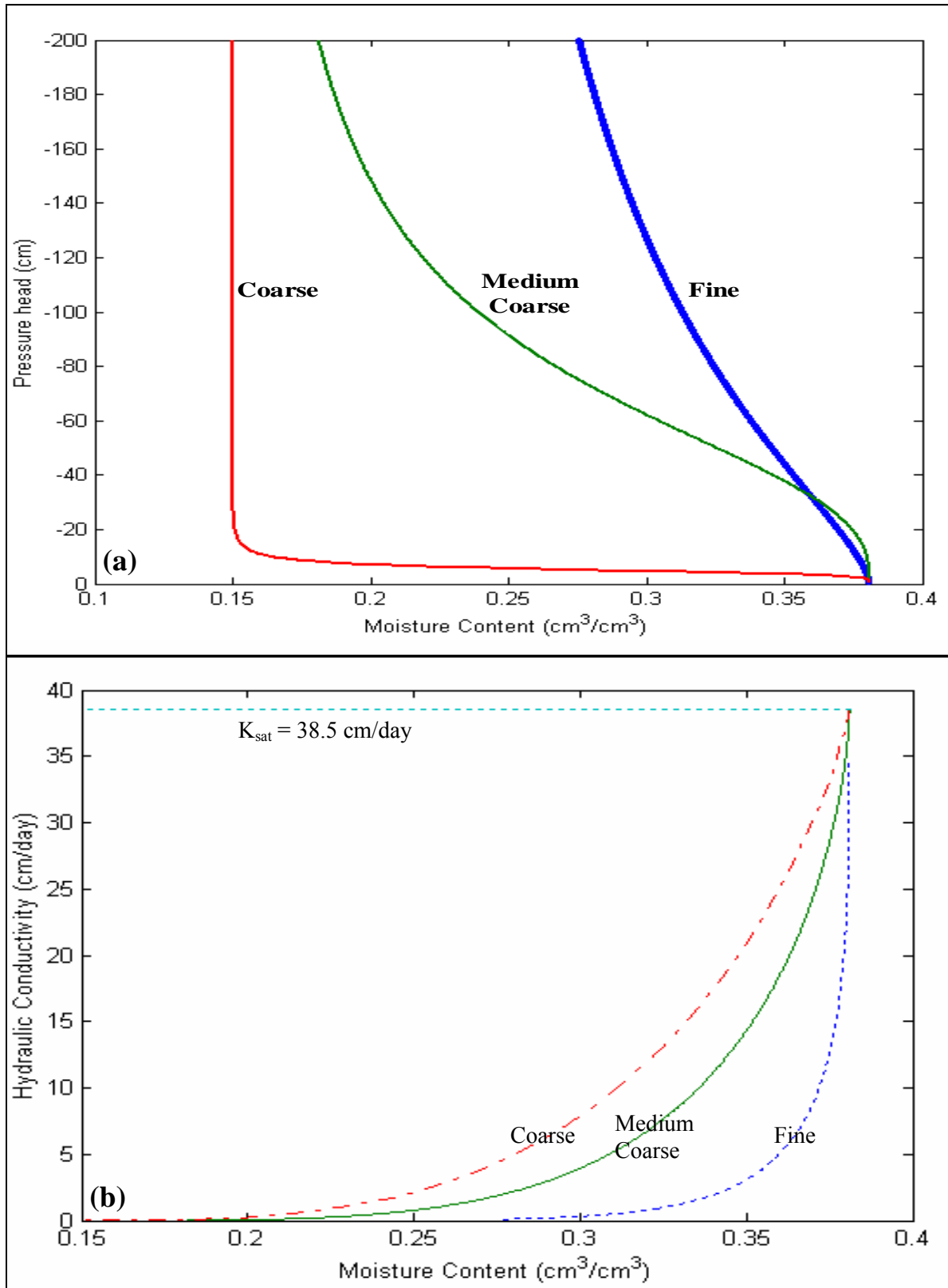


Figure 3.5: A comparison of the (a) capillary saturation and (b) relative permeability characteristics for fine, medium coarse and coarse soil

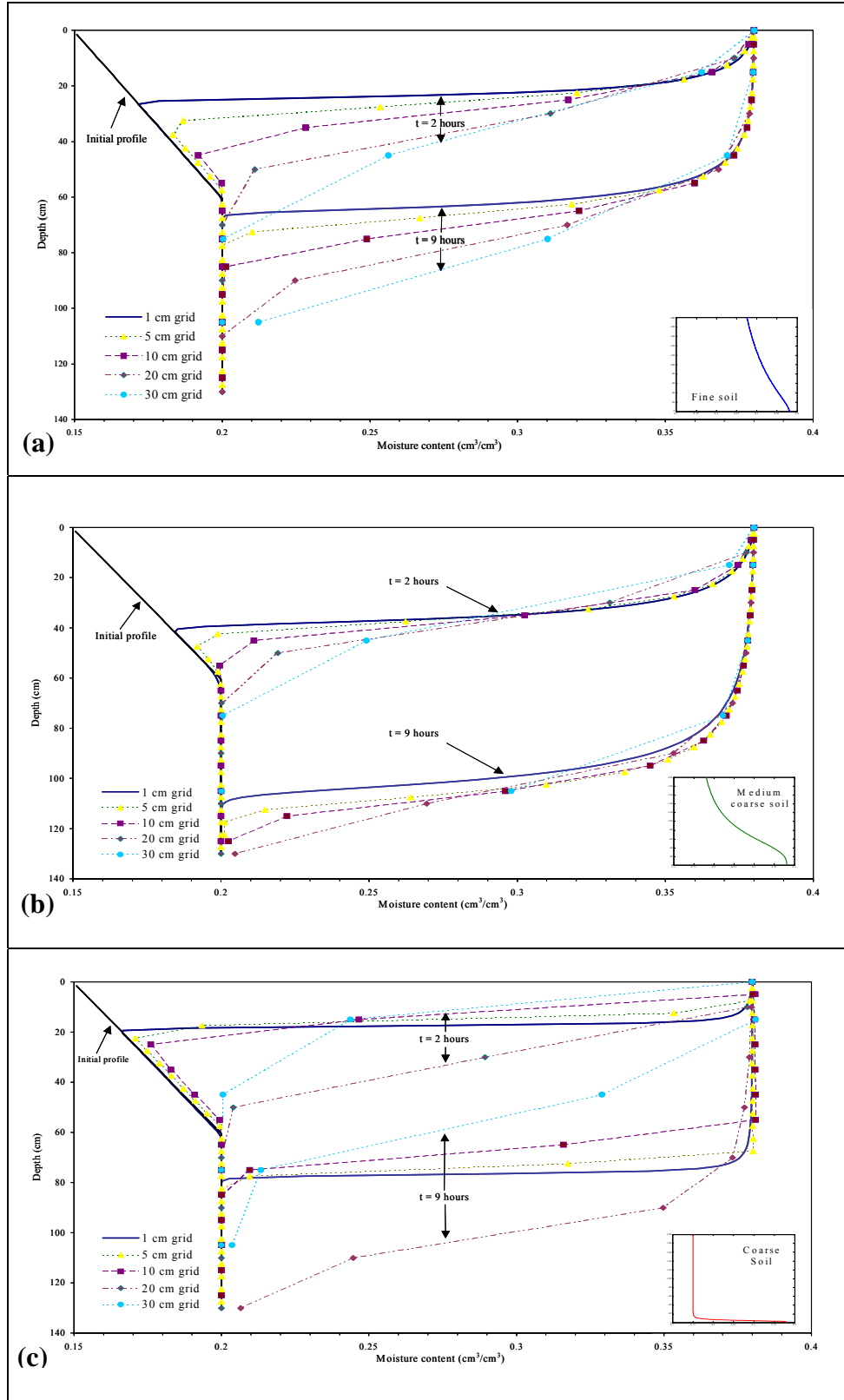


Figure 3.6: Simulation results at $t = 2$ hours and $t = 9$ hours for constant head infiltration of (a) fine soil, (b) medium coarse soil and (c) coarse soil using 5 different spatial grid discretizations. The inset figures are reproduced for reference from figure 3.5(a)

The statistical measures of root mean square error (RMSE; equation 3.2), maximum error (ME; equation 3.3) and coefficient of determination (CD; equation 3.4) were used to evaluate the spatial discretization results presented in **figure 3.6**. The root mean square error is a measure of the model's residual errors or the absolute difference between the observed (in this case the fine grid solution) and the predicted ($\Delta z > 1$ cm). The maximum error identifies the greatest absolute error in each solution set. The coefficient of determination is a measure of the fraction of the total variance of observed data that is explained by the predicted data (*Loague and Green, 1991*). It is noted that the utility of these statistics degrades significantly for data sets where the number of point is small and therefore statistical analysis of the 30 cm grid spacing solutions ($n = 8$) provides little insight into the error trends at that discretization.

$$RMSE = \left[\sum_{i=1}^n \frac{(P_i - O_i)^2}{n} \right]^{\frac{1}{2}} \frac{100}{\bar{O}} \quad (3.2)$$

$$ME = \max |P_i - O_i|_{i=1}^n \quad (3.3)$$

$$CD = \frac{\sum_{i=1}^n (O_i - \bar{O})^2}{\sum_{i=1}^n (P_i - \bar{O})^2} \quad (3.4)$$

where

P_i = predicted value

O_i = observed value

i, n = data indices (n = data set population, $i = 1$ to n)

\bar{O} = arithmetic mean of observed values

The solution for the 1 cm grid spacing was used as the basis for comparison (i.e., the “observed values” in equations 3.2, 3.3 and 3.4). In order to examine possible temporal trends between the solutions at $t = 2$ hours and $t = 9$ hours, the simulation results for each soil were analyzed using RMSE at all four grid spacings ($\Delta z = 5$ cm, 10 cm, 20 cm, and 30 cm). The RMSE for the combined solution sets (both $t = 2$ hours and $t = 9$ hours) was also evaluated and the results from both analyses are plotted against the grid spacing in **figure 3.7 (a) and (b)**. The maximum error for the combined solution

sets is plotted against grid spacing in **figure 3.8**. The coefficient of determination for each solution time is plotted against grid spacing in **figure 3.9 (CD)**.

Several observations can be made from these figures. The residual error increased with grid spacing for all soil types (**figure 3.8a**), with fine soil producing the highest RSME values and the medium coarse soil producing the lowest. There were no significant temporal trends apparent in the RMSE values for the medium and coarse soils between the two simulation times (**figure 3.8b**). However, the fine soil error for the longer simulation time ($t = 9$ hours) increased for all grid discretizations, indicating instability in the model solution. The maximum error results reflected the same general trend of the RMSE (**figure 3.8**). The trends for CD are somewhat less clear (**figure 3.9**). In general, the model's performance was good for all the simulations ($CD \approx 1$) and it tended to degrade with increasing grid size. The model over-predicted the fine and medium-coarse soil solutions, and this over-prediction increased with time as well as with grid spacing. The model performed best for the medium coarse soil, while the coarse soil illustrated the transient nature of model performance due to the non-linearity of the soil's characteristic functions.

Although these results do not suggest any common trend in solution performance (i.e. over- or under-prediction) between the soil types, it is clear that grid spacing causes varying degrees of solution degradation for all three soils. The observed degradation in solution accuracy with increasing grid size reflects the results of *Smith* (1970) who examined the influence of grid-size on infiltration simulations of a medium coarse soil using the Brooks-Corey soil relationships. The results of this study also agree with the findings of *Short et al.* (1995), in which Richard's equation was scaled in order to define a parameter space set by the grid-size and a variable describing the degree of non-linearity in the soil characteristic function. In general, it is concluded that systems containing fine and/or coarse textured soils within the vadose zone require small grid spacing (< 20 cm) in order to insure stable and convergent solutions for this model formulation.

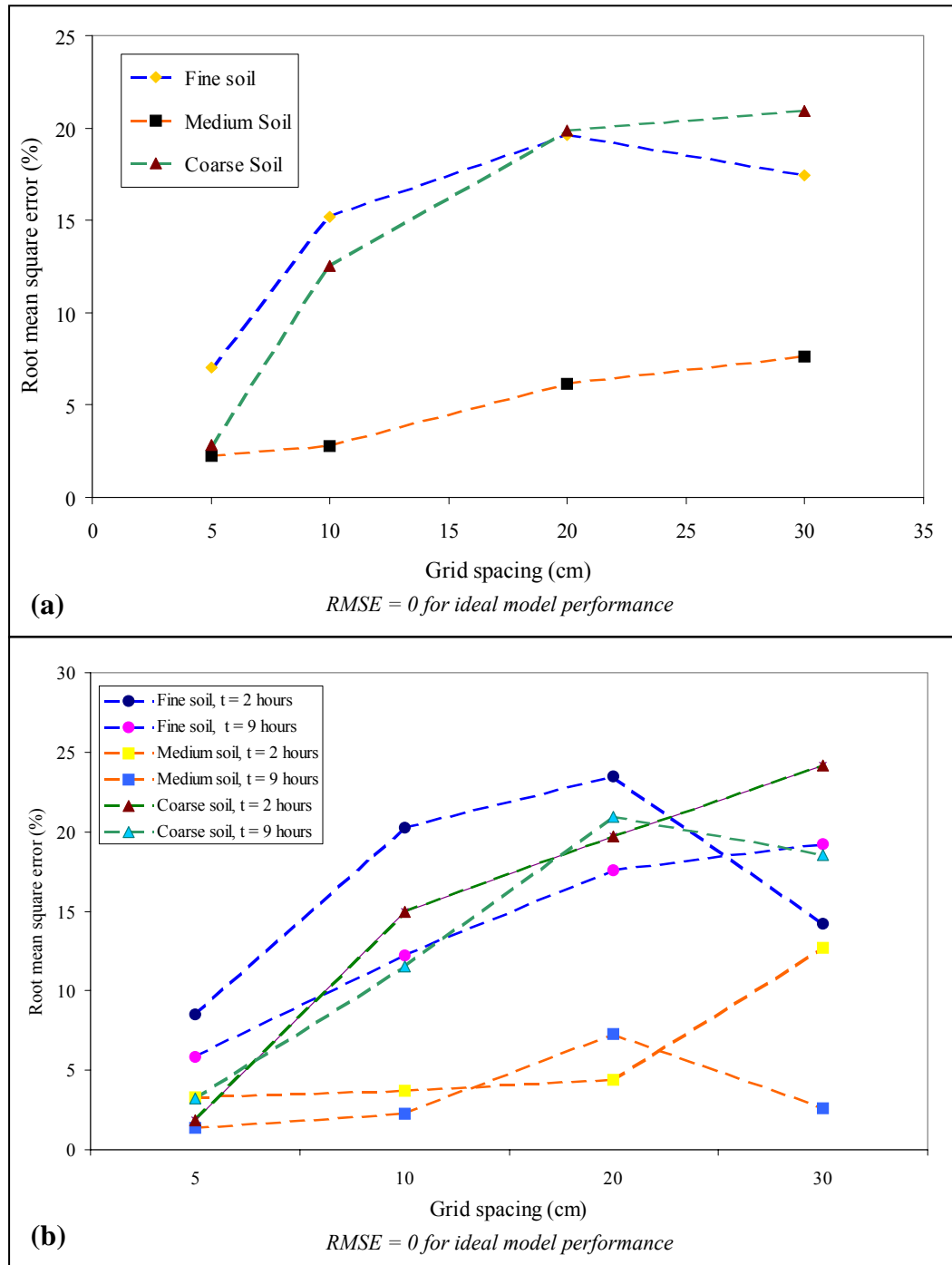


Figure 3.7: Root mean square error of model solutions for three soil types evaluated for (a) the combined solution sets and (b) separately at $t = 2$ hours and $t = 9$ hours, plotted against the grid spacing of each solution. The degradation of solution accuracy with increasing grid size is evident in varying degrees for each soil.

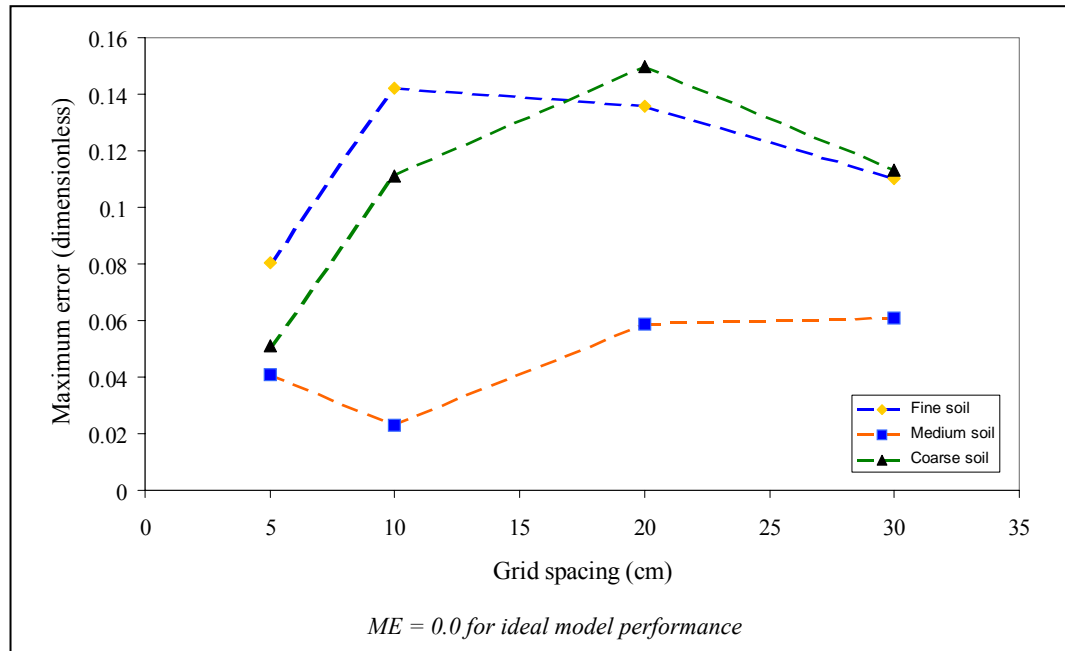


Figure 3.8: Maximum error (ME) of model solutions for three soil types evaluated at both $t = 2$ hours and $t = 9$ hours, plotted against the grid spacing of each solution. The coarse and fine soils show significant increases in deviant solution values as the grid spacing increases.

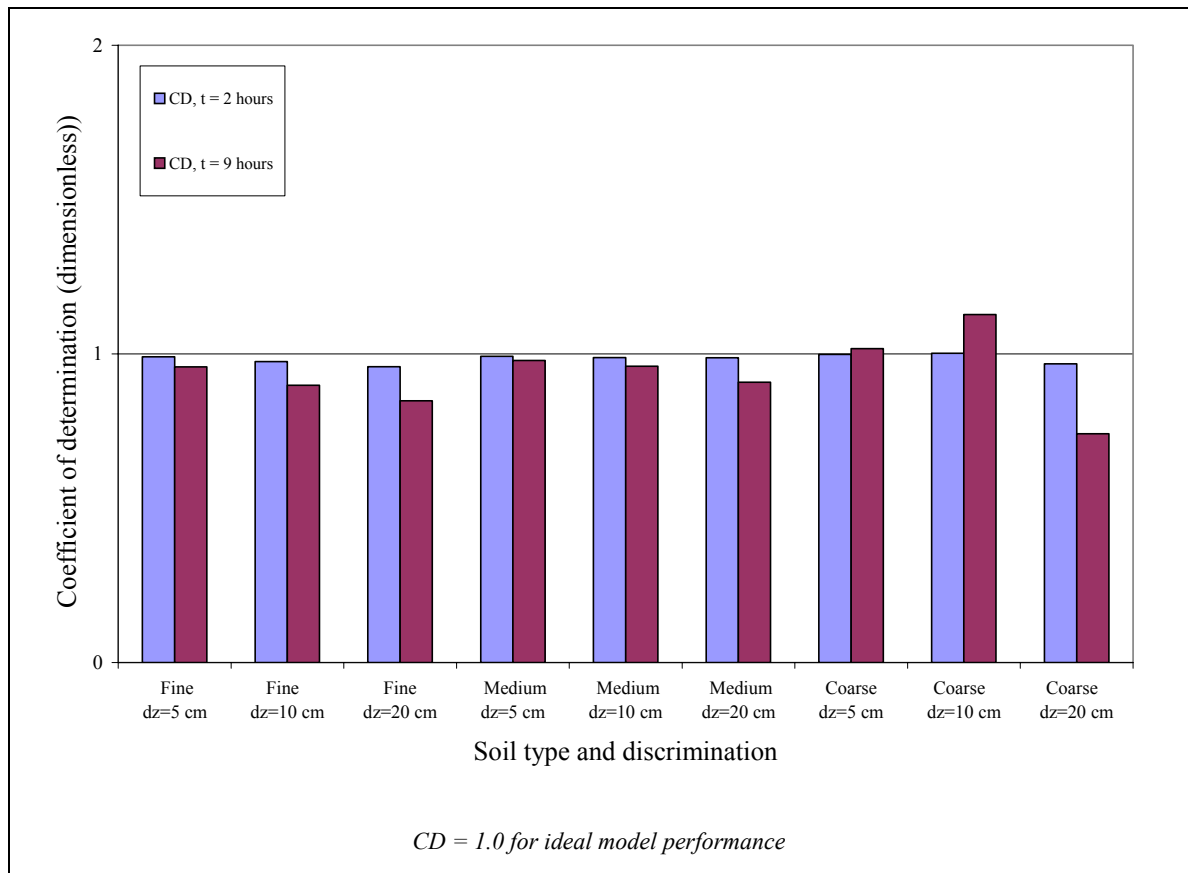


Figure 3.9: Coefficient of determination for three soil types evaluated at t = 2 hours and t = 9 hours. Over-prediction (CD<1.0) increased with increasing grid discretization for the fine and medium coarse soils, while the coarse soil solutions degraded erratically.

3.2 Conjunctive overland and subsurface flow simulation

The classic soil flume experiment of *Smith* (1970) (published as *Smith and Woolhiser* (1971)) is simulated here to confirm proper implementation of the overland flow formulation described in **sections 2.2.1 and 2.2.2**. The experiment examined laminar surface flow of a light oil (kinematic viscosity = $1.94 \times 10^{-4} \text{ m}^2/\text{s}$, about 200 times that of water) across a porous sand under both ‘wet’ and ‘dry’ initial soil conditions. The dry case is simulated here to confirm this model’s ability to properly replicate the numerically difficult infiltration-excess (Hortonian) overland flow.

The soil flume measured 12.2 meters long by 5.1 centimeters thick and 1.22 meters deep and was inclined at a slope of 0.01. The oil was applied evenly across the length of the flume for 15 minutes at a rate of 0.42 cm/min. The soil in the flume was a Poudre fine sand with differing bulk densities. The soil layer and initial saturation distribution data are shown in **figure 3.10**. The soil flume’s imbibition relations ($\theta(\psi), K_r(\psi)$) were determined experimentally. The distinct imbibition behavior of the light oil required the parameters for the capillary-saturation and relative permeability relations to be fit separately (**table 3.3 and figures 3.11, 3.12 and 3.13**).

Previous studies (*Smith*, 1970; *Akan and Yen*, 1981; *Singh and Bhallamudi*, 1998) have used the Brooks-Corey functions to represent the hydraulic properties for low pore pressures ($\psi < -20 \text{ cm}$) and interpolated functions for pore pressures near saturation ($\psi > -15 \text{ cm}$). The governing equation used by those approaches (the “ θ -form” of the Richard’s equation, after *Celia et al.* (1990)) does not simulate the transition into fully-saturated subsurface flow and therefore, any discontinuity in soil saturation and hydraulic conductivity across this transition (e.g. entrapped air) can be incorporated into the soil characteristic functions. The model formulation presented here requires that the soil hydraulic functions are first order continuous across the transition from variably saturated to fully saturated pore space. In order to represent this system accurately, the effects of entrapped air on the soil’s imbibition behavior had to be incorporated into van Genuchten

/ Mualem capillary saturation functions presented to the model (**table 3.3**). For the hydraulic conductivity, an effective saturated conductivity value was determined by interpolation (**figures 3.11(a), 3.12(a) and 3.13(a)**) and used in place of the fully saturated K^S given by *Smith* (1970). The effect of entrapped air on the soil saturation and moisture capacity was incorporated into the model by constraining the capillary-saturation curve to an “effective total porosity” value, θ_s (**figures 3.11(b), 3.12(b) and 3.13(b)**)). The model is given the resultant fitted curve parameters (α and β , **table 3.3**) to define the shape of the curve and the “total porosity” value, n to set the upper bound of available pore space. The resultant model soil saturations are thus defined relative to the “effective total porosity” and are converted into total volumetric saturations by multiplying the ratio of effective total porosity to total porosity. This method allows the model to properly represent the large storage capacity (set by its total porosity) of the soil near saturation while tracking the fluid’s capillary-saturation relative to the estimated “effective total porosity”.

Table 3.3: Model parameters for the conjunctive surface / subsurface flow simulation¹

Soil characteristic function parameter for three bulk densities of Poudre fine sand	
Low Bulk Density (1.25 gm/cm ³)	
$K_{rel}(h_c)$	<i>Mualem model</i> ; $\alpha=0.0548 \text{ cm}^{-1}$, $\beta=2.66$ $K^S=0.394 \text{ cm/min}$ $K_{fit}^S=0.197 \text{ cm/min}$
$\theta(h_c)$	<i>Van Genuchten</i> ; $\alpha=0.069 \text{ cm}^{-1}$, $\beta=4.26$ $n = 0.460$ $\theta_s=0.393$, $\theta_r=0.020$
Medium Bulk Density (1.36 g/ cm ³)	
$K_{rel}(h_c)$	<i>Mualem model</i> ; $\alpha=0.0538 \text{ cm}^{-1}$, $\beta=3.41$ $K^S=0.254 \text{ cm/min}$ $K_{fit}^S=0.149 \text{ cm/min}$
$\theta(h_c)$	<i>Van Genuchten</i> ; $\alpha=0.0582 \text{ cm}^{-1}$, $\beta=3.65$ $n = 0.504$ $\theta_s=0.443$, $\theta_r=0.025$
High Bulk Density (1.48 g/ cm ³)	
$K_{rel}(h_c)$	<i>Mualem model</i> ; $\alpha=0.0434 \text{ cm}^{-1}$, $\beta=4.03$ $K^S=0.186 \text{ cm/min}$ $K_{fit}^S=0.129 \text{ cm/min}$
$\theta(h_c)$	<i>Van Genuchten</i> ; $\alpha=0.051 \text{ cm}^{-1}$, $\beta=3.30$ $n = 0.543$ $\theta_s=0.499$, $\theta_r=0.025$

¹ The saturated hydraulic conductivity K^S values from *Smith* (1970) are assumed to represent the hydraulic conductivity of the soil at total saturation of the pores (no entrapped air). The total porosity n values from *Singh and Bhallamudi* (1998) are assumed to represent total available pore space (including entrapped air) and are used with the effective saturation data from *Smith* (1970) to determine the total effective porosity, θ_s .

