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ESTIMATING ROOT ZONE SOIL WATER CONTENT USING LIMITED SOILS INFORMATION AND SURFACE SOIL MOISTURE DATA ASSIMILATION

A Dissertation

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A Dissertation APPROVED FOR THE
DEPARTMENT OF GEOGRAPHY

BY

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ABSTRACT

The various hydrologic processes of infiltration, redistribution, drainage, evaporation, and water uptake by plants are strongly interdependent, as they occur sequentially or simultaneously. An important state variable that strongly influences the magnitude to which these rate processes occur is the amount of water present within the root zone, and in particular, the top few centimeters near the soil surface. Traditionally, measurements of soil moisture have been limited to point measurements made in the field. In general, averages of point measurements are used to characterize the soil moisture of an area, but these averages seldom yield information that is adequate to characterize large scale hydrologic processes. Recent advancements in remote sensing now make it possible to obtain areal estimates of surface soil moisture. The use of remotely sensed data to estimate surface soil moisture, combined with soil water and hydrologic modeling, provides a unique opportunity to advance our understanding of hydrologic processes at a much larger scale. Standard techniques for measuring soil moisture have been well documented, with commercial instrumentation being widely available. Various computer models have been developed to estimate soil moisture in the root and vadose zone, although their application over large scales is limited due to varying spatial and temporal field conditions. It is the combination of ground-based data (in-situ measurements), near-surface soil moisture data, and modeling that form the basis for this research. The interactive use of field research, remote sensing ground truth data, and integrated systems modeling is used to describe surface and profile soil moisture conditions at several locations within a large watershed. Successful application of this approach should improve

our capabilities for estimating soil hydraulic properties and to better estimate water and chemical transport in the root zone, thus enhancing water use efficiency and plant production. This work demonstrates the applicability of using limited soil data information, in combination with sequential assimilation of surface soil moisture, to adequately model soil water dynamics in the root zone. The results of this research contribute to a better understanding of how the spatial and temporal patterns of surface soil moisture are related to the physical and hydraulic properties of soils. The advantages, limitations, and potential impact of the overall approach are discussed. The Southern Great Plains 1997 (SGP97) Hydrology Experimental data sets, in conjunction with site-specific field data from the Little Washita River Watershed (LWRW) in south central Oklahoma, serve as the data base for this project.

1. INTRODUCTION

1.1 GENERAL

The measurement of soil moisture is fundamental in several disciplines of the geosciences. The use of computational modeling to estimate the spatial and temporal distributions of soil moisture from local or point-scale observations to regional scale applications has increased rapidly during the past decade as computing costs have decreased. However, a unified approach to monitor soil moisture for multiple model applications has not been well defined. Furthermore, the performance of current hydrologic models is strongly dependent on the quality of input data which, in turn, may be enhanced through better measurements of soil moisture spatial characteristics. Currently, microwave remote sensing provides the opportunity to monitor and study the spatial patterns of soil moisture over a range of space and time scales. According to Blyth (1993), there are three distinct areas where remote sensing can provide valuable information for input to hydrological models. These were reported as: 1) the siting of instruments for hydrological observation can be made more representative by the study of areal distributions recorded by remote sensing; 2) catchment physical characteristics, such as watershed boundaries or land use which are required for the estimation of model parameters, may be better defined and; 3) catchment variables, such as soil moisture, which may be measured every few days using cloud-penetrating microwave radiometry. This work will primarily address the last two areas noted, though the first was previously studied and taken into account by Allen and Naney (1991) in their research on the Little Washita River Watershed (LWRW).

An important state variable that strongly influences the magnitude to which hydrologic processes occur is the amount of water present within the top few centimeters near the soil surface. Traditionally, measurements of surface soil moisture have been limited to point measurements made in the field. Such measurements are time consuming, labor intensive, and generate high costs when used to increase instrument network density. Usually, averages of point measurements are used to characterize the soil moisture over a much larger area. Using such averages as additional input to estimate hydrological fluxes over larger areas is sometimes questionable and often inadequate (Jackson, 1986). However, recent advancements in remote sensing now make it possible to obtain areal estimates of surface soil moisture which may then be used to better describe subsurface moisture conditions (Engman and Gurney, 1991; Mattikalli et al., 1996; 1998; Jackson et al., 1999). The use of remotely sensed data to estimate surface soil moisture, combined with soil water and hydrologic modeling, provides a unique opportunity to advance our understanding of subsurface soil moisture dynamics at the watershed scale.