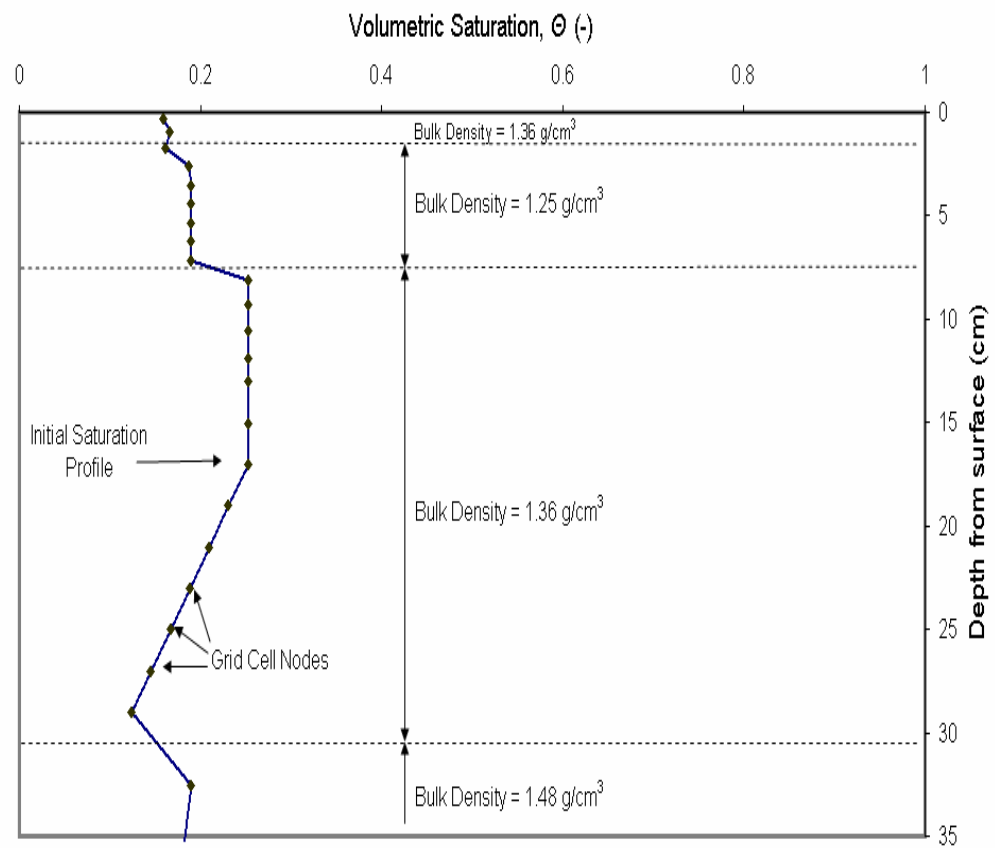


Figure 3.10: Initial saturation profile for the soil flume experiment (*Smith and Woolhiser, 1971*). The three soil layers and vertical model grid spacing are also shown (total depth of the flume equaled 1.22 meters).

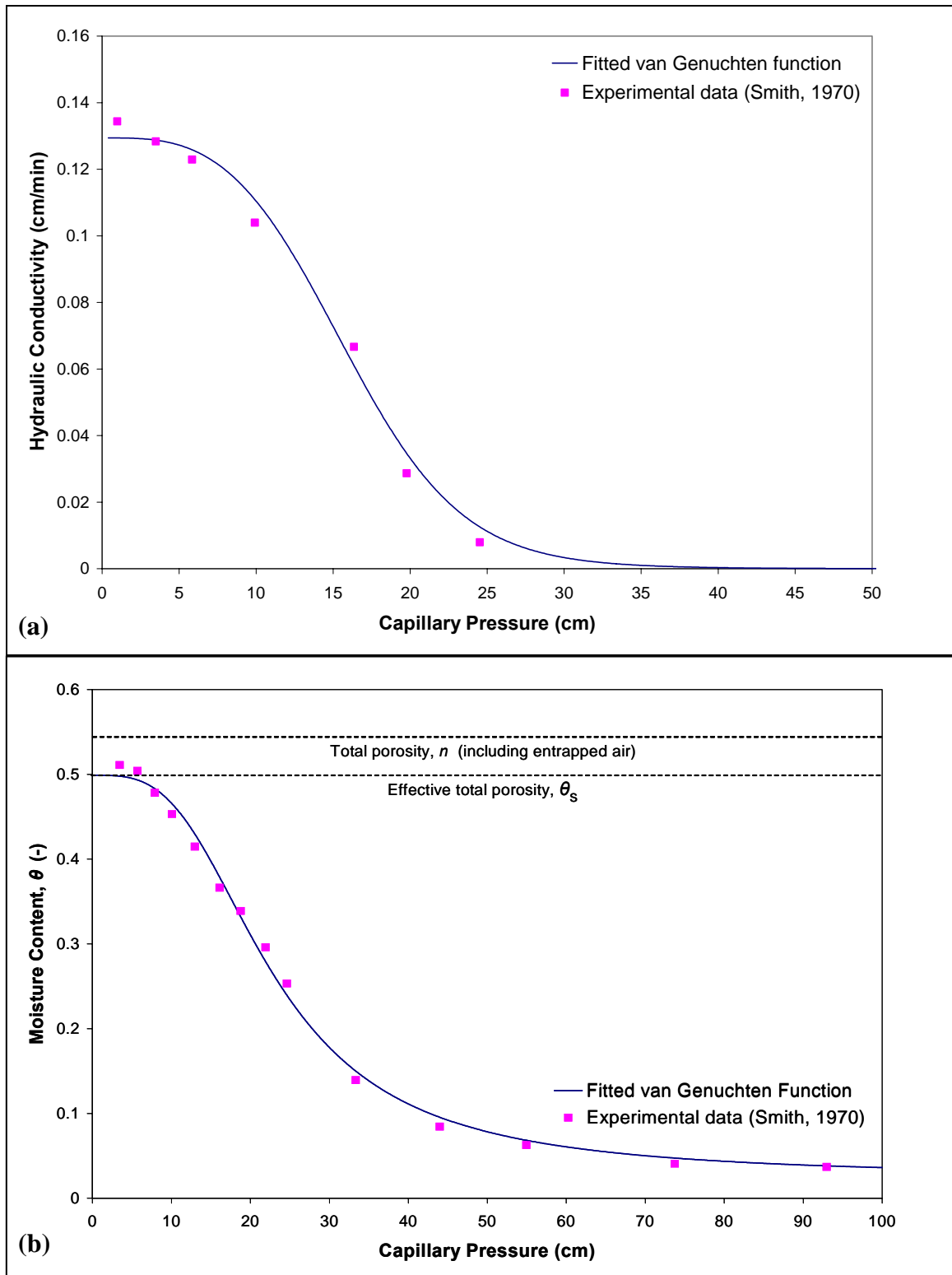


Figure 3.11: Soil characteristic functions for (a) hydraulic conductivity and (b) soil moisture content fitted to the corresponding empirical data for the high bulk density soil layer of *Smith* (1970).

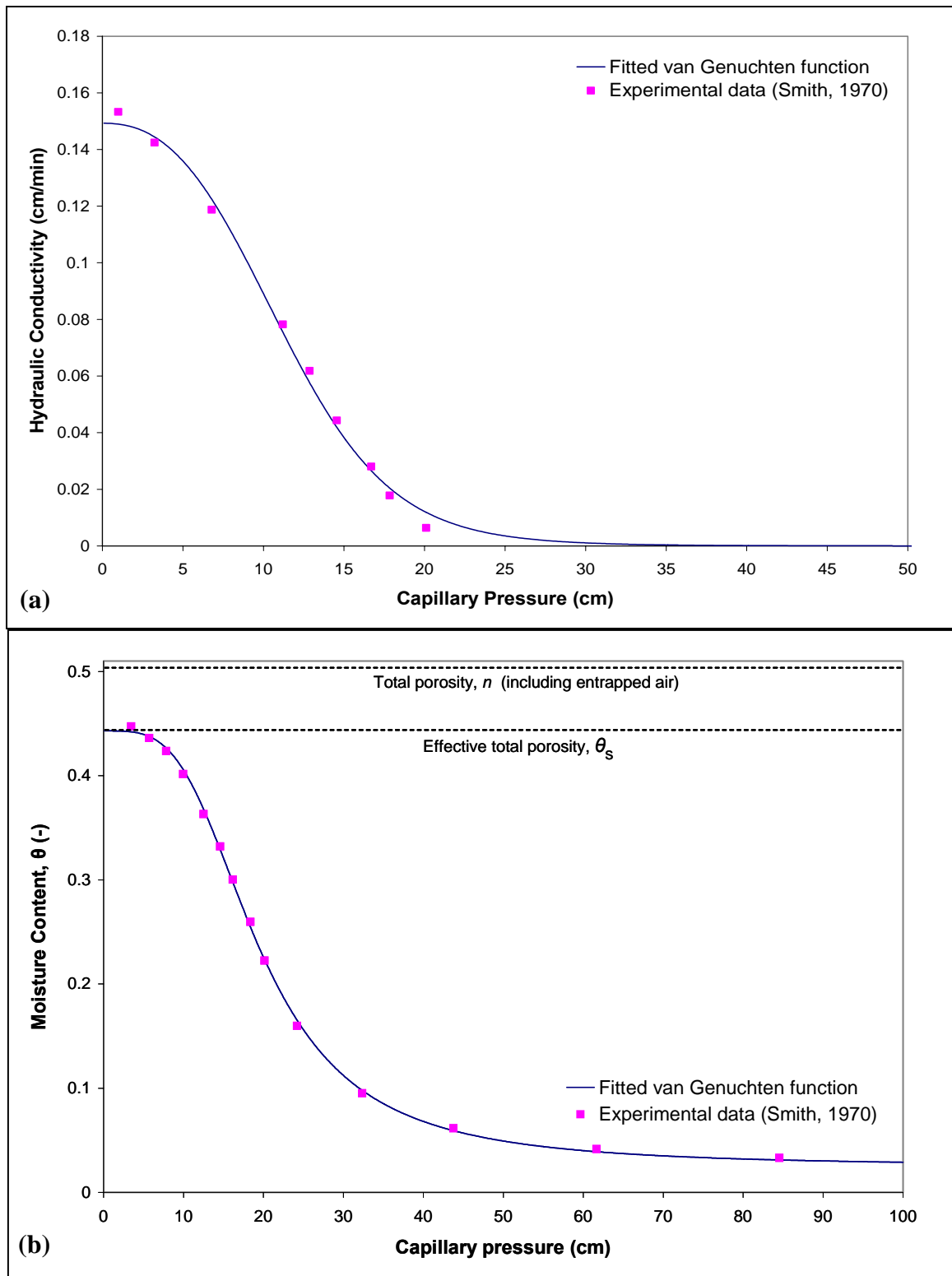


Figure 3.12: Soil characteristic functions for (a) hydraulic conductivity and (b) soil moisture content fitted to the corresponding empirical data for the medium bulk density soil layer of *Smith* (1970).

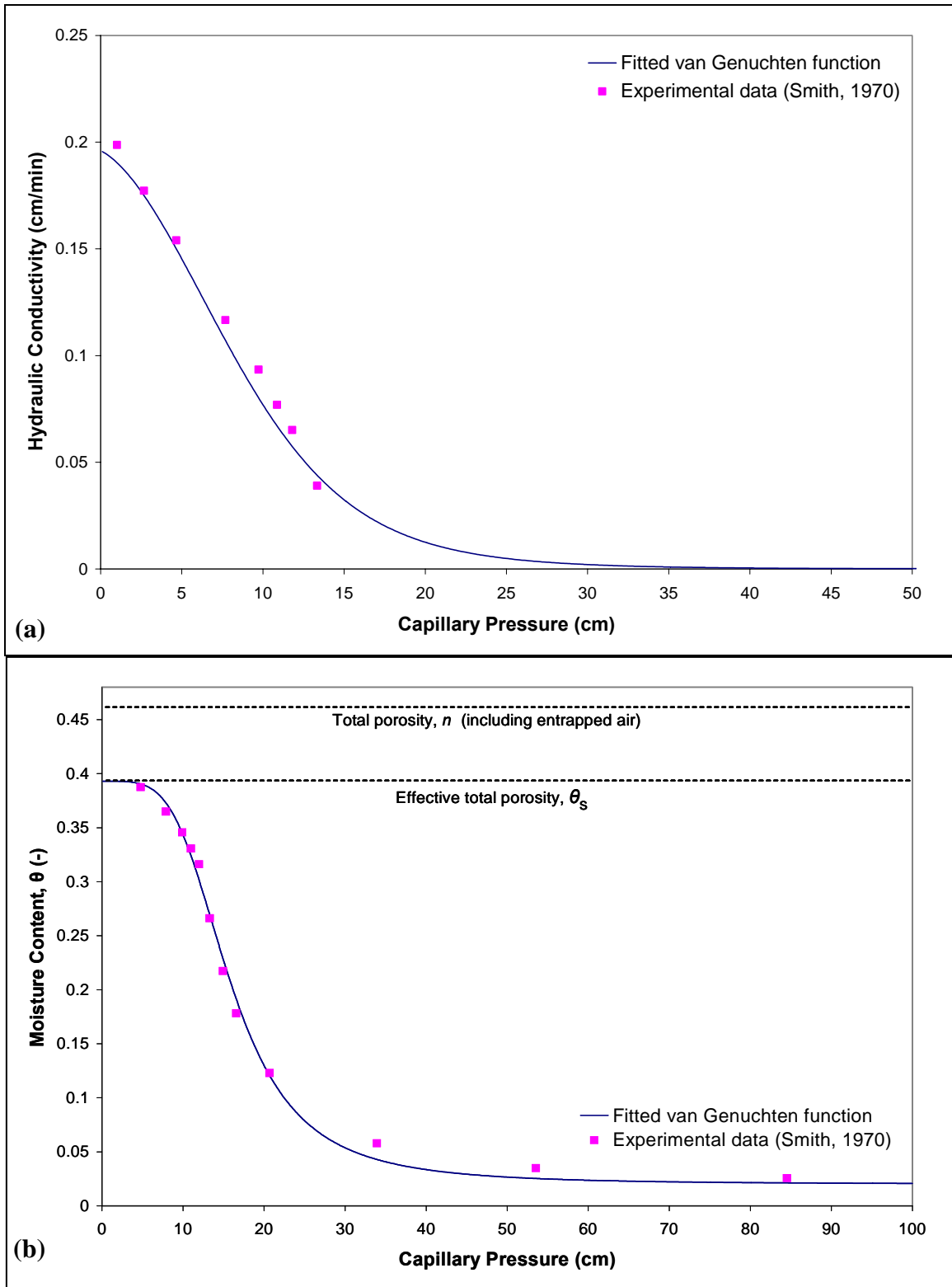


Figure 3.13: Soil characteristic functions for (a) hydraulic conductivity and (b) soil moisture content fitted to the corresponding empirical data for the low bulk density soil layer of *Smith* (1970).

The total simulation time was 18 minutes in order to capture the recession phase of the hydrograph (**figure 3.14**). The simulated soil saturation profiles at four discrete times during the rainfall application are plotted in **figure 3.15** with the corresponding simulation results from *Smith and Woolhiser* (1971). Examining the simulation results, it is immediately obvious that the timing of both the infiltration front (**figure 3.15**) and the initiation of surface runoff (**figure 3.14**) match the results of Smith and Woolhiser (1971) quite well. However, the amplitude of the runoff hydrograph peak is somewhat less than the experimental data. This can be explained by the crude approximation of entrapped air effects used in this study (**figures 3.11b, 3.12b and 3.13b**) that may over-estimate the available specific moisture capacity near saturation. Due to the high viscosity of the light oil, entrapped air in the soil pores prevented the soil from reaching complete saturation (*Smith*, 1970). This entrapped air would reduce the available storage capacity of the soil below the values defined by the capillary saturation functions used in this study (**table 3.3**). Additionally, there is some over-prediction in the lower soil layer of the soil's volumetric saturation, as the infiltration front moves down through the soil column (**figure 3.15**). This loss of water into the soil column causes the model to under-predict the surface runoff in order to maintain overall mass balance (**figure 3.14**). The model also under-estimates the timing of the receding limb of the hydrograph (**figure 3.14**), which may indicate experimental conditions such as hysteresis in the soil drainage due to the persistence of entrapped air or over-prediction by the model of the available soil water capacity. Overall the model captures the hydraulic behavior of the surface runoff hydrograph and subsurface saturation profiles quite well and illustrates the inter-connectivity of surface and subsurface hydrology.

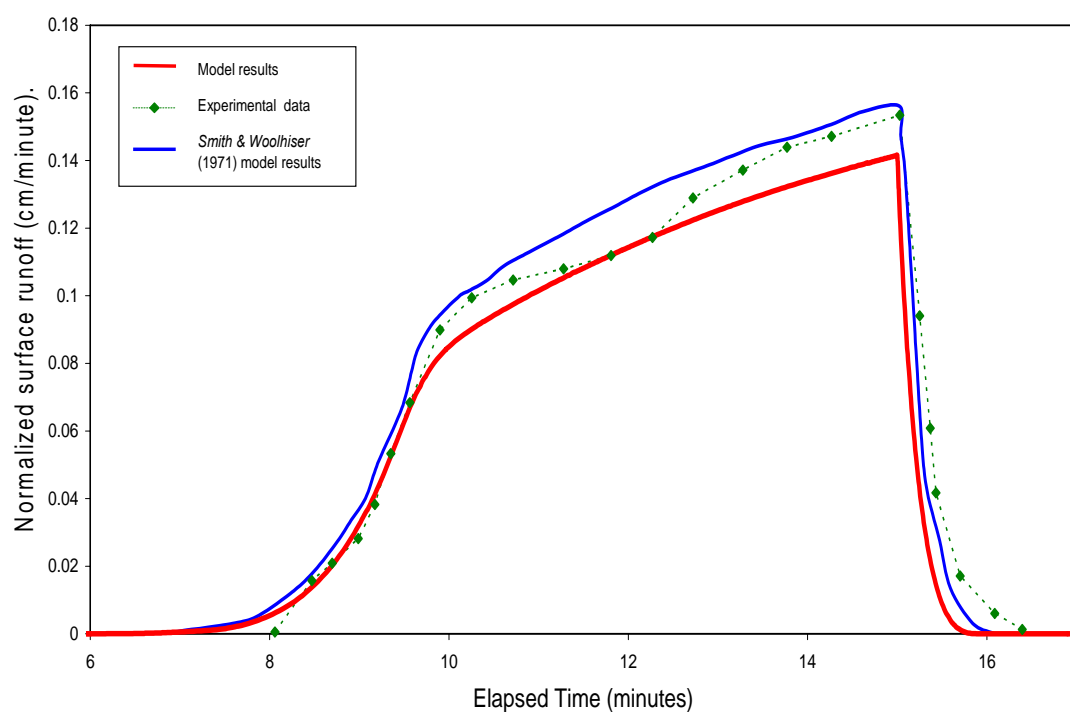


Figure 3.14: Simulated runoff hydrograph plotted against experimental data and model results of *Smith and Woolhiser (1971)* normalized by total surface area.

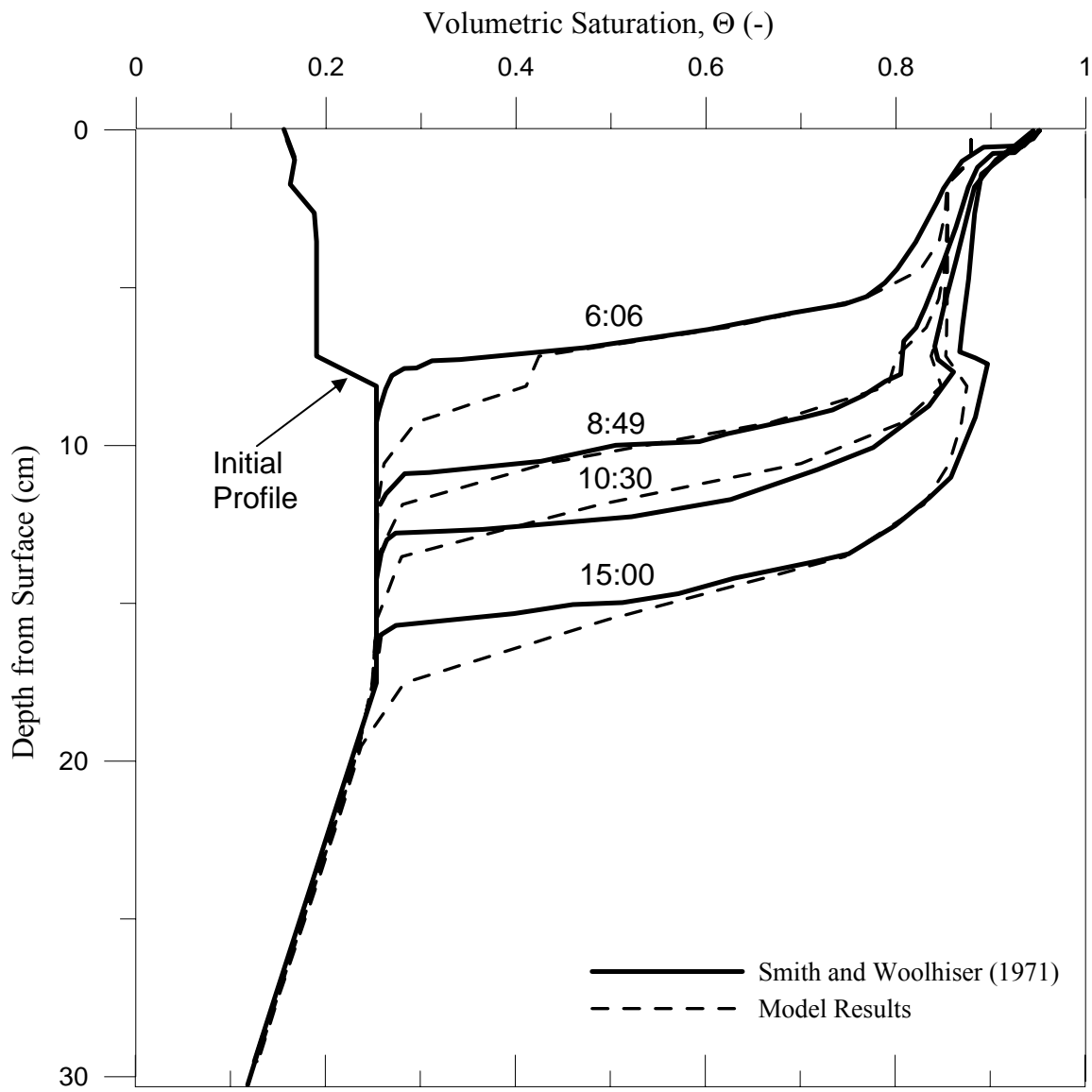


Figure 3.15: Comparison of simulated soil saturation profiles for the soil flume experiment of *Smith and Woolhiser* (1971) (times in minutes and seconds)

3.3 Mass Balance Analysis

Another method of verifying the model's performance is to compare the total mass entering the simulated domain against the total mass leaving the domain (via storage flow or sinks such as constant head cells, drains or wells) plus the change of mass within the domain during the simulation. Mass changes within the domain include flow to and from storage (controlled by the specific storage coefficient) and unsaturated soil moisture flow (controlled by the specific moisture capacity term). It is especially important to examine how the mass balance is affected by the new features presented in this work. The model's mass balance is examined here for both the subsurface simulation of **Section 3.1.3** and the conjunctive surface-subsurface simulation of **Section 3.2**.

The percent discrepancy (PD) of cumulative inflow volume versus outflow volume is used here to examine the model's mass balance as the simulation progresses. The PD tracks the accumulated volumes as the simulation progresses and therefore is a good indicator of the overall mass balance up to that time during the simulation. This metric is defined as the difference between total inflow volume (including flow into storage and soil moisture) and total outflow volume (including flow from storage and soil moisture) divided by the total average volume in the domain:

$$PD = 100 \left(\frac{TIV - TOV}{(TIV + TOV/2)} \right)$$

where:

PD = Percent discrepancy [-]

TIV = Total inflow volume [L^3]

TOV = Total outflow volume [L^3]

The 1-D simulations (**Section 3.1.3**) for the 10 cm and 20 cm grids for all three soil types are run again here with and without the adaptive time stepping algorithm to examine its effects (if any) on the model. The mass balance results (PD) are plotted

against the simulation time for the fine soil (**figure 3.16**), the coarse soil (**figure 3.17**) and the medium coarse soil (**figure 3.18**). Overall the model performs well; none of the 6 simulations examined showed any significant magnitude of PD relative to the model's numerical precision (4 digit precision). All six simulations exhibited similar behavior; the greatest mass balance errors (maxima/minima of PD) occurred early in the simulation and PD converged towards zero as the simulation continued. The model's difficulty with the coarse soil is confirmed by the largest magnitude PD of -0.002% (**figure 3.17**). The adaptive time stepping algorithm slightly increased the PD magnitude for the fine soil (**figure 3.16**) but the mass balance was slightly improved for the coarse (**figure 3.17**) and medium coarse soil (**figure 3.18**) simulations. Overall, it appears that only the coarse soil effects the model's mass balance and the adaptive time stepping algorithm does not seem to have any discernable effects for 1D infiltration with a constant head boundary condition.

The conjunctive surface-subsurface simulation of **Section 3.2** is repeated here with and without the adaptive time stepping algorithm and the mass-balance results are displayed in **figure 3.19**. It is immediately obvious that the initiation of the surface flow at 5.8 minutes causes the model to lose mass. This loss of mass is a singular event that occurs during the time step when surface runoff initiates; the model over-predicts the flow out of the domain for that time step after which the PD slowly converges towards zero as the total simulation volume accumulates. The adaptive time stepping algorithm causes this loss of mass to be significantly larger in magnitude (-3.26% vs -0.056% at the peaks) and despite the continual convergence towards a balance of mass, the final PD was relatively significant (-1.15% of the simulation's average cumulative volume). However, comparing the surface runoff results (the most sensitive to changes in mass) for the two simulations (**figure 3.20**), it is obvious that this loss of mass only has a minor effect on the rising limb of the hydrograph, causing the model to slightly over-predict the initial surface runoff. These results suggest that the adaptive time stepping algorithm may be improved by including a mass balance check in the time step adjustment that is activated with the initiation of surface flow.

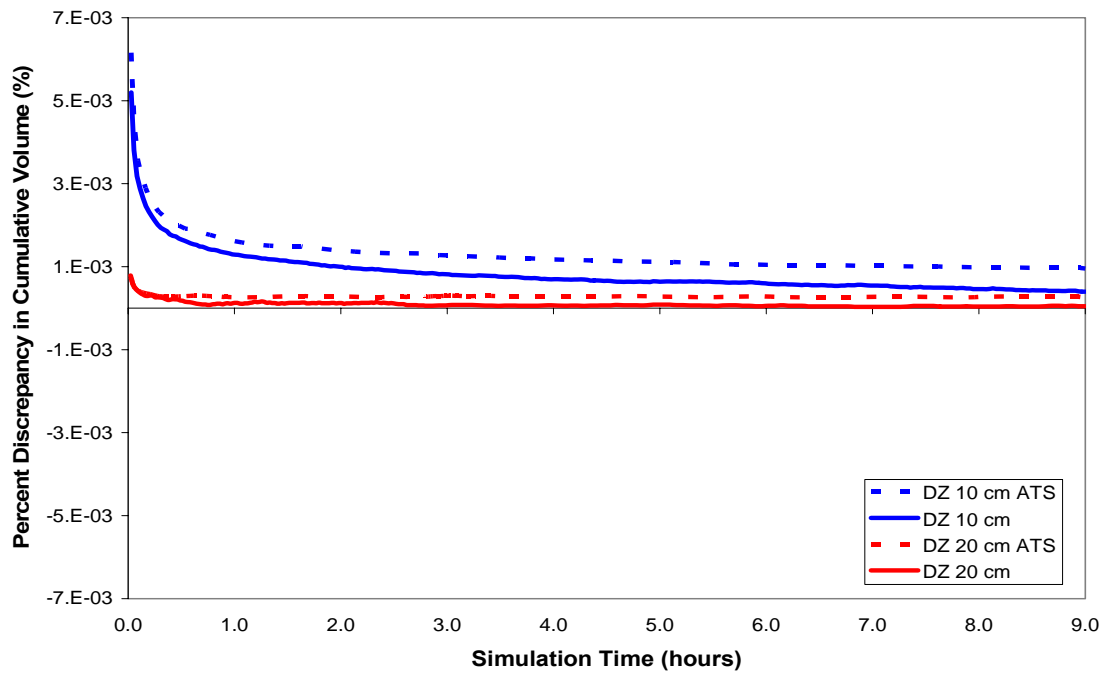


Figure 3.16: Mass balance analysis results for the 1-D fine soil infiltration case of section 3.1.3 with and without the adaptive time stepping algorithm (ATS). The percent discrepancy between cumulative inflow and outflow volumes is plotted against simulation time.

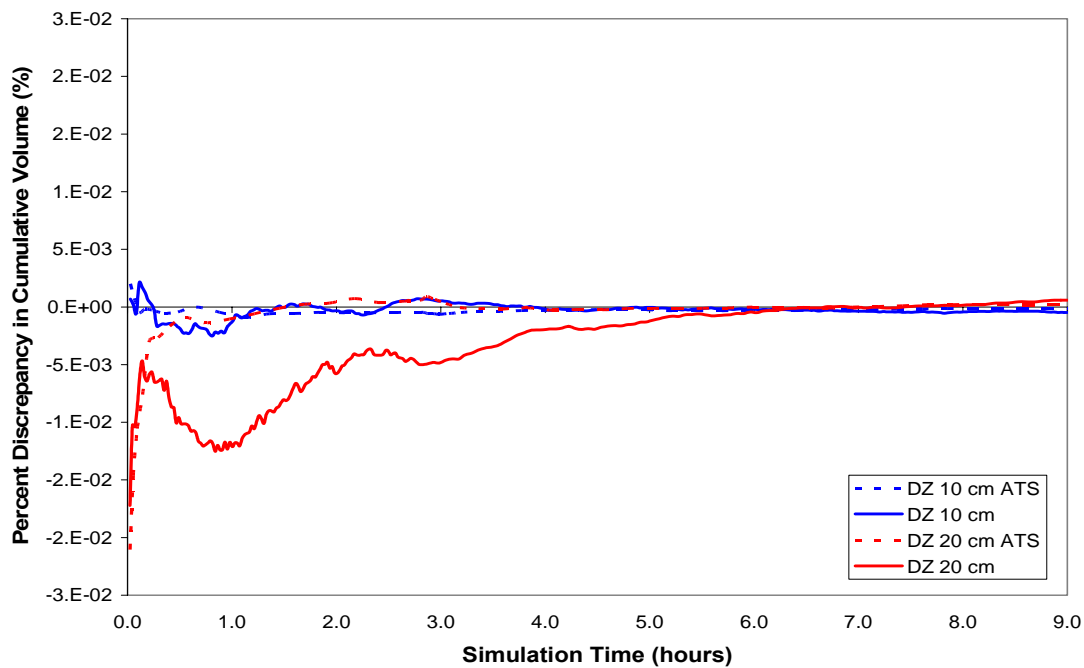


Figure 3.17: Mass balance analysis results for the 1-D coarse soil infiltration case of section 3.1.3 with and without the adaptive time stepping algorithm (ATS). The percent discrepancy between cumulative inflow and outflow volumes is plotted against simulation time.

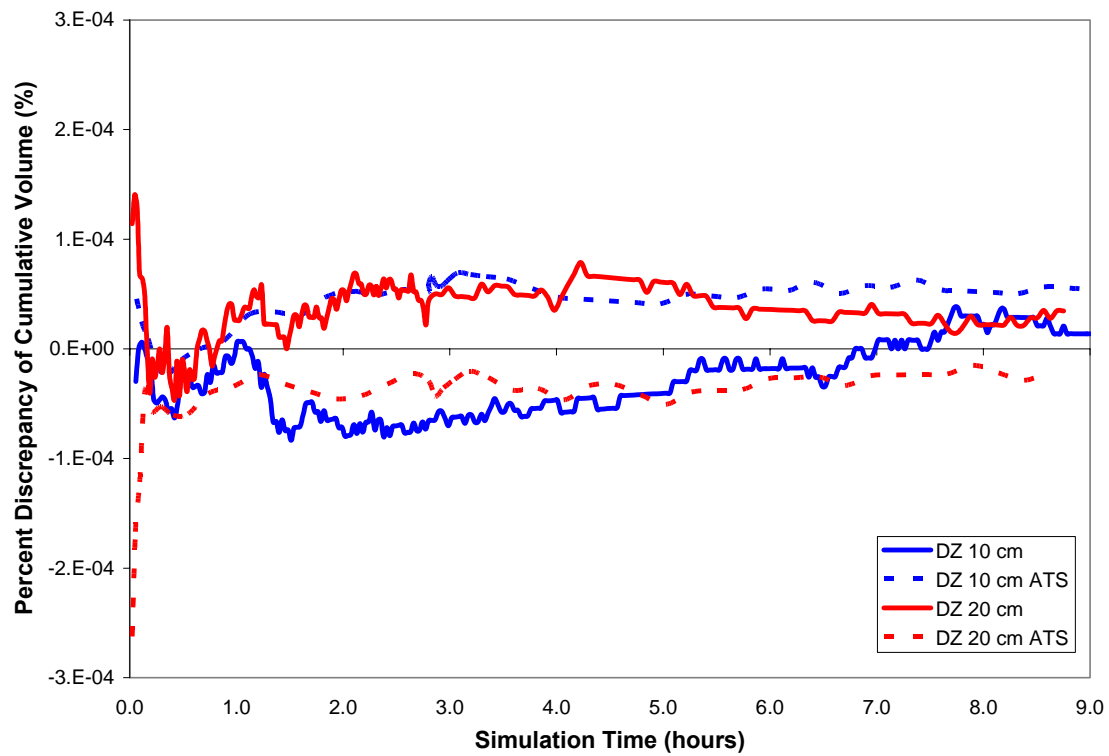


Figure 3.18: Mass balance analysis results for the 1-D medium coarse soil infiltration case of section 3.1.3 with and without the adaptive time stepping algorithm (ATS). The percent discrepancy between cumulative inflow and outflow volumes is plotted against simulation time.

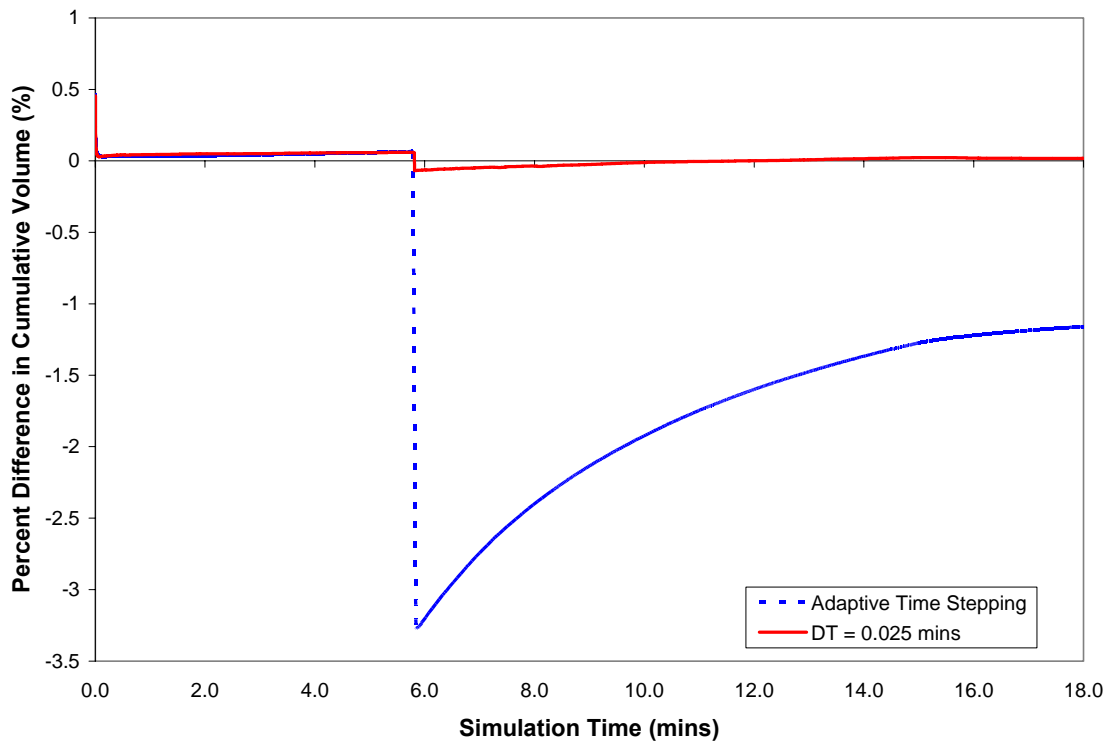


Figure 3.19: Mass balance analysis for the conjunctive surface/subsurface simulation of section 3.2 with and without the adaptive time stepping algorithm (ATS). The percent discrepancy between cumulative inflow and outflow volumes is plotted against simulation time.

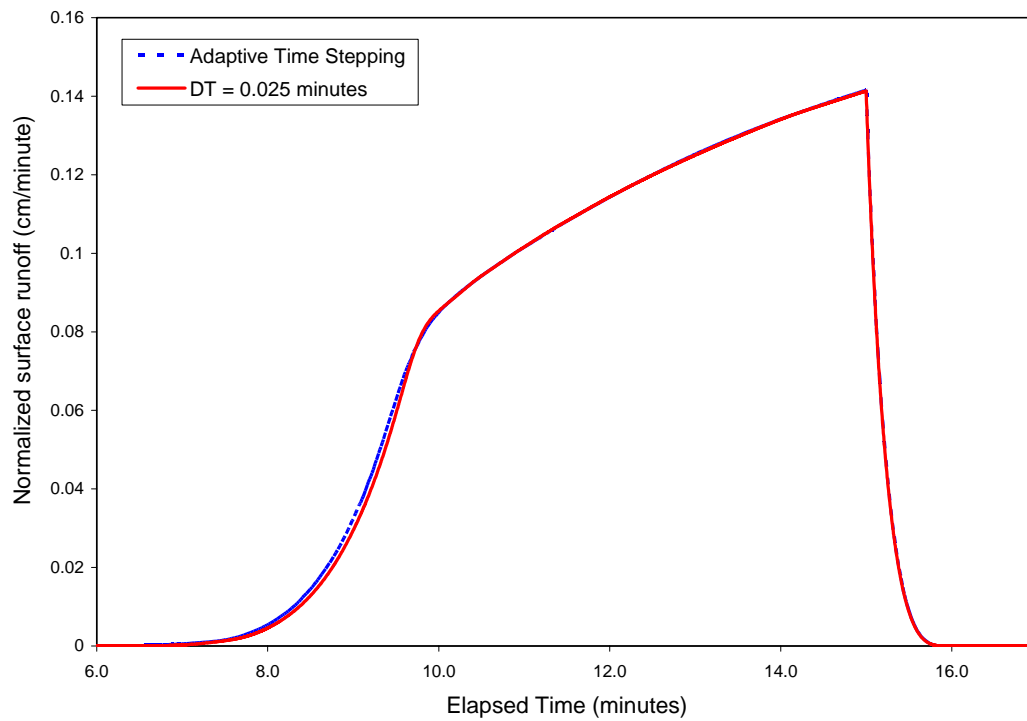


Figure 3.20: Surface runoff hydrograph of conjunctive surface-subsurface simulation (section 3.2) comparing model results with and without the adaptive time stepping algorithm (ATS).

Chapter 4: Conclusions and Future Considerations

In the work presented here, the 3-D saturated ground water flow model MODFLOW was modified to simulate unsaturated flow through porous media using Richards equation and to simulate fully-coupled overland flow using the kinematic wave approximation to the shallow surface flow (Saint Venant) equations. The new capabilities were tested against an analytical solution for 1-dimensional constant head infiltration (Dirichlet boundary condition), results from a field experiment of 1-dimensional constant rainfall infiltration (Neumann boundary condition) and results from a 2-dimensional conjunctive surface-subsurface flow soil flume experiment. The results presented here demonstrate the model's newly enhanced capabilities to simulate vadose zone flow and overland flow as well as to represent the interactions between the surface and subsurface.

As the new MODFLOW capabilities were developed, the primary focus was to retain the flexibility that is at the core of the MODFLOW concept. The resulting code retains the modular structure common to all other features (or 'packages') in MODFLOW. The code is easily adapted to function with a commercial pre/post processing software package and it remains compatible with popular transport codes (i.e. MT3DMS, *Zheng et al.*, 1999; and RT3D, *Clement*, 1997), thus greatly expanding the model's capability to simulate larger, more complex systems. Several improvements will be made in order to facilitate and enhance the model's capabilities. A recently developed

algorithm for local grid refinement ('telescoping grid' capability; *Hill, 2003*) in large (regional) MODFLOW models will be integrated into the model in order to simulate surface-subsurface interactions for a smaller area of interest (e.g. uplands catchment) using the regional model's simulation results as initial and boundary conditions. In order to increase the efficiency of the conceptual model building process, an algorithm for grid optimization will be developed for building the fine space-time grids required for vadose zone modeling. Furthermore, larger systems (i.e. watershed scale) will inevitably require the development of a version of this modeling approach for a parallel network of computers. It is hoped, by introducing these new features (and their source code) into the scientific community, that feedback and discussion will be generated on the model strengths, weaknesses, applicability and possible improvements.

This study is only the first step in establishing the feasibility of this approach as a useful tool for the various scales (i.e. hillslope, catchment, watershed) of hydrologic modeling. Several limitations were made evident in this study that should be considered in future applications of the model. The spatial discretization limitation of Richards equation (**Section 3.1.3**) presents a major consideration in the optimal design of model grids. It was shown that this model requires particularly fine spatial grid resolution in the vadose zone for accurate simulation of systems containing coarse soils. Possible improvements that will be considered to provide the user more options to deal with the error related to a coarse spatial grid include an approximation technique for the unsaturated hydraulic conductivity of gravity-dominated flows (*Zhang, 2000*) as well as additional interblock conductivity schemes (e.g. *Zaidel and Russo, 1992*).

The utility of the kinematic wave approximation across multiple spatial scales and various boundary conditions will have to be investigated in order to develop strategies to address its inherent simplifying assumptions. An algorithm will be developed for building the top model layer using the appropriate physical parameters and boundary conditions that will insure realistic surface response and prevent numerical error from

dominating the runoff signal. Special attention will be paid to hydrologic systems containing dynamic flood plain regions where backwater effects play a dominant role in the system's hydraulics. The incorporation of the turbulent and mixed forms of the Darcy-Weisbach equation into the overland flow package will provide additional flexibility in simulating various surface conditions. Although flood prediction is unlikely, the model should be able to approximate seasonal surface-subsurface interactions on a realistic scale with some degree of accuracy. The task of simulating a natural hydrologic system remains the next obvious step in the model construction and verification process.

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Appendix A

Development of kinematic wave approximation within MODFLOW

Saint Venant equations for shallow surface water flow (*Chin, 2000, pg. 394*):

$$\frac{\partial Q}{\partial x} + \frac{\partial A}{\partial t} = 0 \quad (1-D \text{ continuity})$$

$$\frac{1}{A} \frac{\partial Q}{\partial t} + \frac{1}{A} \frac{\partial}{\partial x} \left(\frac{Q^2}{A} \right) + g \frac{\partial y}{\partial x} - g(S_o - S_f) = 0 \quad (1-D \text{ momentum})$$

where:

- x = distance [L]
- t = time [T]
- Q = volumetric flow rate [L^3/T]
- A = cross sectional area [L^2]
- g = gravity [L^2/T]
- S_o = slope of ground surface [L/L]
- S_f = slope of the energy grade line [-]

For the kinematic wave approximation, inertial and pressure effects are assumed to be negligible compared to the influence of friction and gravity, allowing the conservation of momentum to be approximated by:

$$S_o = S_f$$

Scaling the continuity equation by the horizontal dimensions, x and y , adding rainfall and infiltration terms and rearranging gives:

$$\frac{\partial d}{\partial t} = \frac{\partial q}{\partial x} + \left[\underbrace{R - I}_{\text{precipitation excess}} \right] \quad (1-D \text{ kinematic wave approximation})$$

where:

- q = discharge per unit width of channel [L^2/T]
- d = mean flow depth above ground surface [L]

In the MODFLOW context, the surface depth, d can be considered analogous to pore pressure, ψ in the top model layer: $d = \psi = h - z$, where h is total hydraulic head and z is the ground surface elevation. The precipitation excess is represented in MODFLOW as a source term, P for rainfall and vertical unsaturated flow for infiltration. By using this analogy and recognizing that $\frac{\partial z}{\partial t} = 0$, we can pose the equation as:

$$\frac{\partial h}{\partial t} = \frac{\partial q}{\partial x} + \underbrace{\left[P - K_z(\psi) \frac{\partial h}{\partial z} \right]}_{\text{precipitation excess}} \quad (1\text{-D MODFLOW overland flow})$$

The Darcy-Weisbach equation (*Chin*, 2000 pg 352) is used to approximate the surface discharge per unit width, q :

$$q = \psi^{\frac{1+k}{2-k}} \left[\frac{8gS_o}{k_d} \left(\frac{\rho}{\mu} \right)^k \right]^{\frac{1}{2-k}} \quad (1\text{-D Darcy-Weisbach equation})$$

where:

- k_d = surface roughness parameter [-]
- ρ = fluid density [M/L³]
- μ = dynamic viscosity of fluid [M/LT]
- k = index indicating flow regime, 1 = laminar, 0 = turbulent [-]

Appendix B

One-dimensional simulation of solute transport

To demonstrate the model's compatibility with existing transport model codes, RT3D (Clement, 1997) was modified to simulate solute transport through the vadose zone. The governing equation describing solute transport through saturated soil is (Clement, 1997, pg 7):

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial x_i} \left[n D_{ij} \frac{\partial C}{\partial x_j} \right] - \frac{\partial}{\partial x_i} (v_i C) + \frac{q_s}{n} C_s + r_c$$

(Solute transport through saturated soil)

where:

- C = aqueous-phase concentration of solute [M/L³]
- t = time [T]
- i,j = spatial indices (i,j = 1,2,3) [-]
- x = spatial location [L]
- D_{ij} = hydrodynamic dispersion coefficient [L²/T]
- v = pore velocity [L²/T]
- q_s = volumetric flux of water per unit volume aquifer representing sources and sinks [T⁻¹]
- C_s = concentration of the source/sink [M/L³]
- n = effective porosity [L³/L³]
- r_c = rate of all reactions that occur in the aqueous phase [M/L³/T]

This equation was modified to a form valid for transport through unsaturated soil (*Huyakorn and Pinder, 1983, pg 183*) by including the change in solute mass due to changes in soil water content ($\theta = n\Theta$):

$$\frac{\partial(Cn\Theta)}{\partial t} = \frac{\partial}{\partial x_i} \left[n\Theta D_{ij} \frac{\partial C}{\partial x_j} \right] - \frac{\partial}{\partial x_i} (v_i C_k) + \frac{q_s}{n} C_s + r_c$$

(*Solute transport through variably saturated soil*)

where:

Θ = saturation of the soil (water volume / drainable void volume) [-]

RT3D was modified to read an interface file containing the soil saturation distributions of a MODFLOW simulation and adjust the concentrations in each grid cell with the corresponding soil saturations for each MODFLOW time step.

The field infiltration experiment of *Warrick et al. (1971)* was briefly described and flow simulation results were presented in **Section 3.1.2**. The experiment was performed in a 6.1 meter² soil plot containing tensiometers at 30, 60, 90, 120, 150, 180 cm depths. A conservative tracer solution (0.2 N CaCl₂) was used to track solute transport through the system. Measurements were collected for 17.5 hours during which the soil surface was kept at constant saturation. The tracer solution was applied to the surface for 2.8 hours followed by 15.3 hours of water. The concentration profiles after 2 hours and 9 hours of infiltration are shown in **figure B.1** compared against both the experimental data and the SUMATRA model (*van Genuchten, 1978*). The basic behavior of the solute in the unsaturated soil is represented satisfactorily, demonstrating proper implementation of the unsaturated transport equation.

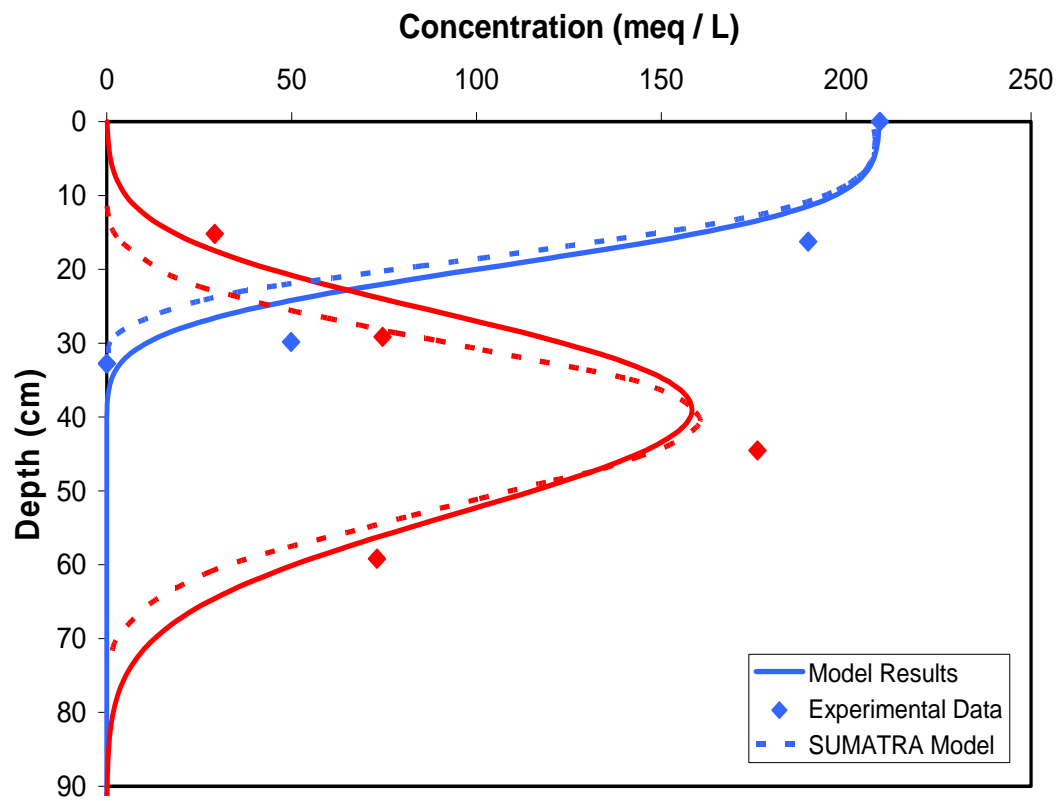


Figure B.1: Simulation results of the solute transport experiment from the *Warrick et al. (1971)* field study

Appendix C

Verification of gas phase diffusion in RT3D

In order to simulate the fate and transport of volatile contaminants through two phase (air/water) systems, the RT3D model code was modified to include gas phase diffusion in the hydrodynamic dispersion coefficient, D_{ij} . To verify proper implementation, a simple simulation was run comparing the RT3D results with an analytical solution for diffusion across a semi-infinite medium from a constant concentration source. The model parameters for this simulation are listed in **table C.1**.

An effective aqueous diffusion coefficient is defined by assuming instantaneous equilibrium between the gas and water phases. The coefficient is computed in RT3D for each MODFLOW time step and added to the apparent hydrodynamic dispersion tensor, $n\theta D_{ij}$. The coefficient takes the form (*Johnson et al.*, 2003):

$$D_e = D_w \Phi_w \tau_w + H D_a \Phi_a \tau_w \quad (\text{Effective aqueous diffusion coefficient})$$

where:

D_w = free-solution aqueous diffusion coefficient [L^2/T]

D_a = free-air gas-phase diffusion coefficient [L^2/T]

Φ_w = water filled porosity [L^3/L^3]

Φ_a = air filled porosity [L^3/L^3]

τ_w = water tortuosity ($\tau_w = [\Phi_w]^{1/3} / n^2$) [-]

τ_a = air tortuosity ($\tau_a = [\Phi_a]^{1/3} / n^2$) [-]

H = Henry's gas constant [-]

Table C.1: Model parameters for verification of gas phase diffusion

Gas phase diffusion from constant concentration source	
Total porosity	0.385 (cm ³ / cm ³)
Gas filled porosity	0.0770 (cm ³ / cm ³)
Water filled porosity	0.308 (cm ³ / cm ³)
Gas tortuosity	0.0170 (-)
Water tortuosity	0.432 (-)
Free-air gas-phase diffusion coefficient	6700 (cm ² /day)
Free solution aqueous diffusion coefficient	0.7 (cm ² /day)
Henry's gas constant	0.39 (-)
Effective gas diffusion	3.42 (cm ² /day)
Effective water diffusion	0.0932 (cm ² /day)
Effective diffusion coefficient	3.51 (cm ² /day)

The equation describing pure diffusion from a constant concentration source on the boundary of a semi-infinite medium can be expressed:

$$\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2} \quad (\text{Diffusion of a solute})$$

where:

$$D = \text{molecular diffusion coefficient [L}^2\text{/T]}$$

with the boundary conditions

$$C = C_0, \quad x = 0 \quad t > 0,$$

and the initial conditions

$$C = 0, \quad x > 0, \quad t = 0.$$

It can be shown (Crank, 1975, pg 20) that this system can be described by:

$$C = C_0 \operatorname{erfc} \frac{x}{2\sqrt{Dt}} \quad (\text{Analytical solution for diffusion})$$

The parameters from **table C.1** were used with the analytical solution to examine the extent of diffusion from a source of unit concentration ($C=1.0$). The effective diffusion coefficient D_e was converted into a valid form for the analytical solution by dividing by an effective porosity defined as $\Phi_e = \Phi_w + H\Phi_a$. The results from the transport simulation are compared with the analytical solution at several simulation times in **figure C.1**. The close match between the simulation and analytical solution confirms that gas phase diffusion is represented properly by the modified version of RT3D.