Remote Sensing Microwave Radiometry and Regional Hydrology

Large-scale soil moisture estimates are an essential component for regional and global hydrologic research studies. At these scales the operational monitoring of soil moisture conditions by in situ methods is not possible due to the large spatial and temporal variability of this parameter. Thus, there has been significant research effort invested in developing the capability of monitoring soil moisture by remote sensing techniques (Jackson et al., 1987; Jackson, 1993). Much of the attention for hydrological research has focused on the use of low-frequency (1.4 GHz) microwave radiometry. The atmosphere and clouds are relatively transparent to radiation in this spectral region. The relationship between the microwave emission of natural surfaces and their inherent moisture content has been studied and well documented (e.g., Schmugge et al., 1992; Jackson et al., 1987; Moran et al., 1989). The fundamentals of this approach are well established (Jackson et al., 1987) and soil water content retrieval algorithms have been verified using high resolution ground based experiments and air craft observations (Jackson et al., 1993). Thus, by using remotely sensed microwave radiometric data, reliable estimates of surface soil moisture over large areas can be obtained. Microwave techniques for measuring soil moisture include the use of either passive or active microwave systems, each having certain advantages (Jackson, 1993). These techniques rely on the large contrast between the dielectric constant of water and that of dry soil (Owe et al., 1992). The large dielectric constant for water is the result of the water molecule's alignment of the electric dipole in response to an applied electromagnetic field (Schmugge et al., 1992). The dielectric constant of water is approximately 80 compared with that of dry soil which ranges from 3 to 5. Thus, as the soil moisture increases, the dielectric constant can increase to a value of almost 30 for wet soils (Jackson, 1993). Microwave techniques for measuring soil moisture are limited to a surface layer about 5 cm thick and must take into account surface roughness and vegetation cover (Engman and Gurney, 1991).

The ability to use remote sensing estimates of soil moisture as input to water and energy balance modeling has important applications to regional-scale hydrology. Much of the research in this area has been concerned with improving spatial parameterization of hydrological models using microwave remote sensing (Camillo et al., 1986; Blyth, 1993; Mattikalli et al., 1998). Modeling optimization techniques and interactive numerical simulation are used in conjunction with remotely sensed data to estimate certain soil hydraulic parameters such as hydraulic conductivity over large areas. Hollenbeck et al., (1996) reported on the ability of passive microwave remote sensing to obtain near-surface soil hydraulic characteristics using relative change detection techniques for filtering out the drydown heterogeneity caused by spatial variability in initial wetness rather than soil heterogeneity. Camillo et al. (1986) used remotely sensed data for estimating hydraulic conductivity, matric potential and soil moisture at saturation, and a soil texture parameter based on model calibration techniques. To better facilitate the spatial and temporal analyses of modeled data, the application of Geographic Information Systems (GIS) has recently become extremely useful in many cases (Ehlers, 1992; Rogowski, 1996). In work by Mattikalli et al. (1998) a GIS-based analysis was used to suggest that two-days initial drainage of soil, measured from remote sensing, was related to the saturated hydraulic conductivity. Chang and Islam (2000) reported that by using a GIS integrated neural network analysis, soil texture could be inferred from remotely sensed drainage patterns of soil moisture.

Surface Soil Moisture Data Assimilation

It is apparent from the literature that there are several unresolved issues concerning the application of remote sensing microwave data to areas other than that of obtaining near surface soil moisture observations. To address them all is beyond the scope of this thesis. However, among the various issues described above, there is currently a question that is of significant interest to many analysts working in areas of hydrologic research. To what extent, if any, does the assimilation of surface soil moisture data into soil water models improve estimates of profile soil water content? To date, there is insufficient field experimental data to adequately support the range of theoretical analyses. Applications of data assimilation arose from the meteorological custom of constructing daily weather maps which show how environmental variables such as pressure and wind velocity vary spatially (Daley, 1991). Analysis using data assimilation provides time-dependent spatially distributed estimates that can be updated whenever new data become available. Thus, the application of different data assimilation techniques has recently become a major area of investigation concerning the integration of remote sensing and soil water modeling (e.g., Calvet et al., 1998; Houser et al., 1998; Wigneron et al., 1999; Hoeben and Troch, 2000; Walker et al., 2001).

A common characteristic of current surface soil moisture data assimilation studies is lack of sufficient field measurements. This is an issue of concern to many research analysts and is most often a matter concerning the time, labor, and cost involved with obtaining reliable and accurate field data. As a result, many investigators are obliged to use artificially generated or synthetic data sets. Furthermore, an important question exist as to what amount of soil data information is needed as model input to adequately describe the status of soil water content in the root zone? A key element of this work is the combined use of an extensive set of quality field measurements and a detailed process-based model to evaluate the potential benefits of remote sensing data assimilation with use of limited soil data information.. The challenge of this work is to effectively link in-situ data, remote sensing measurements at the surface, and modeling techniques to estimate vertical profiles of soil moisture while considering issues of scale and spatial variability. Hopefully, the approach provides better insight to real world applications. Although the work presented here is at the point scale, it is a basic step towards better understanding the application of remote sensing data assimilation to estimate profile soil water content, which should be considered essential before making various assumptions and being applied at larger scales.

Soil Water Modeling and Scaling Issues

Much research, particularly in soil physics, has been devoted to developing numerical models to describe the state and flow of water and its constituents in soil (Ahuja and Hebson, 1992; Pachepsky et al., 1993). Numerical simulation of soil water movement in the unsaturated zone using microwave remote sensing data has been reported by Bernard et al. (1981), Lascano and Van Bavel (1983), and Jackson (1986). Jackson (1986) suggested developing methods for extrapolating remotely sensed surface layer estimates of soil moisture through the root zone. The simplest approach is to develop a regression equation to predict profile soil moisture from surface layer measurements. The results from several investigations evaluating linear correlations between soil layers showed that in general, correlation decreases with depth, the presence of plant cover significantly influences the correlation, and increasing the thickness of the surface layer improves the relationship between the surface and the profile moisture (e.g., Arya et al., 1983; Jackson, 1986). Another approach is the integration of surface observations into more detailed and complex physically-based profile soil moisture models. In this technique, the surface moisture is used as an initial boundary condition in a meteorological driven soil water model that may also require input characterizing the profile hydraulic properties (Bernard et al., 1981; Jackson, 1993; Li and Islam, 1999).

Over the past two decades, scaling of soil water properties and hydrologic processes has become one of the major areas of research in soil physics and hydrology, respectively (Ahuja et al., 1984; Ahuja and Williams, 1991; Wood, 1995; Sivapalan and Kalma, 1995). Scaling encompasses many concepts; soil physical and hydraulic properties, process descriptions, cartographic considerations or pattern analysis, and spatial and temporal effects (Eagleson, 1986; Seyfield and Wilcox, 1995). Scaling may be considered as the transfer of information obtained from local observations to larger regions. An example would be: characterization of spatial and temporal variability of soil properties at the point-scale and scaling of the dynamic behavior of transport processes across larger areas based on local measurements. On one hand, the scaling of soil properties across different soil types such as hydraulic conductivity must be addressed, while on the other hand, it is a matter of scaling processes such as infiltration and redistribution. Bloschl and Sivapalan (1995) give a thorough review of issues regarding scale in hydrologic process modeling. Different approaches are discussed for linking state variables, parameters, inputs and conceptualizations across scales. Ahuja et al., (1984) examined the variability and interrelation of scaling soil water properties and infiltration modeling. Ahuja and Williams (1991) used scaling as a means to relate soil properties of different soil types or spatial locations according to simple conversion factors, called the scaling factors. Although these methods hold much promise, there are still a number of questions to be addressed at the point-scale regarding the use of remote sensing data as model input. Such questions might include determining whether there is a scaling factor among soil types that would account for different drainage characteristics based on point-scale measurements. If so, this type of information could then be applied across soil types on a much larger scale. Therefore, the emphasis of the research presented in this thesis will be modeling at the point-scale with discussions given in Chapters 4 and 5 regarding how the results may be applied to larger areas.