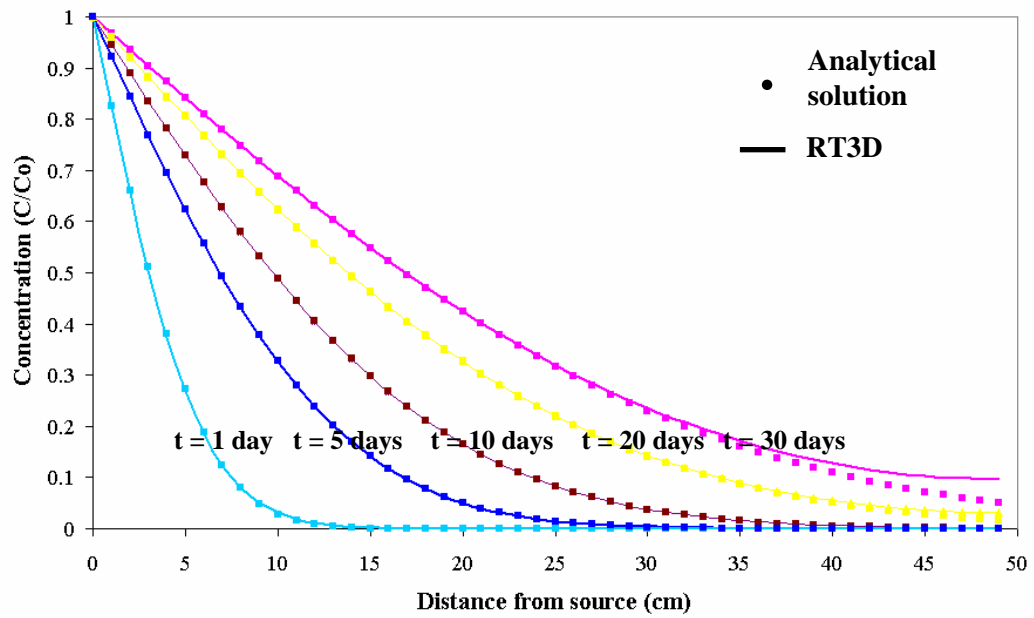


Figure C.1: Comparison between analytical solution and simulation of gas phase diffusion from constant concentration source

Appendix D

2-Dimensional Hypothetical Watershed Flowpath Simulations

In order to verify its functionality in simulating watershed response, a numerical modeling system must be tested under complex boundary conditions at realistic spatial and temporal scales. The watershed flowpath simulations of *Johnson et al. (2003)* provided an opportunity to compare the performance of this modeling system (MFWHT) with the well-established variably-saturated groundwater flow and transport model, MODFLOW-SURFACT 99 (MFS99) (Hydrogeologic, 1999). *Johnson et al. (2003)* examined the flow and transport of two different contaminants within a 2-dimensional hypothetical watershed flowpath using 10 years of precipitation and evapotranspiration data from six different sites. Two of the simulations (New Brunswick, New Jersey and Fort Collins, Colorado) exhibiting fundamentally different behavior are chosen for this comparison study. The daily evapotranspiration and precipitation data for the two cases are shown in **figure D.1**. The two objectives of the comparison are to (1) evaluate and verify the model's performance against an equivalent commercial model for two climatically different scenarios and (2) examine the simulation of overland flow using two different approaches for the top grid layer.

The model domain consisted of a vertical aquifer slice representing a flowpath from the watershed divide at the up-slope end to a constant stage stream downgradient. The slice is discretized into 20 horizontal layers and 36 vertical columns with 15 meter wide grid cells varying from 0.8 meters thick near the surface to 45 meters thick at the bottom of the domain. The top layer is modified to represent overland flow using the method described below. The ground surface is set at the top of the second layer. Layers 2 through 19 of the domain represent a typical alluvial, valley-fill aquifer with a hydraulic conductivity of 0.3 meters/day and the bottom layer represents the aquifer's bedrock ($K_{\text{sat}}=0.01$ m/day). The sides and bottom of the domain are set as no-flow boundaries and the head in the surface soil cell (layer 2) on the down-gradient end is held constant at stream level. The model parameters used in this study are listed in **TABLE D.1**.

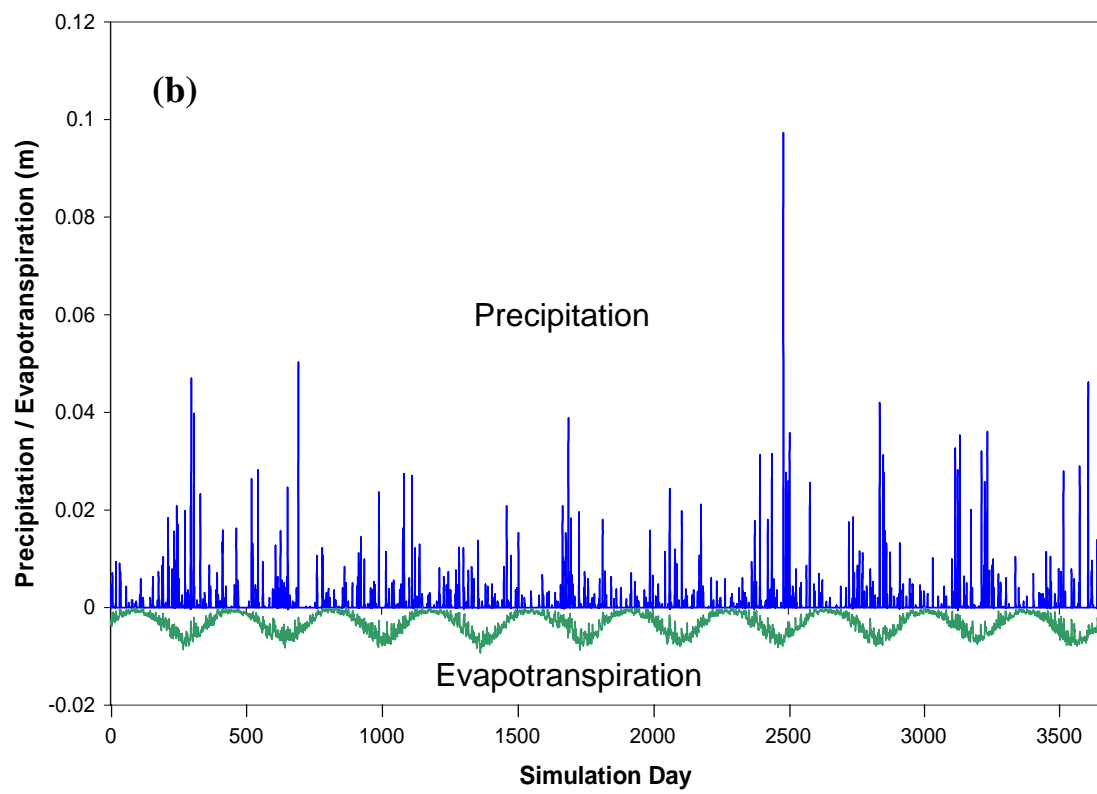
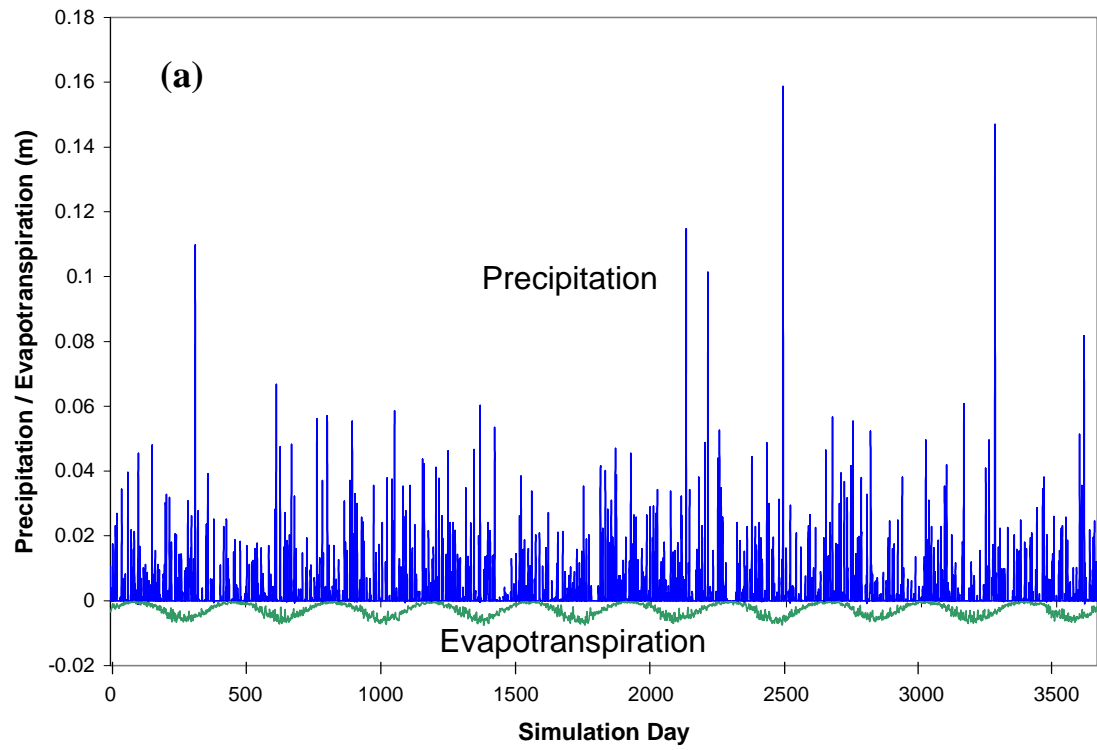


Figure D.1: Daily precipitation and evapotranspiration data for (a) New Brunswick, New Jersey and (b) Fort Collins, Colorado

**Table D.1: Model Parameters for comparison simulations
with MODFLOW-SURFACT 99**

Soil Parameters used by both models	Cap-Sat Parameters	$\alpha = 0.3$ (1/m) $\beta = 4.0$
	Residual Saturation	0.25
	Porosity	0.35
	Aquifer Hydraulic Conductivity	0.3 (m/day)
	Bedrock Hydraulic Conductivity	0.01 (m/day)
MODFLOW-SURFACT (MFS99) Overland flow parameters (top layer) for approximation method of <i>Johnson et al.</i> , 2003	Cap-Sat Parameters	$\alpha = 1.87$ (1/m) $\beta = 2.64$
	Residual Saturation	0.0
	Porosity	1.0
	Effective horizontal hydraulic Conductivity	3000 (m/day)
MODFLOW-WHT (MFWHT) Overland flow parameter (top layer) for kinematic wave method	Surface Roughness Parameter, k_d	12000

Johnson et al. (2003) adjusted the soil hydraulic parameters in the top grid layer of the variably saturated groundwater flow component of MFS99 to approximate overland flow. The top layer was assigned an effective hydraulic conductivity that was four orders of magnitude greater than that of the underlying soil. The soil characteristic parameters α and β were fitted so that the soil drainage and permeability functions approximate laminar surface storage-runoff response (**equation 2.17**). The top layer thickness was set to 1 meter based on the assumption that the surface flow would not exceed this height.

For the simulations using the model presented here (MFWHT), overland flow is assumed to be laminar and the surface roughness parameter is set to a value ($k_d = 12000$) that corresponds with a steep, rough surface (Chen, 1976). It is noted that the boundary rule-set detailed in **section 2.2.1** was active for these two simulations. It was necessary to increase the model grid resolution (106 columns and 24 layers) for the New Jersey simulation using the MFWHT model because of numerical difficulties caused by the increased magnitude of precipitation boundary fluxes.

The model results for the New Jersey case are shown in **figure D.2** and the Colorado case is shown in **figure D.3**. The surface runoff from the down-slope model cell (adjacent to the stream) in the top layer is normalized by the total surface area of the flowpath (**figures D.2a and D.3a**). The water table position is determined relative to the ground surface for the grid column 90 meters up slope from the stream (**figures D.2b and D.3b**). The MFWHT simulation of the New Jersey case exhibits runoff characterized by large peaks that dissipate quickly (**figure D.2a**) and are of the same order of magnitude as the precipitation events that triggered them (**figure D.1a**). This contrasts with the MFS99 runoff results which remain non-zero throughout the entire ten years, rise and fall gradually with the seasonal precipitation and do not exhibit the large peak amplitudes of the MFWHT results (**figure D.2a**). The MFS99 runoff behavior reveals the shortcoming

of the overland flow approximation method that was used. Specifically, the soil permeability function that was used to control the top layer's hydraulic conductivity was non-zero for the majority of the simulation due to the shallow position of the watertable (**figure D.2b**) and resultant low capillary pressure ($(h_c = h_a - \psi)$). This resulted in more total runoff over the course of the simulation, causing less flow to the subsurface and thus a slightly lower water table than the MFWHT results (**figure D.2b**). The MFS99 model results from the Colorado case (**figure D.3a**) show minimal surface flow that is an order of magnitude less than the precipitation events in **figure D.3b**. Again this slight difference in surface flow results in a slightly lower water table position for the MFS99 results (**figure D.3b**). The minimal surface flow influence on the system and strong similarity in water table behavior (**figure D.3b**) for this case confirms the MFWHT model's subsurface performance against the more established MFS99 subsurface model.

Overall, the MFWHT results confirm the model's two dimensional subsurface performance by the close similarity in water table behavior with the MFS99 results for both cases (**figures D.2b and D.3b**). The assumption that the surface runoff method used by *Johnson et al.* (2003) would have minimal impact on subsurface behavior appears valid, as the discrepancy in water table positions for both cases is minimal and is far less than the smallest grid cell thickness of 0.8 m (**figures D.2b and D.3b**). However, the surface runoff behavior of this method does not reflect the daily pulses (or peaks) of runoff inherent to natural systems, especially for systems with shallow water tables and high annual precipitation. Therefore, although the MFS99 results were appropriate in the context of that particular study, the MFWHT results are more representative of a watershed system.

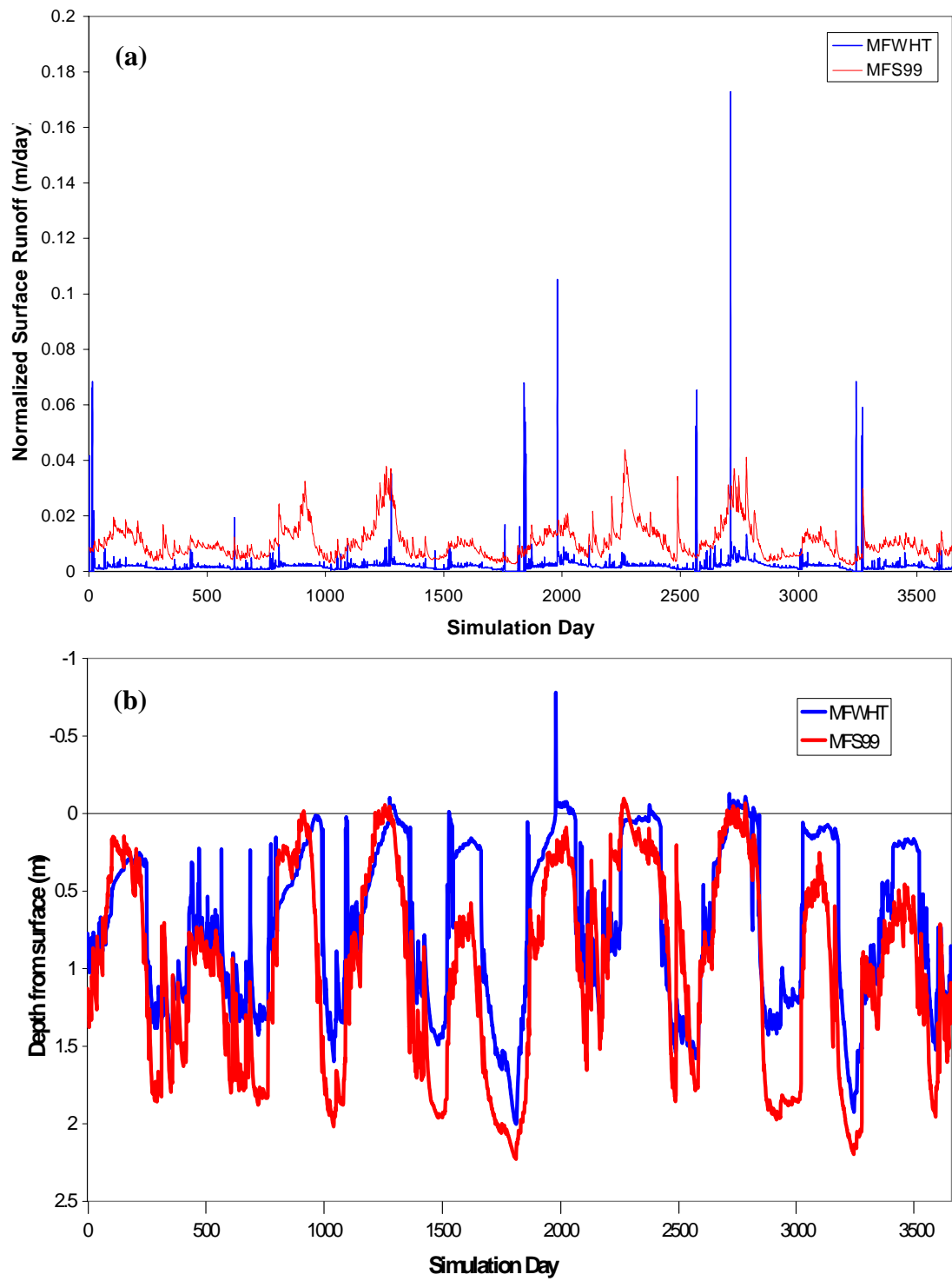


Figure D.2: Comparison of simulated (a) normalized surface runoff and (b) lowland water table position for the New Brunswick, NJ case.

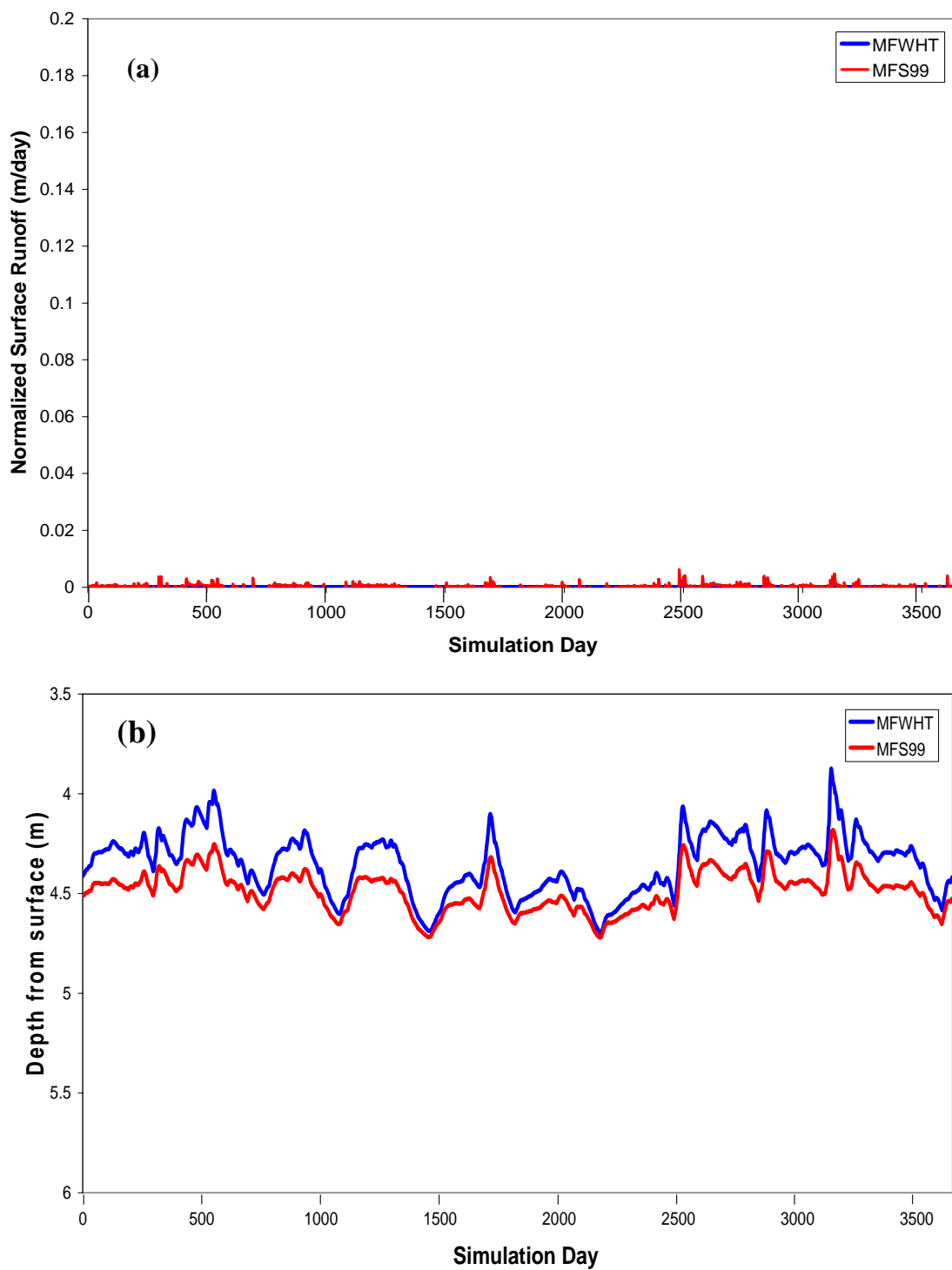


Figure D.3: Comparison of simulated (a) normalized surface runoff and (b) lowland water table position for the Fort Collins, CO case.

Appendix E

Adaptive Time Stepping Scheme

Transient flow simulations of non-linear solutions often have difficulty converging in MODFLOW due to a user-prescribed time step that is too long, causing the simulation to abort. Conversely, for long simulations with multiple stress periods of variable boundary conditions, prescribed time steps that are too short will cause the overall computation time to be unnecessarily long. MODFLOW currently does not have a time stepping scheme that is able to adjust the time step during a simulation based on the computational conditions. An adaptive time stepping scheme was developed to increase the model's efficiency during transient simulations.

The new scheme requires the user to input the maximum time step size (TMX), the minimum time step size (TMN), a time step reduction factor (TSD) and a time step multiplier (TSM), as well as a file number (ITIM) and array size (MXSTP) for recording the time step history of a simulation in an output file (for interfacing with a transport model). The original MODFLOW input files are still used to set the number of time steps (NSTP) for each stress period and to determine the time step size (DELTA). During the simulation, after the computations for each time step are completed, the new scheme evaluates the number of iterations that was required for convergence. If convergence is achieved in more than 65% of the user-defined maximum number of iterations (MXITER), the time step is divided by TSD in anticipation of convergence difficulties in the next time step. If convergence is achieved in less than 35% of MXITER, the time step is multiplied by TSM in order to speed up the simulation. These convergence criteria are recognized to be arbitrary and can be adjusted to meet user demands. If the solution fails to converge within a given time step, the time step is reduced by TSD and the iterative computations are restarted with the reduced time step. If the adjusted time step exceeds the maximum size (TMX), the step is set equal to TMX. Conversely, if the

time step is reduced below the minimum size (TMN), the time step is set equal to TMN. The counter variable that tracks elapsed time in the current stress period (PERTIM) is adjusted using the latest time step (DELT). The last time step of each stress period is adjusted as necessary to prevent exceeding the user-defined stress period length (PERLEN).

Appendix F

FORTRAN Source Code for MODFLOW 2000 Version 1.6

F.1 FORTRAN source code: Unsaturated Flow (UNS) package

The following is the source code developed to simulate unsaturated flow using Richards equation (**equation 2.3**) with MODFLOW 2000 version 1.8 (*Harbaugh et al.*, 2000).

```

C   Last change: RBT  29 OCT 2003 17:00
C=====
      SUBROUTINE GWFIUNSI1AL(ISUM,LCRSW,LCCVS,LCUNSOC,NCOL,NROW,
&                          NLAY,IN,IOUT,IUNSCB,
&                          IUNSOC,LALPHA,LCVGN,IFREFM)
C-----VERSION 29OCT2003 RBT
C   *****
C   READ AND ALLOCATE OUTPUT CONTROL FLAG UNSOC ARRAY (IN RX ARRAY)
C   ALLOCATE ARRAY STORAGE FOR UNSATURATED MODULE RESIDUAL SOIL
C   SATURATIONS (RSW) AND SATURATED VERTICAL CONDUCTANCE (CVS) ARRAYS
C   (IN RX ARRAY).
C   *****
C   SPECIFICATIONS:
C   -----
      INTEGER ZERO
      PARAMETER (ZERO=0)
C   -----
500 FORMAT(1X,/
&1X,'UNSI -- UNSATURATED PACKAGE, VERSION 1,',
&   ' 9/20/2002',/,9X,'INPUT READ FROM UNIT',I3)
570 FORMAT(1X,'CELL-BY-CELL SOIL WATER SATURATIONS WILL BE SAVED ON'
&,' UNIT',I3)
575 FORMAT(1X,'CELL-BY-CELL SOIL WATER SATURATIONS WILL BE SAVED FOR'
&,' ALL TIME STEPS IN EACH STRESS PERIOD')
576 FORMAT(1X,'NO UNSATURATED OUTPUT REQUESTED')
580 FORMAT(1X,'CELL-BY-CELL SOIL WATER SATURATIONS WILL BE SAVED FOR',
&1X,I5,1X,'USER-DEFINED POINTS DURING THE SIMULATION')
585 FORMAT(1X,I10,' ELEMENTS IN X ARRAY ARE USED BY UNS')
C
C1-----IDENTIFY PACKAGE.
      WRITE(IOUT,500)IN
C
C2-----READ UNIT / . FLAG FOR CELL-BY-CELL SOIL SATURATIONS
      IF (IFREFM.EQ.ZERO) THEN
        READ(IN,'(I10)') IUNSCB
      ELSE
        READ(IN,*)IUNSCB
      ENDIF
C
C3-----IF CELL-BY-CELL SOIL WATER SATURATIONS ARE TO BE SAVED THEN
C3-----READ OUTPUT CONTROL FLAG
      IF (IUNSCB.GT.ZERO) THEN
        IF (IFREFM.EQ.ZERO) THEN
          READ(IN,'(I10)') IUNSOC
        ELSE
          READ(IN,*)IUNSOC
        ENDIF
      ENDIF

```

```

      ENDIF
C
C4-----PRINT UNIT NUMBER TO MODFLOW OUTPUT FILE
      WRITE(IOUT,570) IUNSCB
C
C4A-----PRINT OUTPUT CONTROL SETTING TO MODFLOW OUTPUT FILE
      IF (IUNSOC.LT.ZERO) THEN
        WRITE(IOUT,575)
        LCUNSOC=1
      ELSE
        WRITE(IOUT,580)IUNSOC
      ENDIF
C
C5-----IF NO OUTPUT REQUESTED, WRITE NOTICE TO OUTPUT FILE AND SET FLAGS
      ELSE
        WRITE(IOUT,576)
        LCUNSOC=1
        IUNSOC=0
      ENDIF
C
C6-----ALLOCATE SPACE FOR THE ARRAYS CVS, RSW, UNSOC (IF NEEDED), ALPHA, AND VGN
      IRK=ISUM
      LCCVS=ISUM
      ISUM=ISUM+NCOL*NROW*NLAY
      LCRSW=ISUM
      ISUM=ISUM+NCOL*NROW*NLAY
      IF (IUNSCB.GT.ZERO.AND.IUNSOC.GT.ZERO) THEN
        LCUNSOC=ISUM
        ISUM=ISUM+IUNSOC*2
      ENDIF
      LCALPHA=ISUM
      ISUM=ISUM+NCOL*NROW*NLAY
      LCVGN=ISUM
      ISUM=ISUM+NCOL*NROW*NLAY
C
C7-----CALCULATE & PRINT AMOUNT OF SPACE USED BY UNS PACKAGE.
      IRK=ISUM-IRK
      WRITE(IOUT,585)IRK
C
C8-----RETURN.
      RETURN
      END
C=====
      SUBROUTINE GWF1UNSI1RP(IN,IOUT,HNEW,CV,BOTM,NBOTM,ALPHA,VGN,
&                                RSW,SC2,UNSOC,CVS,NCOL,NROW,
&                                NLAY,IUNSCB,IUNSOC,ISWFL,IFREFM,FNAME,
&                                IAVG,IOLF)
C
C-----VERSION 29OCT2003 RBT
C *****
C  READ UNSOC ARRAY (IF NEEDED), INITIAL SW FLAG,
C    VAN GENUCHTEN PARAMETER ARRAY AND SOIL WATER CONTENT ARRAYS
C
C  OPEN OUTPUT FILE
C *****
C  SPECIFICATIONS:
C  -----
      CHARACTER*24 ANAME(4)
      CHARACTER*4 EXT
      CHARACTER*200 OFILE,FNAME
      INTEGER ISWFL,IUNSOC,ZERO,IAVG,IOLF,VGFLG

      DOUBLE PRECISION HNEW
      REAL ALPHA,PRESS,VGN,EFSAT,TTOP,BBOT,SW,RSW,CVS,CV,
1  UNSOC,NODE
C

```

```

        DIMENSION      HNEW(NCOL,NROW,NLAY),SW(NCOL,NROW,NLAY),
1          RSW(NCOL,NROW,NLAY),UNSOC(IUNSOC,2),
2          BOTM(NCOL,NROW,0:NBOTM),BUF(NCOL,NROW,NLAY),
3          CV(NCOL,NROW,NLAY),CVS(NCOL,NROW,NLAY),
4          ALPHA(NCOL,NROW,NLAY),VGN(NCOL,NROW,NLAY)
C
      COMMON /DISCOM/LBOTM(200),LAYCBD(200)
C
      PARAMETER (ZERO=0)
      PARAMETER (ONE=1)
      DATA EXT /'.sat'/
      DATA ANAME(1) /' INITIAL WATER SATURATION'/
      DATA ANAME(2) /' RESIDUAL WATER SATURATION'/
      DATA ANAME(3) /' VAN GENUCHTEN ALPHA'/
      DATA ANAME(4) /' VAN GENUCHTEN N'/
C -----
35      FORMAT (5X,'ERROR IN UNSATURATED INPUT FILE - ALL INITIAL
& WATER SATURATION MUST BE POSITIVE AND NON-ZERO',/)
40      FORMAT (5X,'ERROR IN UNSATURATED INPUT FILE - ALL RESIDUAL
& WATER SATURATION MUST BE POSITIVE AND NON-ZERO',/)
45      FORMAT (5X,'ERROR IN UNSATURATED INPUT FILE - ALL SATURATED
& WATER SATURATION MUST BE POSITIVE AND NON-ZERO',/)
65      FORMAT(5X,'# CELL BY CELL VOLUMETRIC SOIL WATER CONTENTS'
&','5X,'# VAN GENUCHTEN PARAMETERS - ALPHA:',1X,G10.5,2X,
&'N:',1X,G10.5,/)
70      FORMAT (5X,'# INITIAL SOIL WATER CONTENT ARRAY')
C
C1----READ AVERAGING FLAG TO DETERMINE INTERCELL METHOD AND
C1----OVERLAND FLOW FLAG (TO ACTIVATE TOP LAYER)
      IF (IFREFM.EQ.ZERO) THEN
        READ(IN,'(I10)') IAVG
        READ(IN,'(I10)') IOLF
      ELSE
        READ(IN,*) IAVG
        READ(IN,*) IOLF
      ENDIF
C
C2----READ UNSOC ARRAY IF REQUESTED (IUNSOC IS POSITIVE)
      IF (IUNSOC.GT.ZERO) THEN
        DO 1 K=1,IUNSOC
          IF (IFREFM.EQ.ZERO) THEN
            READ(IN,'(G10.3)') (UNSOC(K,J),J=1,2)
          ELSE
            READ(IN,*)(UNSOC(K,J),J=1,2)
          ENDIF
1      CONTINUE
      ENDIF
C
C3----READ INITIAL SATURATIONS FLAG
      IF (IFREFM.EQ.ZERO) THEN
        READ(IN,'(I10)') ISWFL
      ELSE
        READ(IN,*)ISWFL
      ENDIF
C
C3A-- READ VAN GENUCHTEN ARRAY FLAG
      IF (IFREFM.EQ.ZERO) THEN
        READ(IN,'(I10)') VGFLG
      ELSE
        READ(IN,*)VGFLG
      ENDIF
C
C3B-- IF VG FLAG IS POSITIVE,
C3B-- CONSTANT VAN GENUCHTEN PARAMETERS FOR ALL MODEL CELLS
      IF (VGFLG.GT.0) THEN
C

```

```

C3C-- POSITIVE VGFLG; CONSTANT VAN GENUTCHEN PARAMETERS
      IF (IFREFM.EQ.ZERO) THEN
        READ(IN,'(2G10.5)') ALPH,VN
      ELSE
        READ(IN,*)ALPH,VN
      ENDIF
      DO 8 I=1,NROW
      DO 8 J=1,NCOL
      DO 8 K=1,NLAY
        ALPHA(J,I,K)=ALPH
        VGN(J,I,K)=VN
8      CONTINUE
    ELSE
C
C3D---READ VAN GENUCHTEN PARAMETER ARRAYS FROM INPUT FILE
      DO 2 K=1,NLAY
        CALL U2DREL(BUF(1,1,K),ANAME(3),NROW,NCOL,K,IN,IOUT)
2      CONTINUE
        DO 3 I=1,NROW
        DO 3 J=1,NCOL
        DO 3 K=1,NLAY
          ALPHA(J,I,K)=BUF(J,I,K)
3      CONTINUE
        DO 4 K=1,NLAY
          CALL U2DREL(BUF(1,1,K),ANAME(4),NROW,NCOL,K,IN,IOUT)
4      CONTINUE
        DO 6 I=1,NROW
        DO 6 J=1,NCOL
        DO 6 K=1,NLAY
          VGN(J,I,K)=BUF(J,I,K)
6      CONTINUE
    ENDIF
C
C4----IF ISWFL > ZERO, READ INITIAL SATURATIONS
      IF (ISWFL.GT.ZERO) THEN
        DO 5 K=1,NLAY
          CALL U2DREL(BUF(1,1,K),ANAME(1),NROW,NCOL,K,IN,IOUT)
5      CONTINUE
        DO 7 I=1,NROW
        DO 7 J=1,NCOL
        DO 7 K=1,NLAY
          SW(J,I,K)=BUF(J,I,K)
7      CONTINUE
    ENDIF
C
C5----READ RESIDUAL SOIL SATURATION FOR EACH CELL
      DO 10 K=1,NLAY
        CALL U2DREL(BUF(1,1,K),ANAME(2),NROW,NCOL,K,IN,IOUT)
10     CONTINUE
        DO 12 I=1,NROW
        DO 12 J=1,NCOL
        DO 12 K=1,NLAY
          RSW(J,I,K)=BUF(J,I,K)
12     CONTINUE
C
C6----MAKE SURE ALL ARRAYS CONTAIN POSITIVE, NON-ZERO VALUES
      IF (IOLF.GT.0)KK=2
      KK=1
      DO 20 I=1,NROW
      DO 20 J=1,NCOL
      DO 25 K=KK,NLAY
        IF (ISWFL.GT.ZERO.AND.SW(J,I,K).LE.ZERO) THEN
          WRITE(*,35)
          STOP
        ELSEIF (RSW(J,I,K).LE.ZERO) THEN
          WRITE(*,40)

```



```

                                STOP
                                ENDIF
25      CONTINUE
20      CONTINUE
C
C7--OPEN OUTPUT FILE
      IF (IUNSCB.GT.0) THEN
        OFILE=FNAME
        NUM=INDEX(OFILE,' ')
        WRITE(OFILE(NUM-4:NUM),'(A4')EXT
        IF(IUNSOC.EQ.-10)THEN
          OPEN (UNIT=IUNSCB,FILE=OFILE,FORM='BINARY',
&      STATUS='UNKNOWN')
        ELSE
          OPEN (UNIT=IUNSCB,FILE=OFILE,FORM='FORMATTED',
&      STATUS='UNKNOWN')
        ENDIF
      ENDIF
C
C8---- IF INITIAL SOIL SATURATION ARRAY READ,
C8---- ADJUST HEAD IN UNSATURATED CELLS ACCORDINGLY
      IF (ISWFL.GT.ZERO) THEN
C8B-OLF-- DO NOT CALCULATE INITIAL HEADS FOR OLF LAYER
        KK=1
        IF (IOLF.GT.ZERO) KK=2
C8B-OLF
        DO 55 K=KK,NLAY
        DO 55 J=1,NCOL
        DO 55 I=1,NROW
          EFSAT=0.
          BBOT=BOTM(J,I,LBOTM(K))
          TTOP=BOTM(J,I,LBOTM(K)-1)
          EFSAT=(SW(J,I,K)-RSW(J,I,K))/(1-RSW(J,I,K))
          PRESS=UNSPS(EFSAT,ALPHA(J,I,K),VGN(J,I,K))
          NODE=(TTOP+BBOT)/2
          HNEW(J,I,K)=NODE+PRESS
          IF (EFSAT.EQ.1.0) HNEW(J,I,K)=NODE
55      CONTINUE
        ENDIF
C
C9A---- IF REQUESTED,CALCULATE SOIL SATURATIONS FROM INITIAL HEADS
      IF (IUNSOC.EQ.-10.AND.ISWFL.LE.ZERO)THEN
        KK=1
C9-OLF
        IF (IOLF.GT.0) KK=2
        DO 15 K=KK,NLAY
        DO 15 I=1,NROW
        DO 15 J=1,NCOL
          HD=HNEW(J,I,K)
          BBOT=BOTM(J,I,LBOTM(K))
          TTOP=BOTM(J,I,LBOTM(K)-1)
          NODE=(TTOP+BBOT)/2
          PRESS=HD-NODE
          IF (HD.GE.NODE) THEN
            SW(J,I,K)=ONE
          ELSE
            SW(J,I,K)=UNSSP(PRESS,RSW(J,I,K),ALPHA(J,I,K),VGN(J,I,K))
          ENDIF
15      CONTINUE
        ENDIF
C
C9B----IF REQUESTED, WRITE INITIAL SW TO BINARY OUTPUT FILE FOR RT3D
      IF (IUNSOC.EQ.-10) THEN
        L=0
        M=0
        N=0.

```

```

        WRITE (IUNSCB)L,M,N
        WRITE (IUNSCB)((SW(J,I,K),J=1,NCOL),I=1,NROW),K=1,NLAY)
    ENDIF
C
C10--- SET SCV (SATURATED VERTICAL CONDUCTANCE STORAGE ARRAY) EQUAL TO CV VALUES
        DO 80 K=1,NLAY
        DO 80 I=1,NROW
        DO 80 J=1,NCOL
            IF (K.LT.NLAY) CVS(J,I,K)=CV(J,I,K)
80      CONTINUE
C
C11---RETURN
        RETURN
        END
C
C=====
      SUBROUTINE GWF1UNSF1M(ALPHA,VGN,NCOL,NROW,NLAY,HNEW,BOTM,NBOTM,
&                          CVS,CV,IAVG,IOLF,CC,CR)
C
C-----VERSION 29OCT2003 RBT
C *****
C  CALCULATE INTERCELL RELATIVE PERMEABILITY
C    AND USE TO ADJUST CONDUCTANCES
C *****
C  SPECIFICATIONS:
C  -----
        DOUBLE PRECISION HNEW
        REAL HD,BBOT,TTOP,PRESS
        REAL VGN,ALPHA,SPSC
        REAL SAT,KREL,SW,KR1,KR2,NODE
C
        DIMENSION      BOTM(NCOL,NROW,0:NBOTM),HNEW(NCOL,NROW,NLAY),
1          CVS(NCOL,NROW,NLAY),CV(NCOL,NROW,NLAY),
2          TOP(NCOL,NROW,NLAY),KREL(NCOL,NROW,NLAY),
3          ALPHA(NCOL,NROW,NLAY),VGN(NCOL,NROW,NLAY),
4          CC(NCOL,NROW,NLAY), CR(NCOL,NROW,NLAY)
C
        COMMON /DISCOM/LBOTM(200),LAYCBD(200)
C
        PARAMETER (ONE=1.0)
        PARAMETER (ZERO=0.0)
C  -----
C
C1-- CALCULATE RELATIVE PERMEABILITY FROM HEAD OF CURRENT ITERATION
        KK=1
C1-OLF
        IF (IOLF.GT.0.)KK=2
        DO 10 K=KK,NLAY
            DO 10 I=1,NROW
            DO 10 J=1,NCOL
                HD=HNEW(J,I,K)
                BBOT=BOTM(J,I,LBOTM(K))
                TTOP=BOTM(J,I,LBOTM(K)-1)
                NODE=(TTOP+BBOT)/2
                PRESS=HD-NODE
C
C1A-----IF CELL IS SATURATED, SET KREL = 1.0
                IF (HD.GE.NODE) THEN
                    KREL(J,I,K)=ONE
                ELSE
C
C1B-----IF CELL IS UNSATURATED, CALCULATE RELATIVE K
                    KREL(J,I,K)=UNSKP(PRESS,ALPHA(J,I,K),VGN(J,I,K))
                ENDIF
10      CONTINUE
C

```

```

C2---- CALCULATE HORIZONTAL AND VERTICAL CONDUCTANCES FOR ALL CELLS
C2---- USING RELATIVE PERMEABILITY
      KK=1
      DO 20 K=KK,NLAY
        DO 20 I=1,NROW
          DO 20 J=1,NCOL
            KR1=KREL(J,I,K)
C
C2A-OLF--IF OVERLAND FLOW PACKAGE ACTIVE, ONLY ADJUST LEAKANCE
      IF (IOLF.GT.0.)GOTO 50
C
C2B-----IF T=0 THEN SET CONDUCTANCE EQUAL TO 0. GO ON TO VERTICAL CONDUCTANCE
      IF(CC(J,I,K).NE.ZERO) GO TO 30
      CR(J,I,K)=ZERO
      GO TO 50
C
C2B-----ADJUST CONDUCTANCES USING INTERCELL AVERAGING
C2B-----FOR RELATIVE PERMEABILITY
      30          IF(J.EQ.NCOL) GO TO 40
                  KR2=KREL(J+1,I,K)
C
C2B-----OPTIONS FOR INTERCELL AVERAGING OF RELATIVE PERMEABILITY
C2B-----GEOMETRIC MEAN, ARITHMETIC MEAN AND UPSTREAM WEIGHTING
      IF (IAVG.EQ.1) THEN
        CR(J,I,K)=CR(J,I,K)*(KR1*KR2)**(0.5)
      ELSEIF (IAVG.EQ.2)THEN
        CR(J,I,K)=CR(J,I,K)*(KR1+KR2)/2.
      ELSEIF (IAVG.EQ.3)THEN
        HD1 = HNEW(J,I,K)
        HD2 = HNEW(J+1,I,K)
        IF (HD1.GT.HD2) THEN
          CR(J,I,K)=CR(J,I,K)*KR1
        ELSE
          CR(J,I,K)=CR(J,I,K)*KR2
        ENDIF
      ENDIF
C
C2C-----IF THIS IS NOT THE LAST ROW(FRONTMOST) THEN CALCULATE
C2C-----BRANCH CONDUCTANCE IN THE COLUMN DIRECTION (CC) TO THE FRONT.
      40          IF(I.EQ.NROW) GO TO 50
                  KR2=KREL(J,I+1,K)
                  IF (IAVG.EQ.1) THEN
                    CC(J,I,K)=CC(J,I,K)*(KR1*KR2)**(0.5)
                  ELSEIF (IAVG.EQ.2)THEN
                    CC(J,I,K)=CC(J,I,K)*(KR1+KR2)/2.
                  ELSEIF (IAVG.EQ.3)THEN
                    HD1 = HNEW(J,I,K)
                    HD2 = HNEW(J,I+1,K)
                    IF (HD1.GT.HD2) THEN
                      CC(J,I,K)=CC(J,I,K)*KR1
                    ELSE
                      CC(J,I,K)=CC(J,I,K)*KR2
                    ENDIF
                  ENDIF
C
C2D-----IF THIS IS NOT THE LAST LAYER (BOTTOM) THEN ADJUST
C2D-----VERTICAL CONDUCTANCE IN THE LAYER DIRECTION (CV)
      50          IF(K.GE.NLAY) GOTO 20
                  KR2=KREL(J,I,K+1)
C2D-OLF
      IF (IOLF.GT.0.AND.K.EQ.1) KR1=1.0
C2D-OLF
      IF (IAVG.EQ.1) THEN
        CV(J,I,K)=CVS(J,I,K)*(KR1*KR2)**(0.5)
      ELSEIF (IAVG.EQ.2)THEN
        CV(J,I,K)=CVS(J,I,K)*(KR1+KR2)/2.

```

```

                                ELSEIF (IAVG.EQ.3) THEN
                                    HD1 = HNEW(J,I,K)
                                    HD2 = HNEW(J,I,K+1)
                                    IF (HD1.GE.HD2) THEN
                                        CV(J,I,K)=CVS(J,I,K)*KR1
                                    ELSE
                                        CV(J,I,K)=CVS(J,I,K)*KR2
                                    ENDIF
                                ENDIF
                                ENDIF
                                20 CONTINUE
C
C3-----RETURN
                                RETURN
                                END
C
C=====
SUBROUTINE GWF1UNSD1BD(HNEW,SC2,RSW,BOTM,NBOTM,UNSOC,NCOL,NROW,
&                                NLAY,IUNSCB,IUNSOC,KSTP,KPER,ALPHA,VGN,IOLF,
&                                CV,DELR,DELC,PERTIM,NPER,TOTIM,MSUM,VBVL,
&                                VBNM,DELT,HOLD,ICBCFL)
C-----VERSION 29OCT2003 RBT
C *****
C CALCULATE SOIL SATURATION DISTRIBUTION
C AND WRITE TO UNS OUTPUT FILE
C *****
C SPECIFICATIONS:
C -----
C DOUBLE PRECISION HNEW,SSLM,SLMIN,SLMOUT
C CHARACTER*16 VBNM(MSUM),TEXT
C
C REAL TTOP,BBOT,HD,PRESS,VGN,ALPHA,SW,RSW,SC2,PERTIM,USTP,P,NODE,
& UNSOC,LIM,H1,H2,HDIFF,FLUX,WT5,WT30,HD5,HD30,TOTIM,SLM,DSDT
C
C INTEGER UPER,IUNSOC,KSTP,IBD,KPER,KK
C
C DIMENSION HNEW(NCOL,NROW,NLAY),BOTM(NCOL,NROW,0:NBOTM),
1 SW(NCOL,NROW,NLAY),RSW(NCOL,NROW,NLAY),
2 UNSOC(IUNSOC,2),USTP(IUNSOC),UPER(IUNSOC),
3 CV(NCOL,NROW,NLAY),DELR(NCOL),DELC(NROW),
4 ALPHA(NCOL,NROW,NLAY),VGN(NCOL,NROW,NLAY),
5 SLM(NCOL,NROW,NLAY),VBVL(4,MSUM),HOLD(NCOL,NROW,NLAY),
6 SC2(NCOL,NROW,NLAY)
C
C COMMON /DISCOM/LBOTM(200),LAYCBD(200)
C
C PARAMETER (ZERO=0)
C PARAMETER (ONE=1)
C PARAMETER (LIM=0.01)
C DATA TEXT / ' SOIL MOISTURE'/
C -----
C
C1---CALCULATE SOIL SATURATIONS FOR UNSATURATED CELLS
DO 15 K=1,NLAY
DO 15 I=1,NROW
DO 15 J=1,NCOL
HD=HNEW(J,I,K)
BBOT=BOTM(J,I,LBOTM(K))
TTOP=BOTM(J,I,LBOTM(K)-1)
NODE=(TTOP+BBOT)/2
PRESS=HD-NODE
IF (HD.GE.NODE) THEN
SW(J,I,K)=ONE
ELSE
SW(J,I,K)=UNSSP(PRESS,RSW(J,I,K),ALPHA(J,I,K),VGN(J,I,K))
ENDIF
15 CONTINUE

```

```

C
C2----WRITE CELL-BY-CELL SOIL SATURATION VALUES (STRESS PERIOD NUMBER AND TIME)
C2----TO UNS OUTPUT FILE (UNIT = IUNSCB)
      IF (IUNSCB.GT.ZERO.AND.IUNSOC.LT.ZERO) THEN
        IF (IUNSOC.EQ.-10)THEN
          WRITE (IUNSCB)KSTP,KPER,TOTIM
          WRITE (IUNSCB)(((SW(J,I,K),J=1,NCOL),I=1,NROW),K=1,NLAY)
        ELSE
          WRITE (IUNSCB,*)KSTP,KPER,TOTIM
          DO 31 K=1,NLAY
            BBOT=BOTM(55,1,LBOTM(K))
            TTOP=BOTM(55,1,LBOTM(K)-1)
            HD=HNEW(55,1,K)
            NODE=(TTOP+BBOT)/2
            WRITE (IUNSCB,*)NODE,SW(55,1,K),HD
31          CONTINUE
        ENDIF
      C
      C2A---IF REQUESTED (IUNSOC > ZERO), WRITE SW VALUES FOR USER-SPECIFIED
      C2A---TIME STEP AND STRESS PERIOD
        ELSEIF (IUNSCB.GT.ZERO.AND.IUNSOC.GT.ZERO) THEN
          DO 35 L=1,IUNSOC
            UPER(L)=INT(UNSOC(L,1))
            USTP(L)=UNSOC(L,2)
35          CONTINUE
      C
      C2B-- WRITE SATURATION VALUES FOR REQUESTED STRESS PERIOD AND ELAPSED TIME
        DO 40 L=1,IUNSOC
          IF (USTP(L).LT.ZERO) THEN
            STP=INT(ABS(USTP(L)))
            IF (KPER.EQ.UPER(L).AND.KSTP.EQ.STP) THEN
              WRITE (IUNSCB,*)KSTP,KPER,PERTIM
              GOTO 50
            ENDIF
          ELSE
            DIFF=ABS(PERTIM-USTP(L))
            IF (KPER.EQ.UPER(L).AND.DIFF.LE.LIM) THEN
              WRITE (IUNSCB,*)KSTP,KPER,PERTIM
              GOTO 50
            ENDIF
          ENDIF
        ENDIF
      CYCLE
    C
    C2C--- FORMATTING OPTIONS (TO BE DEVELOPED AS NEEDED)
    50      DO 45 J=1,NCOL
            DO 45 I=1,NROW
            DO 45 K=1,NLAY
              WRITE (IUNSCB,*)SW(J,I,K)
45      CONTINUE
40      CONTINUE
    ENDIF
  C
  C3-- STORE SOIL SATURATION FLOW FOR FLOW BUDGET
    SLMIN=ZERO
    SLMOUT=ZERO
    KK=1
  C
  COLF--- IF OLF PACKAGE ACTIVE, DO NOT COMPUTE SOIL SATURATION
  COLF--- BUDGET FOR TOP LAYER
    IF (IOLF.GT.0.) KK=2
  COLF
    DO 60 K=KK,NLAY
      DO 60 I=1,NROW
      DO 60 J=1,NCOL
  C
  C3A-- ASSIGN VALUES

```

```

                P = SC2(J,I,K)
                BBOT=BOTM(J,I,LBOTM(K))
                TTOP=BOTM(J,I,LBOTM(K)-1)
        NODE=(TTOP+BBOT)/2
        THCK=TTOP-BBOT
        TLED=1/DELT
        SWNEW=SW(J,I,K)
C
C3B-- SET SWOLD = SOIL SATURATION FROM PREVIOUS TIME STEP
        HO=HOLD(J,I,K)
        PRESS=HO-NODE
        IF (HO.GE.NODE) THEN
                SWOLD=1.0
        ELSE
                SWOLD=UNSSP(PRESS,RSW(J,I,K),ALPHA(J,I,K),VGN(J,I,K))
        ENDIF
C
C3C-- CALCULATE CHANGE IN SOIL SATURATION OVER TIME STEP
        DSDT=P*DELR(J)*DELC(I)*THCK*(SWOLD-SWNEW)*TLED
C
C3D-- STORE CELL-BY-CELL SOIL SATURATION FLOW IN BUFFER AND ADD TO ACCUMULATORS.

                SLM(J,I,K)=DSDT
                SSLM=DSDT
                IF(DSDT) 295,60,296
295                SLMOUT=SLMOUT-SSLM
                GO TO 60
296                SLMIN=SLMIN+SSLM
C
        60 CONTINUE
C
C3E-- IF CELL-BY-CELL FLOWS WILL BE SAVED, SET FLAG IBD.
        IBD=0
        IF(IBCFCB.GT.0) IBD=ICBCFL
C
C3F-- IF IBD FLAG IS SET AND UNS PACKAGE ACTIVE, RECORD THE CONTENTS OF THE SOIL MOISTURE ARRAY.
        IF(IBD.EQ.1) CALL UBDSV(KSTP,KPER,TEXT,
1                IBCFCB,SLM,NCOL,NROW,NLAY,IOUT)
        IF(IBD.EQ.2) CALL UBDSV1(KSTP,KPER,TEXT,IBCFCB,
1                SLM,NCOL,NROW,NLAY,IOUT,DELT,PERTIM,TOTIM,IBOUND)
C
C3G-- ADD TOTAL SOIL MOISTURE RATES AND VOLUMES TO VBVL & PUT TITLE IN VBNM.
        SMIN=SLMIN
        SMOUT=SLMOUT
        VBVL(1,MSUM)=VBVL(1,MSUM)+SMIN*DELT
        VBVL(2,MSUM)=VBVL(2,MSUM)+SMOUT*DELT
        VBVL(3,MSUM)=SMIN
        VBVL(4,MSUM)=SMOUT
        VBNM(MSUM)=TEXT
        MSUM=MSUM+1
C
C4---RETURN.
        RETURN
        END
C
C=====
        FUNCTION UNSPS(EFSAT,ALPHA,VGN)
C-----VERSION 29OCT2003 RBT
C *****
C  CALCULATE PRESSURE HEAD AS A FUNCTION OF EFFECTIVE SATURATION
C  USING VAN GENUTCHEN FUNCTION
C
C *****
C  SPECIFICATIONS:
        REAL EFSAT,ALPHA,VGN,M
C -----

```

```

C
    M=1-(1/VGN)
    PRESS=(1./ALPHA)*(1./(EFSAT**(1/M))-1)**(1./VGN)
    UNSPS=-PRESS
C
    END
C
=====
C      FUNCTION UNSKP(PRESS,ALPHA,VGN)
C-----VERSION 29OCT2003 RBT
C      *****
C      CALCULATE RELATIVE HYDRAULIC CONDUCTIVITY AS A FUNCTION OF
C      PRESSURE USING VAN GENUTCHEN FUNCTION
C      *****
C      SPECIFICATIONS:
C      REAL PRESS,ALPHA,VGN,M
C      -----
C
    M=1-(1./VGN)
    PRESS=-PRESS
    TOP=(1-(ALPHA*PRESS)**(VGN-1)*(1+(ALPHA*PRESS)**VGN)**(-M))**2
    UNSKP=TOP/((1+(ALPHA*PRESS)**VGN)**(M/2))
    PRESS=-PRESS
C
    END
C
=====
C      FUNCTION UNSSP(PRESS,RSW,ALPHA,VGN)
C-----VERSION 29OCT2003 RBT
C      *****
C      CALCULATE SOIL WATER SATURATION AS A FUNCTION OF PRESSURE HEAD
C      USING VAN GENUTCHEN FUNCTION
C
C      NOTE: PRESSURE MUST BE POSITIVE FOR
C      VAN GENUTCHEN RELATIONSHIP
C      *****
C      SPECIFICATIONS:
C      REAL PRESS,RSW,ALPHA,VGN,M
C      -----
C
    M=1-(1./VGN)
    PRESS=-PRESS
    UNSSP=RSW+(1.-RSW)/((1+(ALPHA*PRESS)**VGN)**M)
    PRESS=-PRESS
    END
C
=====
C      FUNCTION UNSCP(PRESS,RSW,SC2,ALPHA,VGN)
C-----VERSION 29OCT2003 RBT
C      *****
C      CALCULATE SPECIFIC SOIL WATER CAPACITY (DERIVATIVE OF SOIL WATER
C      CONTENTS WITH RESPECT TO PRESSURE) USING VAN GENUTCHEN FUNCTION
C      *****
C      SPECIFICATIONS
C      REAL SW,RSW,SC2,ALPHA,VGN,M,EFSAT,BUFF
C      -----
C
    M=1-(1./VGN)
    PRESS=-PRESS
    EFSAT=(1./(1+(PRESS*ALPHA)**VGN))**M
    BUFF=(1./(1.-M))*ALPHA*M*(SC2-RSW)*(EFSAT**(1/M))
    UNSCP=BUFF*((1.-EFSAT**(1/M))**M)
    PRESS=-PRESS
C
    END

```

F.2 FORTRAN Source Code: Overland Flow (OLF) package

The following is the source code developed to simulate overland flow using the laminar form of the kinematic wave approximation (**equation 2.18**) with MODFLOW 2000 version 1.6 (*Harbaugh et al.*, 2000).

```

C   Last change: RBT 30OCTOBER2003 4:30 PM
C=====
      SUBROUTINE GWF1OLFRP(NCOL,NROW,NLAY,CV,BOTM,NBOTM,CVS)

C
C-----VERSION 30OCTOBER2003
C *****
C   ADJUST VERTICAL LEAKANCE FOR OVERLAND FLOW CELLS (ZERO SOIL THICKNESS)
C *****
C
C   SPECIFICATIONS:
C   -----
C
      REAL ADJUST,THCK1,THCK2
      DIMENSION      BOTM(NCOL,NROW,0:NBOTM),CV(NCOL,NROW,NLAY),
&                  CVS(NCOL,NROW,NLAY)
C
      COMMON /DISCOM/LBOTM(200),LAYCBD(200)
C   -----

C1-- CALCULATE ADJUSTMENT FACTOR
C1-- (INTERCELL THICKNESS / HALF CELL THICKNESS LAYER 2)
C1-- AND MULTIPLY LEAKANCE
C1-- **ASSUMES VERTICAL CONDUCTIVITY EQUAL FOR BOTH LAYERS**
C
      DO 10 I=1,NROW
      DO 10 J=1,NCOL
          THCK1=BOTM(NCOL,NROW,LBOTM(1)-1)-BOTM(NCOL,NROW,LBOTM(1))
          THCK2=BOTM(NCOL,NROW,LBOTM(1))-BOTM(NCOL,NROW,LBOTM(2))
          ADJUST=((THCK1+THCK2)/2.)/(THCK2/2.)
          CV(J,I,1)=CV(J,I,1)*ADJUST
          CVS(J,I,1)=CV(J,I,1)
10      CONTINUE

C2-- RETURN
      RETURN
      END
C
C=====
      SUBROUTINE GWF1OLF1AD(HNEW,IRCH,RECH,CV,NCOL,NROW,NLAY,BOTM,NBOTM)

C
C-----VERSION 30OCTOBER2003
C *****
C   ADJUST RECHARGE BOUNDARY CONDITION BASED ON
C   VERTICAL CONDUCTANCE IN LAYER 2
C *****
C
C   SPECIFICATIONS:
C   -----
C
      DOUBLE PRECISION HNEW
C
      DIMENSION      HNEW(NCOL,NROW,NLAY),CV(NCOL,NROW,NLAY),

```



```

1          IRCH(NCOL,NROW),RECH(NCOL,NROW),
2          BOTM(NCOL,NROW,0:NBOTM)
C          REAL          RRATE,VCOND,THCK,THCK1,THCK2
C          COMMON /DISCOM/LBOTM(200),LAYCBD(200)
C          PARAMETER (ONE=1.0)
C          PARAMETER (ZERO=0.0)
C          -----
C
C1-- USE VERTICAL CONDUCTANCE TO PARTITION RECHARGE
      DO 50 I=1,NROW
      DO 50 J=1,NCOL
      RRATE=RECH(J,I)
      THCK1=(BOTM(J,I,LBOTM(1))-BOTM(J,I,LBOTM(2)))/2.
      THCK2=(BOTM(J,I,LBOTM(2))-BOTM(J,I,LBOTM(3)))/2.
      THCK=THCK1+THCK2
      VCOND=CV(J,I,2)*THCK
C
C3-- IF RECHARGE RATE LESS THAN VERTICAL CONDUCTANCE, APPLY IN SOIL LAYER (2)
      IF (RRATE.LT.VCOND) THEN
        IRCH(J,I) = 2
C
C4-- ELSE APPLY IN TOP LAYER (EXFILTRATING OR SMALL CONDUCTANCE TERM)
        ELSE
          IRCH(J,I) = 1
        ENDIF
50      CONTINUE
C
C5-- RETURN
      RETURN
      END

C
C=====
C          SUBROUTINE GWF1OLFFM(NCOL,NROW,NLAY,HNEW,BOTM,NBOTM,HY,IOLF,CV,
1          CR,CC,DELC,DELR,CVS)

C
C-----VERSION 30OCTOBER2003
C          *****
C          CALCULATE INTERCELL RELATIVE PERMEABILITY FOR OVERLAND FLOW CELLS
C          IN TOP LAYER
C          *****
C
C          SPECIFICATIONS:
C          -----
C
C          DOUBLE PRECISION HNEW
C
C          REAL MINFLW, COEF, MINDPH,FLWDPH,T1,T2,HD1,HD2,THCK,GRAD,RESIST
C
C          DIMENSION      HNEW(NCOL,NROW,NLAY),IBOUND(NCOL,NROW,NLAY),
1          HY(NCOL,NROW,NLAY),BOTM(NCOL,NROW,0:NBOTM),
2          CR(NCOL,NROW,NLAY),CC(NCOL,NROW,NLAY),
3          CV(NCOL,NROW,NLAY),DELC(NROW),
4          DELR(NCOL),CVS(NCOL,NROW,NLAY),
C
C          COMMON /DISCOM/LBOTM(200),LAYCBD(200)
C
C          PARAMETER (ONE=1.0)
C          PARAMETER (ZERO=0.0)
C          -----
C
C1-- SET MINIMUM FLOW DEPTH AND COEFFICIENT VALUE BASED ON UNITS (OLF)
C

```

```

IF (IOLF.EQ.1) THEN
    MINFLW = 3.28E-5
    COEF = 5980.2
ELSEIF (IOLF.EQ.2) THEN
    MINFLW = 0.005
    COEF = 56505600
ELSEIF (IOLF.EQ.3) THEN
    MINFLW=0.01
    COEF = 800000.
ELSE
    WRITE (*,*)'INPUT ERROR FOR OVERLAND FLOW PACKAGE UNITS FLAG'
    STOP
ENDIF

C
C2--- IF HEAD BELOW MINIMUM FLOW DEPTH, SET HORIZONTAL CONDUCTANCES = 0
C
    DO 10 I=1,NROW
    DO 10 J=1,NCOL
        HD=HNEW(J,I,1)
        MINDPTH=BOTM(J,I,LBOTM(1))+MINFLW

        IF (HD.LT.MINDPTH) THEN
            CC(J,I,1)=ZERO
        ELSE

C
C3--- IF FLOWDEPTH IS EXCEEDED, COMPUTE OVERLAND FLOW CONDUCTANCES
C3--- NOTE: THE HY ARRAY MUST CONTAIN RESISTANCE FACTOR FOR TOP LAYER
C
            FLWDPH=HD-BOTM(J,I,LBOTM(1))
            CC(J,I,1)=FLWDPH*COEF*(FLWDPH**2.)/HY(J,I,1)

C
            ENDIF
10    CONTINUE
C
C4--- COMPUTE INTERCELL TRANSMISSIVITIES USING ARITHMETIC AVERAGE
C
    DO 40 I=1,NROW
    DO 40 J=1,NCOL
C5-----FOR EACH CELL CALCULATE BRANCH CONDUCTANCES FROM THAT CELL
C5-----TO THE ONE ON THE RIGHT AND THE ONE IN FRONT.
        T1=CC(J,I,1)
C
C6-----IF T=0 THEN SET CONDUCTANCE EQUAL TO 0. GO ON TO NEXT CELL.
        IF(T1.NE.ZERO) GO TO 20
        CR(J,I,1)=ZERO
        GO TO 40
C
C7-----IF THIS IS NOT THE LAST COLUMN(RIGHTMOST) THEN CALCULATE
C7-----BRANCH CONDUCTANCE IN THE ROW DIRECTION (CR) TO THE RIGHT.
20    IF(J.EQ.NCOL) GO TO 30
        T2=CC(J+1,I,1)
        IF(T2.EQ.ZERO) THEN
            CR(J,I,1)=ZERO
        ELSE
C7A-----ARITHMETIC MEAN INTERBLOCK TRANSMISSIVITY
            CR(J,I,1)=DELC(I)*(T1+T2)/(DELR(J+1)+DELR(J))
C7A-----HARMONIC MEAN INTERBLOCK TRANSMISSIVITY
c        CR(J,I,1)=2*T2*T1*DELC(I)/(T1*DELR(J+1)+T2*DELR(J))
        END IF
C
C8-----IF THIS IS NOT THE LAST ROW(FRONTMOST) THEN CALCULATE
C8-----BRANCH CONDUCTANCE IN THE COLUMN DIRECTION (CC) TO THE FRONT.
30    IF(I.EQ.NROW) GO TO 40
        T2=CC(J,I+1,1)
        IF(T2.EQ.ZERO) THEN
            CC(J,I,1)=ZERO

```

```

                                ELSE
                                CC(J,I,1)=DEL R(J)*(T1+T2)/(DEL C(I+1)+DEL C(I))
c                                CC(J,I,1)=2*T2*T1*DEL R(J)/(T1*DEL C(I+1)+T2*DEL C(I))
                                END IF
C
C 40 CONTINUE
C
c
C10-- RETURN
      RETURN
      END
```

F.3 FORTRAN source code: Adaptive time stepping scheme

The following is the source code developed for an adaptive time stepping scheme within MODFLOW 2000 version 1.8 (*Harbaugh et al.*, 2000).

```

C   Last change: RBT  6JUNE2003  2:30 PM
C=====
      SUBROUTINE ATSI1AL(ISUM,LCTIM,MXSTP,ITIM,FNAME,IFREFM,IATS,IOUT)
C-----VERSION 10DEC2002 RBT
C   *****
C   READ OUTPUT FLAG AND OPEN TIME STEP INFO FILE
C   ALLOCATE ARRAY STORAGE FOR ADAPTIVE TIME STEPPING MODULE
C   *****
C
C   SPECIFICATIONS:
C   -----
      CHARACTER*200 LINE
      CHARACTER*200 OFILE,FNAME
      CHARACTER*80 HEADNG(2)
      INTEGER ZERO,LCTIM,MXSTP,IFREFM,IRK,IOUT,IATS,ITIM
      PARAMETER (ZERO=0)
      DATA EXT /'.tim'/
C   -----
500 FORMAT(1X,/
&1X,'ATS1 -- ADAPTIVE TIME STEPPING PACKAGE, VERSION 1,',
& ' 9/20/2002',/,9X,'INPUT READ FROM UNIT',I3)
570 FORMAT(1X,'TIME STEP INFORMATION WILL BE SAVED ON UNIT'
&,I3)
585 FORMAT(1X,I10,' ELEMENTS IN X ARRAY ARE USED BY ATS')
590 FORMAT(1X,'TIME STEP INFORMATION WILL NOT BE SAVED')
C
C1-----IDENTIFY PACKAGE.
      WRITE(IOUT,500)IATS
C
C2-----READ UNIT / FLAG FOR OUTPUT FILE AND TIME STEP ARRAY DIMENSION (MXSTP)
      ITIM=0
      IF (IFREFM.EQ.ZERO) THEN
        READ(IATS,'(I10)') ITIM
        READ(IATS,'(I10)') MXSTP
      ELSE
        READ (IATS,*)ITIM
        READ (IATS,*)MXSTP
      ENDIF
C
C3-- IF TIME FILE REQUESTED (ITIM>0) OPEN BINARY OUTPUT FILE
      IF (ITIM.GT.0) THEN
C3A-- PRINT OUTPUT FILE NUMBER
        WRITE (IOUT,570) ITIM
C
        OFILE=FNAME
        NUM=INDEX(OFILE,'')
        WRITE(OFILE(NUM-4:NUM),'(A4)')EXT
        OPEN (UNIT=ITIM,FILE=OFILE,FORM='BINARY',STATUS='UNKNOWN')
C
C4-----ALLOCATE SPACE FOR THE ARRAY TIM(IF REQUESTED)
        IRK=ISUM
        LCTIM=ISUM
        ISUM=ISUM+MXSTP
C
C5-----CALCULATE & PRINT AMOUNT OF SPACE USED BY ATS PACKAGE.

```

```

        IRK=ISUM-IRK
        WRITE(IOUT,585)IRK
    ELSE
        WRITE(IOUT,590)
        LCTIM=1
    ENDIF
C
C6-----RETURN.
    RETURN
    END
C
C=====
    SUBROUTINE ATS1RP(IATS,TMX,TMN,TSM,TSD)
C-----VERSION 29SEPT2002 RBT
C *****
C     READ PARAMETERS FOR ADAPTIVE TIME STEPPING PACKAGE
C *****
C
C     SPECIFICATIONS:
C -----
C     REAL TMX,TMN,TSMULT,TSDIV
C     INTEGER IATS,NUM
C -----
C
C-- READ MAX AND MIN TIMESTEPS
    READ (IATS,*)TMX
    READ (IATS,*)TMN
C
C-- READ TIME STEP MULTIPLIER AND REDUCER
    READ (IATS,*)TSM
    READ (IATS,*)TSD
C
C-- RETURN
    RETURN
    END SUBROUTINE
C=====
    SUBROUTINE ATS1RST(DELT,TMX,TMN,TSD,IRST,ICNVG,TIM,MXSTP,
    & KSTP,ITIM,HNEW,NROW,NCOL,NLAY,PERTIM,TOTIM)
C-----VERSION 6JUNE2003 RBT
C *****
C     NON-CONVERGENCE: ADJUST TIME STEP ACCORDINGLY
C *****
C
C     SPECIFICATIONS:
C -----
C     DOUBLE PRECISION HNEW
C     REAL TMX,TMN,TSD
C     INTEGER IRST,ICNVG,MXSTP,KSTP,ITIM
C     DIMENSION TIM(MXSTP),HNEW(NCOL,NROW,NLAY)
C -----
C     IRST=0
C
C1-- DID NOT CONVERGE, CHECK DELT AND REDUCE IF POSSIBLE
    IF (ICNVG.NE.1) THEN
        IF (DELT.LE.TMN) THEN
            WRITE(*,5)
            5 FORMAT ('Simulation aborted: ATS - Did not converge with minimum
            & time step')
            STOP
        ELSEIF (DELT.GT.TMN) THEN
            PERTIM=PERTIM-DELT
            TOTIM=TOTIM-DELT
            DELT=DELT/TSD
            IF(DELT.LT.TMN)DELT=TMN
        ENDIF
C2-- ADJUST TO MINIMIZE ROUND-OFF ERRORS

```

```

10          DT=FLOAT(IFIX(1.E5*DELT))
          DELT=DT/1.E5
C3-- RESET PERIOD AND TOTAL SIMULATION TIME COUNTERS
          PERTIM=PERTIM+DELT
          TOTIM=TOTIM+DELT

c
C4-- SET RESTART FLAG
          IRST=1
          ELSE
C5-- CONVERGED? STORE DELT VALUE IN TIME OUTPUT ARRAY (IF ACTIVATED)
          IF(ITIM.GT.0) TIM(KSTP)=DELT
          ENDIF
C
C6-- RETURN
          RETURN
          END

C=====
C      SUBROUTINE ATSIAD(DELT,TMX,TMN,TSM,TSD,KKITER,MXITER,PERTIM,
C      &                  PERLEN,ENDPER,KPER,KSTP,TIM,MXSTP,ITIM,RST)

C-----VERSION 6JUNE2002 RBT
C      *****
C      ADJUST TIME STEP BASED ON CURRENT TIME STEP'S ITERATION RATIO
C      *****
C
C      SPECIFICATIONS:
C      -----
C      REAL TMX,TMN,TSM,TSD,MINCV,MAXCV,RATIO,KI,MI,PL,TIM,DT
C      INTEGER KKITER,MXITER,ENDPER,NUMSTP,KSTP,ITIM,MXSTP,FLG,RST
C      DIMENSION TIM(MXSTP)
C      -----
C
C      ONE=1.0
C      ENDPER=0
C      FLG=0
C      RST=0
C      KI=KKITER
C      MI=MXITER
C      MINCV=0.35
C      MAXCV=0.65
C      RATIO=KI/MI
C
C
C1-- IF CONVERGENCE IS WITHIN 35% OF MAXIMUM NUMBER OF ITERATIONS,
C1-- INCREASE BY TSMULT
          IF (RATIO.LT.MINCV) THEN
              DELT=DELT*TSM
C2-- IF CONVERGENCE IS ABOVE 65% OF MAXIMUM, REDUCE BY TSDIV
          ELSEIF (RATIO.GT.MAXCV) THEN
              DELT=DELT/TSD
          ENDIF
C3-- MAKE SURE TMN<DELT<TMX
10      IF(DELT.GT.TMX)DELT=TMX
          IF(DELT.LT.TMN)DELT=TMN
C4-- ADJUST TO MINIMIZE ROUND-OFF ERRORS
          DT=FLOAT(IFIX(1.E5*DELT))
          DELT=DT/1.E5
C5-- IF PERIOD LENGTH IS EXCEEDED, ADJUST DELT
          PL=DELT+PERTIM
          IF (PL.GT.PERLEN) THEN
              DELT=PERLEN-PERTIM
          ENDIF
C6-- IF DELT IS LAST STEP IN CURRENT STRESS PERIOD SET FLAG AND RETURN
          IF (PERTIM.GE.PERLEN) THEN
              ENDPER=1
              NUMSTP=KSTP

```

```
C6-- IF OUTPUT ACTIVATED, WRITE TIME INFORMATION FOR CURRENT STRESS PERIOD TO OUTPUT FILE
      IF (ITIM.GT.0) THEN
            WRITE (ITIM)KPER,PERLEN,NUMSTP
            WRITE (ITIM)(TIM(I),I=1,NUMSTP)
C6-- RE-INITIALIZE TIME STEP ARRAY
            TIM=0.
      ENDIF
ENDIF
C
C-- RETURN
100  RETURN
      END
```

F.4 Implementation in MODFLOW

F.4.1 Installation instructions

F.4.1.1 Unsaturated flow (UNS) package

This section lists the changes and additional subroutine call statements that are needed for using the unsaturated flow package presented in this work. The sections of code are formatted for cutting and pasting directly into the MODFLOW (**MODFLOW 2000 Version 1.6, compiled October 21, 2001**) files. It is suggested that the user first marks the locations of the changes in the code (listed here by line number) and then inserts the modifications at those marked locations.

Modifications to Main Code (mf2k.f):

1. Insert 'UNS' label as element 50 in the option array, CUNIT.

<LINE 96>¹

```
DATA CUNIT/BCF6,'WEL','DRN','RIV','EVT',' ','GHB',
& 'RCH','SIP','DE4','SOR','OC','PCG','LMG',
& 'GWT','FHB','RES','STR','IBS','CHD','HFB6',
& 'LAK','LPF','DIS','SEN','PES','OBS','HOB',
& 'ADV2','COB','ZONE','MULT','DROB','RVOB','GBOB',
& 'STOB','HUF','CHOB','ETS','DRT','DTOB',' ','',
& 'HYD',' ','SFOB','GAGE',' ',' ','LMT6',
& 'UNS',50* ' ' /
```

2. Insert call statement for UNS allocation subroutine and dummy variables.

<LINE 627>

```
IF (IUNIT(50).GT.0) THEN
  CALL GWF1UNSIAL(ISUMRX,LCRSW,LCCVS,
& LCUNSOC,NCOL,NROW,NLAY,IUNIT(50),IOUT,
& IUNSCB,IUNSOC,LCALPHA,LCVGN,IFREFM)
ELSEIF (IUNIT(50).LE.0) THEN
  LCRSW=LENRX+1
  LCALPHA=LENRX+2
  LCVGN=LENRX+3
  IUNSCB=0
  IOLF=0
ENDIF
```

3. Insert UNS activation flag (IUNIT(50))into BCF read and prepare subroutine:

<LINE 652>

```
1 CALL GWF1BCF6RP(IG(LCIBOU),GZ(LCHNEW),RX(LCSC1),RX(LCHY),
2   GX(LCCR),GX(LCCC),GX(LCCV),GX(LCDELR),
3   GX(LCDELC),RX(LCSC2),RX(LCTRPY),IUNIT(1),
4   ISS,NCOL,NROW,NLAY,IOUT,RX(LCWETD),IWDFLG,
5   RX(LCCVWD),IUNIT(50))
```

4. Insert call statement for UNS read and prepare subroutine.

¹ Note that line numbers refer to original mf2k.f file positions before UNS modifications are made.

<LINE 739>

```

IF (IUNIT(50).GT.0)
& CALL GWF1UNSRP(IUNIT(50),IOUT,GZ(LCHNEW),GX(LCCV),
& GX(LCBOTM),NBOTM,RX(LCALPHA),
& RX(LCVGN),RX(LCRSW),RX(LCSC2),RX(LCUNSOC),
& RX(LCCVS),NCOL,NROW,NLAY,IUNSCB,
& IUNSOC,ISWCFM,IFREFM,FNAME,IAVG,IOLF)

```

5. Insert UNS variables into BCF formulate subroutine.

<LINE 900>

```
&          CALL GWF1BCF6FM(GX(LCHCOF),GX(LCRHS),GX(LCHOLD),
&          RX(LCSC1),GZ(LCHNEW),IG(LCIBOU),
&          GX(LCCR),GX(LCCC),GX(LCCV),RX(LCHY),
&          RX(LCTRPY),GX(LCBOTM),NBOTM,RX(LCSC2),
&          GX(LCDELRL),GX(LCDELCL),DELT,
&          ISSFLG(KKPER),KKITER,KKSTP,KKPER,NCOL,
&          NROW,NLAY,IOUT,RX(LCWETD),IWDFLG,
&          RX(LCCVWD),WETFCT,IWETIT,IHDWET,HDRY,
&          GX(LCBUFF),IUNIT(50),RX(LCRSW),
&          RX(LCALPHA),RX(LCVGN),IUNSCB,IOLF)
```

6. Insert call statement for UNS formulate subroutine.

<LINE 909>

```

&      IF (IUNIT(50).GT.0)
&      CALL GWF1UNSI FM(RX(LC ALPHA),RX(LCVGN),NCOL,NROW,NLAY,
&                      GZ(LCHNEW),GX(LCBOTM),N BOTM,RX(LCCVS),
&                      GX(LCCV),I AVG,IOLF,GX(LCCC),
&                      GX(LCCR))

```

7. Insert UNS variables into BCF budget subroutines.

<LINE 1138>

```

IF (IUNIT(1).GT.0) THEN
  CALL SGWF1BCF6S(VBNM,VBVL,MSUM,GZ(LCHNEW),IG(LCIBOU),
    &      GX(LCHOLD),RX(LCSC1),GX(LCBOTM),NBOTM,
    &      RX(LCSC2),DELT,ISSFLG(KKPER),NCOL,NROW,
    &      NLAY,KKSTP,KKPER,IBCFCB,ICBCFL,GX(LCBUFF),
    &      IOUT,PERTIM,TOTIM,IUNIT(50),RX(LCRSW),
    &      RX(LCALPHA),RX(LCVGN),
    &      GX(LCDELR),GX(LCDELC),IOLF)
  CALL SGWF1BCF6F(VBNM,VBVL,MSUM,GZ(LCHNEW),IG(LCIBOU),
    &      GX(LCCR),GX(LCCC),GX(LCCV),DELT,NCOL,NROW,
    &      NLAY,KKSTP,KKPER,IBCFCB,GX(LCBUFF),IOUT,
    &      ICBCFL,PERTIM,TOTIM,GX(LCBOTM),NBOTM,
    &      ICHFLG,IUNIT(50))
  IBDRET=0
  IC1=1
  IC2=NCOL
  IR1=1
  IR2=NROW
  IL1=1
  IL2=NLAY
  DO 36 IDIR = 1,3
    CALL SGWF1BCF6B(GZ(LCHNEW),IG(LCIBOU),GX(LCCR),GX(LCCC),
    &      GX(LCCV),NCOL,NROW,NLAY,KKSTP,KKPER,
    &      IBCFCB,GX(LCBUFF),IOUT,ICBCFL,DELT,
    &      PERTIM,TOTIM,IDIR,IBDRET,ICHFLG,IC1,IC2,
    &      IR1,IR2,IL1,IL2,GX(LCBOTM),NBOTM,
    &      IUNIT(50))
36  CONTINUE
  ENDIF

```

8. Insert UNS budget subroutine.

<LINE 1346>

```

IF (IUNIT(50).GT.0)
&   CALL GWF1UNSI BD(GZ(LCHNEW),RX(LCSC2),RX(LCRSW),GX(LCBOTM),
&                   NBOTM,RX(LCUNSOC),NCOL,NROW,NLAY.

```

```

&                                IUNSCB,IUNSOC,KSTP,KPER,RX(LCALPHA),
&                                RX(LCVGN),IOLF,GX(LCCV),GX(LCDELR),
&                                GX(LCDELC),PERTIM,NPER,TOTIM,MSUM,
&                                VBVL,VBNM,DELT,GX(LCHOLD),ICBCFL)

```

9. Close UNS cell-by-cell output file (if output was requested).

<LINE 2056>

```
IF (IUNIT(50).GT.0.AND.IUNSCB.GT.0) CLOSE(IUNSCB)
```

Modifications to Block-Centered Flow (BCF) Package (gwflbcf6.f):

1. Insert UNS activation flag (IUNS) into BCF read and prepare subroutine.

<LINE 184>²

```
SUBROUTINE GWF1BCF6RP(BOUND,HNEW,SC1,HY,CR,CC,CV,DELR,DELC,
1 SC2,TRPY,IN,ISS,NCOL,NROW,NLAY,IOUT,WETDRY,IWDFLG,CVWD,IUNS)
```

2. Insert UNS activation flag (IUNS) into BCF check and prepare utility subroutine.

<LINE 256>

```
CALL SGWF1BCF6N(HNEW,BOUND,SC1,SC2,CR,CC,CV,HY,TRPY,DELR,DELC,
1 ISS,NCOL,NROW,NLAY,IOUT,WETDRY,IWDFLG,CVWD,IUNS)
```

3. Insert UNS variables IUNS,RSW,ALPHA,VGN,IUNSCB,IOLF into BCF formulate subroutine.

<LINE 306>

```
SUBROUTINE GWF1BCF6FM(HCOF,RHS,HOLD,SC1,HNEW,BOUND,CR,CC,CV,HY,
1 TRPY,BOTM,NBOTM,SC2,DELR,DELC,DELT,ISS,KITER,
2 KSTP,KPER,NCOL,NROW,NLAY,IOUT,WETDRY,IWDFLG,CVWD,
3 WETFCT,IWETIT,IHDWET,HDRY,BUFF,IUNS,RSW,
4 ALPHA,VGN,IUNSCB,IOLF)
```

<LINE 327>

```
7 RSW(NCOL,NROW,NLAY),ALPHA(NCOL,NROW,NLAY),VGN(NCOL,NROW,NLAY)
```

C

REAL NODE

4. Insert UNS activation flag (IUNS) into BCF horizontal conductance calculation subroutine.

<LINE 346>

```
CALL SGWF1BCF6H(HNEW,BOUND,CR,CC,CV,HY,TRPY,DELR,DELC,BOTM,NBOTM,
1 KK,KB,KITER,KSTP,KPER,NCOL,NROW,NLAY,IOUT,WETDRY,IWDFLG,
2 CVWD,WETFCT,IWETIT,IHDWET,HDRY,BUFF,IUNS)
```

5. Formulate storage flow due to soil moisture changes and overland flow formulation.

<REPLACE LINES 355-364>

C2UNS-- UNSATURATED FORMULATION

DO 140 I=1,NROW

DO 140 J=1,NCOL

IF(BOUND(J,I,K).LE.0) GO TO 140

C

C3UNS--IF UNS PACKAGE IS ACTIVE, MODIFIED PICARD ITERATION TERM ADDED

IF (IUNS.GE.1) THEN

BBOT=BOTM(J,I,LBOTM(K))

TTOP=BOTM(J,I,LBOTM(K)-1)

THCK=TTOP-BBOT

HD=HNEW(J,I,K)

NODE=(TTOP+BBOT)/2

C

C4UNS-- IF OVERLAND FLOW ACTIVATED,

C4OLF-- STORAGE IN TOP LAYER = 1 UNIT DEPTH PER UNIT HEAD CHANGE

IF (IOLF.GT.0.AND.K.EQ.1.AND.HD.GT.BBOT)THEN

DSDT=0.

SSTO=DELR(J)*DELC(I)*TLED

SPSC=0.

GOTO 777

ELSEIF(IOLF.GT.0.AND.K.EQ.1.AND.HD.LE.BBOT)THEN

DSDT=0.

SSTO=0.

² Note that line numbers refer to original gwflbcf6.f file positions before UNS modifications are made.

```

                SPSC=0.
                GOTO 777
            ENDIF
C4UNS1--CALCULATE SOIL SATURATION FROM PREVIOUS ITERATION (SWNEW)
    PRESS=HD-NODE
    IF (HD.GE.NODE) THEN
        SWNEW=ONE
    ELSE
        SWNEW=UNSSP(PRESS,RSW(J,I,K),ALPHA(J,I,K),VGN(J,I,K))
    ENDIF
C4UNS2--SET SW = SOIL SATURATION FROM PREVIOUS TIME STEP
    HD=HOLD(J,I,K)
    PRESS=HD-NODE
    IF (HD.GE.NODE) THEN
        SWOLD=ONE
    ELSE
        SWOLD=UNSSP(PRESS,RSW(J,I,K),ALPHA(J,I,K),VGN(J,I,K))
    ENDIF
C
C4UNS3-- CALCULATE SW TIME DERIVATIVE TERM FOR MODIFIED PICARD ITERATION
    P=SC2(J,I,K)
    DSDT=P*(SWNEW-SWOLD)*TLED*DEL R(J)*DEL C(I)*THCK
C
C4UNS4-- CALCULATE SOIL WATER CAPACITY AND SPECIFIC STORAGE FOR RHS
C4UNS4-- USING THE HEAD VALUE FROM THE CURRENT ITERATION
    HD=HNEW(J,I,K)
    PRESS=HD-NODE
    IF (HD.GE.NODE) THEN
        SPSC=0.0
        SSTO=SC1(J,I,K)*TLED
    ELSE
        RSWC=RSW(J,I,K)*P
        SPSC=UNSCP(PRESS,RSWC,P,ALPHA(J,I,K),VGN(J,I,K))
        SPSC=SPSC*DEL R(J)*DEL C(I)*THCK*TLED
C
C4UNS4A-- ADJUST SPECIFIC STORAGE TERM WITH AVERAGE SOIL SATURATION
    SWAVG=(SWNEW+SWOLD)/2.
    SSTO=TLED*SC1(J,I,K)*SWAVG
    ENDIF
C
C4UNS5-- ADD DERIVATIVE TERM TO RHS; USE HEAD FROM PREVIOUS ITERATION
777    RHO=SPSC+SSTO
        HCOF(J,I,K)=HCOF(J,I,K)-RHO
        RHS(J,I,K)=RHS(J,I,K)+DSDT-SPSC*HNEW(J,I,K)-SSTO*HOLD(J,I,K)
C
C4UNS6-- USE ORIGINAL FORMULATION IF UNS PACKAGE IS NOT ACTIVATED
    ELSE
C4UNS7-----SEE IF THIS LAYER IS CONVERTIBLE OR NON-CONVERTIBLE.
        IF(LAYCON(K).EQ.3 .OR. LAYCON(K).EQ.2) GO TO 150
        RHO=SC1(J,I,K)*TLED
        HCOF(J,I,K)=HCOF(J,I,K)-RHO
        RHS(J,I,K)=RHS(J,I,K)-RHO*HOLD(J,I,K)
    ENDIF
C4UNS8-- END UNS CHANGES

```

6. Insert IUNS flag into leakance corrections.

<LINE 403>

IF(LAYCON(K).NE.3 .AND. LAYCON(K).NE.2.OR.IUNS.GE.ONE) GO TO 250

<LINE 425>

IF(LAYCON(K+1).NE.3 .AND. LAYCON(K+1).NE.2.OR.IUNS.GE.ONE)
&GO TO 300

7. Insert IUNS flag into inter-cell flow budget subroutine.

<LINE 494>

SUBROUTINE SGWF1BCF6B(HNEW,IBOUND,CR,CC,CV,NCOL,NROW,NLAY,KSTP,
1 KPER,IBCFCB,BUFF,IOUT,ICBCFL,DELT,PERTIM,TOTIM,

```
2 IDIR,IBDRET,ICHFLG,IC1,IC2,IR1,IR2,IL1,IL2,BOTM,NBOTM,IUNS)
```

<LINE 657>

```
IF(LAYCON(K+1).NE.3 .AND. LAYCON(K+1).NE.2.OR.IUNS.GT.0) GO TO 580
```

8. Insert UNS variables IUNS,RSW,ALPHA,VGN,DELR,DELC,IOLF into BCF storage budget subroutine.

<LINE 673>

```
SUBROUTINE SGWF1BCF6S(VBNM,VBVL,MSUM,HNEW,IBOUND,HOLD,SC1,
1 BOTM,NBOTM,SC2,DELT,ISS,NCOL,NROW,NLAY,KSTP,KPER,IBCFCB,
2 ICBCFL,BUFF,IOUT,PERTIM,TOTIM,IUNS,RSW,ALPHA,VGN,
3 DELR,DELC,IOLF)
```

<LINE 689>

```
4 ,RSW(NCOL,NROW,NLAY),DELR(NCOL),DELC(NROW),
5 ALPHA(NCOL,NROW,NLAY),VGN(NCOL,NROW,NLAY)
```

```
REAL NODE
```

9. Insert IUNS flag into layer check.

<LINE 730>

```
IF(LC.NE.3 .AND. LC.NE.2.OR.IUNS.GT.0) GO TO 285
```

10. Insert unsaturated storage calculations.

<REPLACE LINES 744-745>

```
285 IF (IUNS.GT.0) THEN
C
C7B-OLF- STORAGE IN TOP LAYER = 1 FOR OVERLAND FLOW PACKAGE
IF (IOLF.GT.ZERO.AND.K.EQ.1.AND.HSING.GT.BOTM(J,I,1))THEN
    RHO=TLED*DELC(I)*DELR(J)
c    RHO=TLED
    STRG=RHO*(HOLD(J,I,K)-HSING)
    GOTO 288
ELSEIF(IOLF.GT.ZERO.AND.K.EQ.1.AND.HSING.LE.BOTM(J,I,1))THEN
    STRG=0.
    GOTO 288
ENDIF
C
C7B-UNS1--- SOIL WATER CAPACITY AND ADJUSTED SPECIFIC STORAGE TERMS
C7B-UNS1--- USED FOR UNSATURATED LAYERS
    BBOT=BOTM(J,I,1)
    TTOP=BOTM(J,I,1)-1
    THCK=TTOP-BBOT
    NODE=(TTOP+BBOT)/2
    P=SC2(J,I,K)
C
C7B-UNS2--CALCULATE SOIL SATURATION FROM CURRENT HEAD(SWNEW)
    HN=HNEW(J,I,K)
    PRESS=HN-NODE
    IF (HN.GE.NODE) THEN
        SWNEW=1.0
    ELSE
        SWNEW=UNSSP(PRESS,RSW(J,I,K),ALPHA(J,I,K),VGN(J,I,K))
    ENDIF
C
C7B-UNS3--SET SWOLD = SOIL SATURATION FROM PREVIOUS TIME STEP
    HO=HOLD(J,I,K)
    PRESS=HO-NODE
    IF (HO.GE.NODE) THEN
        SWOLD=1.0
    ELSE
        SWOLD=UNSSP(PRESS,RSW(J,I,K),ALPHA(J,I,K),VGN(J,I,K))
    ENDIF
C
C7B-UNS4-- CALCULATE SPECIFIC STORAGE FOR PREVIOUS TIME STEP
    IF (HO.GE.NODE) THEN
        OLDRHO=SC1(J,I,K)*TLED
    ELSE
```

```

                                OLDRHO=TLED*SC1(J,I,K)*SWOLD
                                ENDIF
C
C7B-UNS5-- CALCULATE SPECIFIC STORAGE FOR CURRENT TIME STEP
                                IF (HN.GE.NODE) THEN
                                    NEWRHO=SC1(J,I,K)*TLED
                                ELSE
                                    NEWRHO=TLED*SC1(J,I,K)*SWNEW
                                ENDIF
C
C7B-UNS6-- CALCULATE CHANGE IN SOIL SATURATION
C                                DSDT=P*DELR(J)*DELC(I)*THCK*TLED*(SWNEW-SWOLD)
C
C7B-UNS7-- STORAGE FLOW = OLD STORAGE MINUS NEW STORAGE
                                STRG=(HOLD(J,I,K)-HSING)*(OLDRHO+NEWRHO)/2
                                ELSE
                                    RHO=SC1(J,I,K)*TLED
                                    STRG=RHO*HOLD(J,I,K) - RHO*HSING
                                ENDIF

```

11. Insert IUNS flag into constant head budget subroutine.

```

<LINE 778>
SUBROUTINE SGWF1BCF6F(VBNM,VBVL,MSUM,HNEW,IBOUND,CR,CC,CV,DELT,
1                                NCOL,NROW,NLAY,KSTP,KPER,IBCF6B,BUFF,IOUT,ICBCFL,
2                                PERTIM,TOTIM,BOTM,NBOTM,ICHFLG,IUNS)

<LINE 930>
                                IF(TMP.LT.BOTM(J,I,LBOTM(K)-1).AND.IUNS.LE.0)
                                    & HD=BOTM(J,I,LBOTM(K)-1)

<LINE 948>
                                IF(TMP.LT.BOTM(J,I,LBOTM(K+1)-1).AND.IUNS.LE.0)
                                    & HD=BOTM(J,I,LBOTM(K+1)-1)

```

12. Insert IUNS flag into conductance computation. subroutine.

```

<LINE 996>
SUBROUTINE SGWF1BCF6H(HNEW,IBOUND,CR,CC,CV,HY,TRPY,DELR,DELC
1                                ,BOTM,NBOTM,K,KB,KITER,KSTP,KPER,NCOL,NROW,NLAY,IOUT
2                                ,WETDRY,IWDFLG,CVWD,WETFCT,IWETIT,IHDWET,HDRY,BUFF,IUNS)

<REPLACE LINE 1118>
                                IF(IUNS.GT.0) THEN
                                    THCK=TTOP-BBOT
                                ELSEIF (THCK.LE.ZERO.AND.IUNS.LT.1) THEN
                                    GO TO 100
                                ENDIF

```

13. Insert IUNS flag into initialization subroutine.

```

<LINE 1186>
SUBROUTINE SGWF1BCF6N(HNEW,IBOUND,SC1,SC2,CR,CC,CV,HY,TRPY,DELR,
1                                DELC,ISS,NCOL,NROW,NLAY,IOUT,WETDRY,IWDFLG,CVWD,IUNS)

<LINE 1327>
                                IF (IUNS.GT.0) CYCLE

```

F4.1.2 Overland Flow and Adaptive Time Stepping Packages

Modifications to Main Code (mf2k.f):

1. Insert ATS input file unit into label array CUNIT and define ATS variables.

<LINES 96-103>

```
DATA CUNIT/BCF6,'WEL','DRN','RIV','EVT',' ','GHB',
& 'RCH','SIP','DE4','SOR','OC','PCG','LMG',
& 'GWT','FHB','RES','STR','IBS','CHD','HFB6',
& 'LAK','LPF','DIS','SEN','PES','OBS','HOB',
& 'ADV2','COB','ZONE','MULT','DROB','RVOB','GBOB',
& 'STOB','HUF','CHOB','ETS','DRT','DTOB',' ',' ',
& 'HYD',' ','SFOB','GAGE',' ',' ','LMT6',
& 'UNS','ATS',49* ' ' /
```

<LINE 104>

```
INTEGER KSTP,MXSTP,RST,ENDPER
```

2. Insert ATS allocation subroutine.

<LINE 628>

```
IF (IUNIT(51).GT.0)
& CALL ATS1AL(ISUMRX,LCTIM,MXSTP,ITIM,FNAME,IFREFM,
& IUNIT(51),IOUT)
```

3. Insert OLF and ATS read and prepare subroutines.

<LINE 740>

```
IF (IOLF.GT.0)
& CALL GWF1OLFRP(NCOL,NROW,NLAY,GX(LCCV),GX(LCBOTM),NBOTM,
& RX(LCCVS))
IF (IUNIT(51).GT.0)
& CALL ATS1RP (IUNIT(51),TMX,TMN,TSM,TSD)
```

4. Insert ATS flag into BASIC timing information subroutine.

<LINE 743>

```
CALL GWF1BAS6ST(NSTP(KKPER),DELT,TSMULT(KKPER),PERTIM,KKPER,
& IOUT,PERLEN(KKPER),IUNIT(51))
```

5. Replace time step DO loop with a WHILE loop.

<REPLACE LINES 851-852>

```
IF(IUNIT(51).LE.0)MXSTP=NSTP(KKPER)
DO 91 WHILE (PERTIM,LT.PERLEN(KKPER).AND.KSTP,LT.MXSTP)
KSTP=KSTP+1
KKSTP = KSTP
```

6. Insert OLF adjustment subroutine and restart location.

<LINE 888>

```
IF(IOLF.GT.0.AND.IUNIT(8).GT.0)
& CALL GWF1OLF1AD(GZ(LCHNEW),
& IR(LCIRCH),RX(LCRECH),GX(LCCV),
& NCOL,NROW,NLAY,GX(LCBOTM),NBOTM)
```

7. Insert OLF formulate subroutine.

<LINE 910>

```
IF (IOLF.GT.0)
& CALL GWF1OLFFM(NCOL,NROW,NLAY,GZ(LCHNEW),GX(LCBOTM),
& NBOTM,RX(LCHY),IOLF,GX(LCCV),GX(LCCR),
& GX(LCCC),GX(LCDELC),GX(LCDELR),
& RX(LCCVS))
```

8. Insert ATS restart subroutine.

<LINE 1128>

```
IF (IUNIT(51).GT.0) THEN
CALL ATS1RST(DELT,TMX,TMN,TSD,IRST,ICNVG,RX(LCTIM),MXSTP,
```

```

&                                KSTP,ITIM,GZ(LCHNEW),NROW,NCOL,NLAY,PERTIM,TOTIM)
                                IF (IRST.EQ.1) GOTO 99
                                ENDIF
9. Insert ATS adjustment subroutine.
                                <REPLACE LINE 1853>
90                                IF (IUNIT(51).GT.0) THEN
                                CALL ATSIAD(DELT,TMX,TMN,TSM,TSD,KKITER,MXITER,PERTIM,
&                                PERLEN(KKPER),ENDPER,KPER,KSTP,RX(LCTIM),MXSTP,ITIM,RST)
C-ATS-- IF STRESS PERIOD ENDED AND TIMESTEP WAS ADJUSTED,
C-ATS-- RESTART ITERATION LOOP
                                IF (RST.GT.0) GOTO 99
C-ATS-- IF STRESS PERIOD ENDED, EXIT TIMESTEP LOOP
                                IF (ENDPER.GT.0) EXIT
                                ENDIF
C
C-ATS-TIME STEP LOOP CHANGED TO A WHILE LOOP
C 90 CONTINUE
91 END DO
                                <LINE 1855>
                                IF (KSTP.GT.MXSTP.AND.PERTIM.LT.PERLEN(KKPER))THEN
                                    WRITE (*,101)
                                    STOP
                                ENDIF
101 FORMAT(2X,'MAXIMUM TIME STEPS SPECIFIED BY ATS MODULE EXCEEDED.'
&/,2X,'SIMULATION ABORTED.')
```

Modifications to BASIC Package Code (gwflbas6.f):

1. Insert the ATS activation flag (IATS) into BASIC setup subroutine statement.

```

                                <LINE 179>
                                SUBROUTINE GWFLBAS6ST(NSTP,DELT,TSMULT,PERTIM,KPER,IOUT,PERLEN,
&                                IATS)
```

2. Announce ATS package if activated.

```

                                <REPLACE LINES 192-196>
                                IF (IATS.LT.ONE) THEN
                                    WRITE (IOUT,1) KPER,PERLEN,NSTP,TSMULT
                                ELSE
                                    WRITE (IOUT,5)KPER,PERLEN
                                ENDIF
1 FORMAT('1',/28X,'STRESS PERIOD NO.',I4,' LENGTH =',G15.7,/
1      28X,46('-'),//
2      30X,'NUMBER OF TIME STEPS =',I6,//
3      31X,'MULTIPLIER FOR DELT =',F10.3)
5 FORMAT('1',/28X,'STRESS PERIOD NO.',I4,' LENGTH =',G15.7,/
1      28X,46('-'),/30X,'ADAPTIVE TIME STEPPING',
2      ' PACKAGE IS ACTIVE')
```

3. Adjust TSMULT to 1 if ATS package is activated.

```

                                <REPLACE LINE 206>
                                IF(TSMULT.NE.ONE.AND.IATS.LT.ONE) THEN
                                    DELT=PERLEN*(ONE-TSMULT)/(ONE-TSMULT**NSTP)
                                ELSEIF (TSMULT.NE.ONE.AND.IATS.GE.ONE) THEN
                                    TSMULT = 1.0
                                ENDIF
```


F.4.2 Input instructions

Unsaturated Flow package

Input for the unsaturated flow (UNS) package is read from a file specified in the MODFLOW name file with “UNS” file type. Real arrays are read using the U2DREL array reader utility subroutine except for the output control array (UNSOC). UNSOC is read as a real two dimensional array containing the stress period in the first column and the time step in the second column. These parameters are free format if the word FREE is specified in item 4 of the Basic Package input file; otherwise, the parameters all have 10-character fields.

FOR EACH SIMULATION

1. IUNSCB
2. IUNSOC
3. IAVG
4. IOLF
5. UNSOC (IUNSOC, 2). Only read if IUNSOC is greater than zero.
6. ISWFL
7. VGFLG

If VGFLG is greater than zero, the soil characteristic parameters are read as two constants:

8. ALPHA VGN

Otherwise the parameters are read in as a real array for all cells;

8. ALPHA (NCOL, NROW, NLAY) -- U2DREL
9. VGN (NCOL, NROW, NLAY) -- U2DREL

10. SWC (NCOL, NROW, NLAY) -- U2DREL. Only read if ISWFL is greater than zero.

11. RSW (NCOL, NROW, NLAY) -- U2DREL.

Explanation of the parameters read by UNS package

IUNSCB – The flag containing the file unit for saving cell-by-cell soil saturations.

> 0, output will be saved to unit IUNSCB in a file specified as “SAT” type.
 ≤ 0, no output

IUNSOC – The flag for UNS cell-by-cell output control.

>0, output recorded at IUNSOC specified times
 <0, output recorded at all times

= -10, output recorded in binary interface file for RT3D transport simulations.

IAVG -- The flag specifying the intercell averaging of the relative permeability.
 = 1, Geometric mean
 = 2, Arithmetic mean
 = 3, Upstream weighted

IOLF – The flag for overland flow package (OLF) activation.
 > 0, OLF active; top model layer is not used by UNS package
 ≤ 0, OLF inactive

UNSOC – The output control array containing stress period and time step or specified simulation time.

ISWFL – The flag indicating if initial soil saturations are to be read to set the initial head distribution.
 < 0, initial heads read in the BAS file are used
 > 0, initial saturations read as an array for all model cells

VGFLG – The flag indicating if van Genuchten soil parameters are to be read in as an array or as a constant for all model cells.
 < 0, van Genuchten soil parameters constant for all model cells.
 > 0, van Genuchten soil parameters read in as an array for all model cells.

ALPHA (NCOL,NROW,NLAY) – The array containing van Genuchten soil parameter, α

VGN (NCOL,NROW,NLAY) – The array containing van Genuchten soil parameter, n

SW (NCOL,NROW,NLAY) – The array containing initial soil saturations.

RSW (NCOL,NROW,NLAY) – The array containing residual soil saturations.

Overland Flow (OLF) package

The Overland Flow package is activated through the IOLF flag in the unsaturated flow input file (UNS). If activated, the user should store the surface roughness parameter k_d in the hydraulic conductivity array for the top layer which is read by the Block Centered Flow package in the file specified with the BC6 file type.

Adaptive Time Stepping (ATS) package

Input for the adaptive time stepping (ATS) package is read from a file specified in the MODFLOW name file with “ATS” file type. The time units must be consistent with model units specified in discretization (DIS) file. Real arrays are read using the U2DREL array reader utility subroutine. These parameters are free format if the word FREE is specified in item 4 of the Basic Package input file; otherwise, the parameters all have 10-character fields.

FOR EACH SIMULATION

1. ITIM
2. MXSTP
3. TMX
4. TMN
5. TSM
6. TSD

Explanation of the parameters read by the ATS package

ITIM – The flag containing the file unit of binary output file that is used for interfacing with a transport code such as RT3D. If ITIM is greater than zero, a TIM file is created.

MXSTP – Maximum number of time steps (during a given stress period) expected for entire simulation. Used to allocate the time step array that is saved to the output (TIM) file.

TMX – Maximum allowable time step size.

TMN – Minimum allowable time step size.

TSM – Time step multiplication factor.

TSD – Time step reduction (division) factor.

F.5 RT3D Modifications

The following is the source code for the modifications of RT3D version 2.5 (Clement, 1997) to simulate vadose zone transport and gas-phase diffusion.

```

C   Last change: RBT 15 DEC 2002  2:15 PM
C=====
      SUBROUTINE UNS1AL(ISUM,INUNS,IOUT,LCSATP,LCSW,LCSLP,LCINT,
&                      NCOL,NROW,NLAY)
C-----VERSION 15DEC2002 RBT
C *****
C   ALLOCATE ARRAY STORAGE FOR SATURATED POROSITY ARRAY
C *****
C   SPECIFICATIONS:
C -----
      INTEGER ISUM,INUNS,IOUT,LCSATP,LCSW,NCOL,NROW,NLAY,IRK
C -----
10  FORMAT(1X,'UNS1 -- UNSATURATED TRANSPORT PACKAGE',
& ', VER 1.0, NOV 2002', ' INPUT READ FROM UNIT',I3)
20  FORMAT(1X,I10,'ELEMENTS OF THE X ARRAY USED BY THE UNS PACKAGE')
c
C1-----IDENTIFY PACKAGE.
      WRITE(IOUT,10)INUNS
C2-----ALLOCATE SPACE FOR THE ARRAYS SATP,SW,SLOPE AND INTER
      IRK=ISUM
      LCSATP=ISUM
      ISUM=ISUM+NCOL*NROW*NLAY
      LCSW=ISUM
      ISUM=ISUM+NCOL*NROW*NLAY
      LCSLP=ISUM
      ISUM=ISUM+NCOL*NROW*NLAY
      LCINT=ISUM
      ISUM=ISUM+NCOL*NROW*NLAY
C
C3-----CALCULATE & PRINT AMOUNT OF SPACE USED BY UNS PACKAGE.
      IRK=ISUM-IRK
      WRITE(IOUT,20)IRK
C
C4-----RETURN.
      RETURN
      END
C=====
      SUBROUTINE UNS1RP1(INUNS,SATP,SW,PRSITY,NCOL,NROW,NLAY)
C-----VERSION 19NOV2002 RBT
C *****
C   STORE SATURATED POROSITY IN SATP ARRAY; READ INITIAL SATURATIONS
C *****
C   SPECIFICATIONS:
C -----
      DIMENSION PRSITY(NCOL,NROW,NLAY),SATP(NCOL,NROW,NLAY),
&              SW(NCOL,NROW,NLAY)
      REAL      TTIME, PERTIM, TOTIM,SW
      INTEGER   KKSTP, KKPER, INUNS
      CHARACTER*8 TEXT
C -----
5  FORMAT(/,1X,'Soil saturation time step does not match for step ',
& I4,' period ',I4,' and elapsed time ',G10.5)
10 FORMAT(/,1X,'Soil saturation period does not match for step ',

```

```

&I4,' period ',I4,' and elapsed time ',G10.5)
15 FORMAT(/,1X,'Soil saturation time does not match for step',
&I4,' period ',I4,' and elapsed time ',G10.5)
C
C1-- STORE DRAINABLE POROSITY
      DO 20 I=1,NROW
      DO 20 J=1,NCOL
      DO 20 K=1,NLAY
          SATP(J,I,K)=PRSITY(J,I,K)
20 CONTINUE
C2--- READ IDENTIFICATION LINE FOR INITIAL SATURATIONS
      READ(INUNS)KKSTP,KKPER,TTIME
      IF (KKSTP.NE.0) THEN
          WRITE(*,5)KKSTP,KKPER,TTIME
          STOP
      ELSEIF (KKPER.NE.0) THEN
          WRITE(*,10)KKSTP,KKPER,TTIME
          STOP
      ENDIF
C3-- READ INITIAL SATURATIONS
      READ(INUNS)((SW(IC,IR,IL),IC=1,NCOL),IR=1,NROW),IL=1,NLAY)
C
      RETURN
      END
C=====
      SUBROUTINE UNS1RP2 (INUNS,SW,PRSITY,NCOL,NROW,NLAY,KSTP,KPER,
&                          SATP)
C-----VERSION 12DEC2002 RBT
C *****
C READ SATURATION ARRAY AND ADJUST WATER-FILLED POROSITY
C *****
C
C SPECIFICATIONS:
C -----
      REAL TTIME,SWNEW,SW,PRSITY
      INTEGER KKSTP,KKPER
      DIMENSION SW(NCOL,NROW,NLAY),SWNEW(NCOL,NROW,NLAY),
& PRSITY(NCOL,NROW,NLAY),SATP(NCOL,NROW,NLAY)
C -----
5 FORMAT(/,1X,'Soil saturation time step does not match for step ',
&I4,' period ',I4,' and elapsed time ',G10.5)
10 FORMAT(/,1X,'Soil saturation period does not match for step ',
&I4,' period ',I4,' and elapsed time ',G10.5)
15 FORMAT(/,1X,'Soil saturation time does not match for step',
&I4,' period ',I4,' and elapsed time ',G10.5)
C
C1--- READ IDENTIFICATION LINE
      READ (INUNS)KKSTP,KKPER,TTIME
      IF (KKSTP.NE.KSTP) THEN
          WRITE(*,5)KSTP,KPER,TTIME
          STOP
      ELSEIF (KKPER.NE.KPER) THEN
          WRITE(*,10)KSTP,KPER,TTIME
          STOP
      ENDIF
C2-- READ SATURATIONS
      READ(INUNS)((SWNEW(IC,IR,IL),IC=1,NCOL),IR=1,NROW),IL=1,NLAY)
C3-- ADJUST POROSITY ARRAY USING OLD SATURATIONS
      DO 20 I=1,NROW
      DO 20 J=1,NCOL
      DO 20 K=1,NLAY
          PRSITY(J,I,K) = SW(J,I,K)*SATP(J,I,K)
20 CONTINUE
C4-- SET OLD SATURATIONS = NEW SATURATIONS
      SW=SWNEW
C5-- RETURN

```

```

      RETURN
      END
C=====
      SUBROUTINE UNS1RP3 (INUNS,SW,PRSITY,NCOL,NROW,NLAY,KSTP,KPER,
&      HT1,HT2,SLOPE,INTER,SATP)
C-----VERSION 12DEC2002 RBT
C *****
C COMPUTE INTERPOLATION FACTORS FOR TRANSPORT TIME STEP
C *****
C
C SPECIFICATIONS:
C -----
      REAL SLOPE,INTER,SW,PRSITY,HT1,HT2,SAT2
      INTEGER KKSTP,KKPER
      DIMENSION SW(NCOL,NROW,NLAY),
&      SLOPE(NCOL,NROW,NLAY),INTER(NCOL,NROW,NLAY),
&      PRSITY(NCOL,NROW,NLAY),SATP(NCOL,NROW,NLAY)
C -----
C1-- USE OLD AND NEW SATURATIONS TO COMPUTE SLOPE AND INTERCEPT FOR EACH CELL
C1-- (SATURATIONS FOR PREVIOUS TIME STEP STORED IN PRSITY ARRAY)
      DO 20 I=1,NROW
      DO 20 J=1,NCOL
      DO 20 K=1,NLAY
          SWOLD = PRSITY(J,I,K)/SATP(J,I,K)
          SLOPE (J,I,K) = (SW(J,I,K)-SWOLD)/(HT2-HT1)
          INTER (J,I,K) = SWOLD - SLOPE(J,I,K)*HT1
      20 CONTINUE
C
C2-- RETURN
      RETURN
      END
C=====
      SUBROUTINE UNS1FM(SATP,PRSITY,SLOPE,INTER,NCOL,NROW,NLAY,
&      TIME2)
C-----VERSION 19NOV2002 RBT
C *****
C USE INTERPOLATION FACTORS TO ADJUST POROSITY FOR CURRENT TRANSPORT
C TIME STEP (TIME2)
C *****
C
C SPECIFICATIONS:
C -----
      REAL SAT,SATP,PRSITY,SLOPE,INTER,TIME2
      DIMENSION PRSITY(NCOL,NROW,NLAY),SATP(NCOL,NROW,NLAY),
&      SLOPE(NCOL,NROW,NLAY),INTER(NCOL,NROW,NLAY)
C -----
C
C1-- ADJUST POROSITY USING SATURATION VALUE AT END OF TRANSPORT STEP
      SAT=0.
      DO 20 I=1,NROW
      DO 20 J=1,NCOL
      DO 20 K=1,NLAY
          SAT = SLOPE(J,I,K)*TIME2 + INTER(J,I,K)
          PRSITY(J,I,K) = SAT*SATP(J,I,K)
      20 CONTINUE
C
C2-- RETURN
      RETURN
      END

```

```

C   Last change: RBT 25 NOV 2002 3:15 PM
C=====
      SUBROUTINE GPD1AL(ISUM,INGPD,IOUT,LCDCA,LCKPA,LCGCOMP,
      &NGCOMP,NCOL,NROW,NLAY)
C-----VERSION 25NOV2002 RBT
C   *****
C   ALLOCATE ARRAY FOR GAS/WATER PARTITIONING COEFFICIENTS
C   *****
C   SPECIFICATIONS:
C   -----
      INTEGER ISUM,INGPD,IOUT,LCDCA,LCKPA,NGCOMP,NCOMP,NCOL,NROW,NLAY,
      & IRK,LCGCOMP
C   -----
      10 FORMAT(1X,'GPD1 -- GAS PHASE DIFFUSION PACKAGE',
      & ', VER 1.0, NOV 2002', ' INPUT READ FROM UNIT',I3)
      20 FORMAT(1X,I10,'ELEMENTS OF THE X ARRAY USED BY THE GPD PACKAGE')
C1-----IDENTIFY PACKAGE.
      WRITE(IOUT,10)INGPD
C2-----READ NUMBER OF GAS PHASE COMPONENTS
      READ (INGPD,*)NGCOMP
C3-----ALLOCATE SPACE FOR THE COEFFICIENT ARRAYS
      IRK=ISUM
      LCDCA=ISUM
      ISUM=ISUM+NGCOMP
      LCKPA=ISUM
      ISUM=ISUM+NGCOMP
      LCGCOMP=ISUM
      ISUM=ISUM+NGCOMP
C4-----CALCULATE & PRINT AMOUNT OF SPACE USED BY GPD PACKAGE.
      IRK=ISUM-IRK
      WRITE(IOUT,20)IRK
C
C5-----RETURN.
      RETURN
      END
C=====
      SUBROUTINE GPD1RP(INGPD,OUTGPD,DCA,KPA,GCOMP,NGCOMP,NCOMP,IACT)
C-----VERSION 25NOV2002 RBT
C   *****
C   READ AND STORE GAS PHASE DIFFUSION PARAMETERS
C   *****
C   SPECIFICATIONS:
C   -----
      REAL          DCA,KPA
      INTEGER       NGCOMP,INGPD,OUTGPD,GCOMP,IC,NCOMP,IACT
      CHARACTER*15 FNAME
      DIMENSION     DCA(NGCOMP),KPA(NGCOMP),GCOMP(NGCOMP)
C   -----
C
C1--   CHECK NGCOMP
      IF (NGCOMP.GT.NCOMP) THEN
         WRITE(*,*)'GPD input error: number of gas components >
         &number of model components'
         STOP
      ELSEIF (NGCOMP.EQ.0) THEN
         WRITE(*,*)'GPD input error: number of gas components = 0'
         STOP
      ENDIF
C2-- READ OUTPUT FILE NAME AND NUMBER
      READ (INGPD,*)OUTGPD,FNAME
C2A-- OPEN OUTPUT FILE IF REQUESTED
      IF (OUTGPD.GT.0) THEN
         OPEN(UNIT=OUTGPD,FILE=FNAME,STATUS='UNKNOWN')
      ENDIF
C3-- READ ACTIVE PHASE FLAG
      READ (INGPD,*)IACT

```

```

C4-- READ GAS COMPONENT LOCATOR ARRAY
      READ (INGPD,*)(GCOMP(IC),IC=1,NGCOMP)
C5-- READ AIR DIFFUSION COEFFICIENT ARRAY
      READ (INGPD,*)(DCA(IC),IC=1,NGCOMP)
C6-- READ GAS/AQUEOUS PARTITIONING COEFFICIENT ARRAY
      READ (INGPD,*)(KPA(IC),IC=1,NGCOMP)
C7-- RETURN
      RETURN
      END

C=====
      SUBROUTINE GPD1CF(DCA,KPA,SATP,PRSITY,DXX,DXY,DZX,DYX,DYY,DYZ,DZX,
& DZY,DZZ,NCOL,NROW,NLAY,ICBUND,DELR,DELC,DZ,NGCOMP,NCOMP,
& DMCOEF,SW,KSTP,KPER)
C-----VERSION 25NOV2002 RBT
C *****
C   ADD EFFECTIVE GAS DIFFUSION TERMS TO MODEL ARRAYS
C   NOTE: EXPLICIT FORMULATION - DIFFUSION TERM CALCULATED USING
C   SATURATIONS FOR OLD FLOW TIME STEP
C *****
C   SPECIFICATIONS:
C   -----
      REAL          DCA,KPA,SATP,PRSITY,DXX,DXY,DZX,DYX,DYY,DYZ,DZX,
& DZY,DZZ,TORT,PAVG,PSAVG,P1,P2,DZ,DMG,DMA,DM,AREA,DMCOEF,SW
& SWNEW
      INTEGER       NCOL,NROW,NLAY,K,I,J,L,ICBUND,KM1,IM1,JM1,
&
      DIMENSION     DCA(NGCOMP),KPA(NGCOMP),PRSITY(NCOL,NROW,NLAY),
& DXX(NCOL,NROW,NLAY),DXY(NCOL,NROW,NLAY),DXZ(NCOL,NROW,NLAY),
& DYX(NCOL,NROW,NLAY),DYY(NCOL,NROW,NLAY),DYZ(NCOL,NROW,NLAY),
& DZX(NCOL,NROW,NLAY),DZY(NCOL,NROW,NLAY),DZZ(NCOL,NROW,NLAY),
& ICBUND(NCOL,NROW,NLAY),DELR(NCOL),DELC(NROW),SW(NCOL,NROW,NLAY),
& DZ(NCOL,NROW,NLAY),SATP(NCOL,NROW,NLAY),DMCOEF(NLAY),
& SWNEW(NCOL,NROW,NLAY)
C   -----
c
C1-- CALCULATE WATER SATURATION FOR CURRENT TRANSPORT TIME STEP USING EFFECTIVE POROSITY
      DO I=1,NROW
      DO J=1,NCOL
      DO K=1,NLAY
      WSAT=PRSITY(J,I,K)/SATP(J,I,K)
      ESAT=WSAT
      DO L=1,NGCOMP
      GSAT=KPA(L)*(1.-WSAT)
      ESAT=ESAT-GSAT
      ENDDO
      SWNEW(J,I,K)=ESAT
      ENDDO
      ENDDO
      ENDDO

C2-- ADD EFFECTIVE GAS PHASE DIFFUSION TERMS TO DISPERSION CONDUCTANCE ARRAYS
C2--FOR THE COMPONENTS ALONG THE X DIRECTION
C=====
      IF(NCOL.LT.2) GOTO 100
      DO L=1,NGCOMP
      DO K=1,NLAY
      KP1=MIN(K+1,NLAY)
      KM1=MAX(1,K-1)
      DO I=1,NROW
      IP1=MIN(I+1,NROW)
      IM1=MAX(1,I-1)
      DO J=1,NCOL
      JP1=MIN(J+1,NCOL)
      JM1=MAX(1,J-1)
      IF(ICBUND(J,I,K).EQ.0.OR.ICBUND(JP1,I,K).EQ.0) GOTO 80
C2A--CALCULATE VALUES AT INTERFACES

```



```

      WW=DEL R(JP1)/(DEL R(J)+DEL R(JP1))
C2B-- COMPUTE EFFECTIVE GAS PHASE DIFFUSION USING
C2B-- AIR TORTUOSITY
      P1=SATP(J,I,K)*(1.-SWNEW(J,I,K))
      P2=SATP(JP1,I,K)*(1.-SWNEW(JP1,I,K))
      PAVG=(P1*WW+P2*(1.-WW))
      PSAVG=(SATP(J,I,K)*WW+SATP(JP1,I,K)*(1.-WW))
      TORT=(PAVG**(7./3.))/(PSAVG**2.)
      DMG=KPA(L)*DCA(L)*PAVG*TORT
C2C-- COMPUTE EFFECTIVE AQUEOUS PHASE DIFFUSION USING
C2C-- WATER TORTUOSITY
      P1=SATP(J,I,K)*(SWNEW(J,I,K))
      P2=SATP(JP1,I,K)*(SWNEW(JP1,I,K))
      PAVG=(P1*WW+P2*(1.-WW))
      PSAVG=(SATP(J,I,K)*WW+SATP(JP1,I,K)*(1.-WW))
      TORT=(PAVG**(7./3.))/(PSAVG**2.)
      DMA=DMCOEF(K)*PAVG*TORT
C2D-- SUM DIFFUSION TERMS
      DM=DMG+DMA
C
C2E-- CONVERT TERMS INTO CONDUCTANCES AND ADD TO DXX CONDUCTANCE ARRAY
      AREA=DEL C(I)*(DZ(J,I,K)*WW+DZ(JP1,I,K)*(1.-WW))
      IF(NCOL.GT.1.AND.AREA.GT.0) THEN
        DXX(J,I,K)=DXX(J,I,K)+AREA*DM/(0.5*DEL R(JP1)+0.5*DEL R(J))
      ENDIF
80  ENDDO
    ENDDO
  ENDDO
    ENDDO
C3--FOR THE COMPONENTS ALONG THE Y DIRECTION
C =====
100 IF(NROW.LT.2) GOTO 200
    DO L=1,NGCOMP
      DO K=1,NLAY
        KP1=MIN(K+1,NLAY)
        KM1=MAX(1,K-1)
        DO J=1,NCOL
          JP1=MIN(J+1,NCOL)
          JM1=MAX(1,J-1)
          DO I=1,NROW
            IP1=MIN(I+1,NROW)
            IM1=MAX(1,I-1)
            IF(ICBUND(J,I,K).EQ.0.OR.ICBUND(J,IP1,K).EQ.0) GOTO 180
C3A--CALCULATE VALUES AT INTERFACES
            WW=DEL C(IP1)/(DEL C(I)+DEL C(IP1))
C3B-- COMPUTE EFFECTIVE GAS PHASE DIFFUSION USING
C3B-- AIR TORTUOSITY
            P1=SATP(J,I,K)*(1.-SWNEW(J,I,K))
            P2=SATP(J,IP1,K)*(1.-SWNEW(J,IP1,K))
            PAVG=(P1*WW+P2*(1.-WW))
            PSAVG=(SATP(J,I,K)*WW+SATP(J,IP1,K)*(1.-WW))
            TORT=(PAVG**(7./3.))/(PSAVG**2.)
            DMG=KPA(L)*DCA(L)*PAVG*TORT
C3C-- COMPUTE EFFECTIVE AQUEOUS PHASE DIFFUSION USING
C3C-- WATER TORTUOSITY
            P1=SATP(J,I,K)*(SWNEW(J,I,K))
            P2=SATP(J,IP1,K)*(SWNEW(J,IP1,K))
            PAVG=(P1*WW+P2*(1.-WW))
            PSAVG=(SATP(J,I,K)*WW+SATP(J,IP1,K)*(1.-WW))
            TORT=(PAVG**(7./3.))/(PSAVG**2.)
            DMA=DMCOEF(K)*PAVG*TORT
C3D-- SUM DIFFUSION TERMS
            DM=DMG+DMA
C3E-- CONVERT TERMS INTO CONDUCTANCES AND ADD TO DYY CONDUCTANCE ARRAY
            AREA=DEL R(J)*(DZ(J,I,K)*WW+DZ(J,IP1,K)*(1.-WW))
            IF(NROW.GT.1.AND.AREA.GT.0) THEN

```

```

        DYY(J,I,K)=DYY(J,I,K)+AREA*DM/(0.5*DELC(IP1)+0.5*DELC(I))
        ENDIF
180  ENDDO
    ENDDO
ENDDO
    ENDDO
C4--FOR THE COMPONENTS ALONG THE Z DIRECTION
C=====
200 IF(NLAY.LT.2) GOTO 300
    DO L=1,NGCOMP
        DO I=1,NROW
            IP1=MIN(I+1,NROW)
            IM1=MAX(I,I-1)
            DO J=1,NCOL
                JP1=MIN(J+1,NCOL)
                JM1=MAX(J,J-1)
                DO K=1,NLAY
                    KP1=MIN(K+1,NLAY)
                    KM1=MAX(K,K-1)
                    IF(ICBUND(J,I,K).EQ.0.OR.ICBUND(J,I,KP1).EQ.0) GOTO 280
C4A--CALCULATE VALUES AT INTERFACES
                    WW=DZ(J,I,KP1)/(DZ(J,I,K)+DZ(J,I,KP1))
C4B-- COMPUTE EFFECTIVE GAS PHASE DIFFUSION USING
C4B-- AIR TORTUOSITY
                    P1=SATP(J,I,K)*(1.-SWNEW(J,I,K))
                    P2=SATP(J,I,KP1)*(1.-SWNEW(J,I,KP1))
                    PAVG=(P1*WW+P2*(1.-WW))
                    PSAVG=SATP(J,I,K)*WW+SATP(J,I,KP1)*(1.-WW)
                    TORT=(PAVG**(7./3.))/(PSAVG**2.)
                    DMG=KPA(L)*DCA(L)*PAVG*TORT
C4C-- COMPUTE EFFECTIVE AQUEOUS PHASE DIFFUSION USING
C4C-- WATER TORTUOSITY
                    P1=SATP(J,I,K)*(SWNEW(J,I,K))
                    P2=SATP(J,I,KP1)*(SWNEW(J,I,KP1))
                    PAVG=(P1*WW+P2*(1.-WW))
                    PSAVG=(SATP(J,I,K)*WW+SATP(J,I,KP1)*(1.-WW))
                    TORT=(PAVG**(7./3.))/(PSAVG**2.)
                    DMA=DMCOEF(K)*PAVG*TORT
C4D-- SUM DIFFUSION TERMS
                    DM=DMG+DMA
C4E-- CONVERT TERMS INTO CONDUCTANCES AND ADD TO DXX CONDUCTANCE ARRAY
                    AREA=DELR(J)*DELC(I)
                    IF(NLAY.GT.1.AND.AREA.GT.0) THEN
                        DZZ(J,I,K)=DZZ(J,I,K)+AREA*DM/
&      (0.5*DZ(J,I,KP1)+0.5*DZ(J,I,K))
                    ENDIF
280  ENDDO
        ENDDO
    ENDDO
    ENDDO

300 CONTINUE
C
C5--RETURN
    RETURN
    END
C=====
SUBROUTINE GPD1FM(KPA,SATP,PRSITY,NCOL,NROW,NLAY,NGCOMP,
& SW,KSTP,KPER)
C-----VERSION 25NOV2002 RBT
C *****
C ADD EFFECTIVE SATURATION TERMS TO MODEL ARRAYS
C *****
C SPECIFICATIONS:
C -----
REAL          KPA,SATP,PRSITY,WSAT,GSAT,ESAT,SW

```

```

      INTEGER          NCOL,NROW,NLAY,K,NGCOMP,KSTP,KPER
      DIMENSION       KPA(NGCOMP),PRSITY(NCOL,NROW,NLAY),
& SATP(NCOL,NROW,NLAY),SW(NCOL,NROW,NLAY)
C -----
C
C1-- IF BEGINING OF SIMULATION,
C1-- ADD EFFECTIVE GAS SATURATION TO POROSITY ARRAY
      DO I=1,NROW
      DO J=1,NCOL
      DO K=1,NLAY
      IF (KSTP.EQ.1.AND.KPER.EQ.1) THEN
        WSAT=SW(J,I,K)
        ESAT=WSAT
        DO L=1,NGCOMP
          GSAT=KPA(L)*(1.-WSAT)
          ESAT=ESAT+GSAT
        ENDDO
        PRSITY(J,I,K)=SATP(J,I,K)*ESAT
      ENDIF
      ENDDO
      ENDDO
      ENDDO
C1-- ADD EFFECTIVE GAS SATURATION TO SATURATION ARRAY
      DO I=1,NROW
      DO J=1,NCOL
      DO K=1,NLAY
        WSAT=SW(J,I,K)
        ESAT=WSAT
        DO L=1,NGCOMP
          GSAT=KPA(L)*(1.-WSAT)
          ESAT=ESAT+GSAT
        ENDDO
        SW(J,I,K)=ESAT
      ENDDO
      ENDDO
      ENDDO
C2--RETURN
      RETURN
      END
C=====
      SUBROUTINE GPD1BD(KPA,GCOMP,CNEW,NCOL,NROW,NLAY,OUTGPD,NGCOMP,
& ICOMP,KSTP,KPER,TIME1,TIME2,IACT)
C-----VERSION 25NOV2002 RBT
C *****
C  CONVERT MODEL CONCENTRATIONS TO AQUEOUS CONCENTRATIONS AND OUTPUT
C    GAS PHASE CONCENTRATIONS
C *****
C  SPECIFICATIONS:
C -----
      REAL          CNEW,KPA,CGNEW,TIME1,TIME2
      INTEGER       GCOMP,NGCOMP,NCOL,NROW,NLAY,OUTGPD,KSTP,KPER
      DIMENSION     CNEW(NCOL,NROW,NLAY),KPA(NGCOMP),
& CGNEW(NCOL,NROW,NLAY),GCOMP(NGCOMP)
C -----
      10 FORMAT(1X,'Gas phase concentrations for component #',I3,
& /1X,'for time step ',I3,' stress period ',I3/,1X,
& 'Starting time: ',G10.5,1X,'Ending time:',G10.5)
C
C1-- IF OUTPUT FILE INACTIVE, RETURN
      IF (OUTGPD.LT.0) RETURN
C2-- STORE GASEOUS CONCENTRATIONS IN CGNEW ARRAY
      DO L=1,NGCOMP
        IF(ICOMP.EQ.GCOMP(L))THEN
          DO I=1,NROW
          DO J=1,NCOL
          DO K=1,NLAY

```

```

C2A-- CONVERT CNEW VALUES TO AQUEOUS CONCENTRATIONS IF AIR IS ACTIVE PHASE
      IF (IACT.GT.0) THEN  !WATER IS ACTIVE PHASE
        CGNEW(J,I,K)=CNEW(J,I,K)*KPA(L)
      ELSE
        CGNEW(J,I,K)=CNEW(J,I,K)/KPA(L)  ! GAS IS ACTIVE PHASE
      ENDIF
    ENDDO
  ENDDO
ENDIF
ENDDO
C3-- OUTPUT GASEOUS CONCENTRATION OF COMPONENT (ICOMP)
c  WRITE(OUTGPD,10)ICOMP,KSTP,KPER,TIME1,TIME2
   WRITE(OUTGPD,*)ICOMP,KSTP,KPER,TIME1,TIME2
   WRITE(OUTGPD,'(G)')CGNEW
C4-- RETURN
   RETURN
END

```

BIOGRAPHICAL SKETCH

R. Brad Thoms grew up in beautiful rural Maryland on a 60-acre horse farm. His interest in hydrology is rooted in childhood experiences on the Potomac and Monocacy rivers. He obtained a Bachelors of Science in Civil and Environmental Engineering from Duke University in 1997 with the intention of becoming a practicing hydrologist. After moving to Portland, Oregon, he decided to pursue an advanced degree in order to further this career goal. The path of graduate school has led him to a job as a Research Associate and hydrologic modeler in the Center for Groundwater Research at OGI/OHSU under the direction of Dr. Richard Johnson. His current research interests include surface-subsurface flow and transport interactions, numerical modeling of watershed systems at various scales, rainfall-runoff relationships of different climatic systems, and reactive transport modeling of permeable reactive barriers.