The recently developed Root Zone Water Quality Model (RZWQM), Version 3.2, was the model chosen for this study and is described in greater detail in Chapter 3. The RZWQM is a comprehensive, one-dimensional model that integrates physical, biological, and chemical processes to simulate plant growth and predict the effects of agricultural management practices on the movement of water and chemicals through the root zone (Hanson et al., 1999).

1.2 STUDY AREA DESCRIPTION AND SITE SELECTION

The 611 km^2 Little Washita River Watershed (LWRW), located in south central Oklahoma, was selected as the study site for this research due to availability of meteorological and soil data sets and diversity of soil types and land cover. A map of the watershed in reference to the entire SGP97 experimental region (discussed below) is shown in Figure 1.1. Topography may be characterized as gently to moderately sloping, with a maximum relief of approximately 200 m. Uplands consist in the west primarily of loamy soils overlying gypsum beds. In the east, loamy or sandy soils overlie brick-red sandy shale. There are 64 defined soil series in the LWRW, with fine sand, loamy fine sand, fine sandy loam, loam and silty loams being the predominant textures of the soil surface. The climate is classified as subhumid with total annual precipitation of about 75 cm, which largely comes during the spring and fall months. Land use consisted originally of range grasses in uplands with hardwood riparian zones. Intensive cultivation occurred in the first half of this century and was largely discontinued by the 1950's. Currently land use is approximately 66% range, 18% cultivated, 5% dense timber, and miscellaneous land uses (Allen and Naney, 1991).

Soils in the watershed have been grouped into one of four hydrologic groups on the basis of the soil properties that are known to influence infiltration and runoff. These soil properties include depth to the water table, infiltration rate, and low permeability of subsurface soil layers. In general, most soils have moderate infiltration rates and cover approximately 70% of the watershed. Certain areas of shallow soils in the western portion of the watershed have high runoff potential. Due to low permeability, a few soils in the eastern end of the region have high runoff potential. Dispersed throughout the central portion of the watershed are areas with very low runoff potential because the soils are predominately sandy and, thus, have higher infiltration rates.

LWRW Research Projects and Activities

Research and demonstration projects in the LWRW date to 1936, when a portion of the watershed was selected to study erosion control practices. The USDA-ARS began hydrologic monitoring in 1961 to assess the effectiveness of flood-control practices. In 1978 the watershed was selected as one of seven sites nationwide for the Model Implementation Project (MIP), jointly sponsored by the USDA and USEPA. The primary objective of the MIP was to demonstrate the effects of land conservation measures on water quality in watersheds larger than approximately 50 km^2. An extensive network of rain gages was established along with stream gaging and monitoring for water quality, sediment transport, and groundwater levels (Allen and Naney, 1991).

A meteorological network (*Micronet*) of 45 stations is distributed across the watershed on approximately a 5 km spacing (Fig. 1.1). Forty two of these stations measure a basic suite of meteorological data: rainfall, incoming solar radiation, air temperature, relative humidity, and soil temperature at three depths. At three stations, windspeed and wind direction at two heights and barometric pressure are also recorded in addition to the basic suite of data. The meteorological data are measured every five minutes and reported every 15 minutes to a central archiving facility via radio telemetry.

The data are quality controlled and final output is written in both 5-minute and daily summary files (Elliot, et al. 1994). Meteorological data from selected sites were used to determine break point precipitation required by the model, and to supply the required model inputs to calculate evapotranspiration. Soil profile moisture is measured weekly at 13 sites using time-domain reflectometry (see below). Time-domain reflectometry (TDR) is commonly used to measure volumetric water content in soils. It is based on the relationship between the soil dielectric constant (K) measured by TDR, and the soil volumetric water content (θ_v). Additionally, the watershed is observed by the Next Generation Radar (NEXRAD) system, providing spatial distributions of rainfall intensity on approximately a 4 km by 4 km grid (Klazura and Imy, 1993).

Nine *Micronet* sites were selected (Fig.2.1) in this study for TDR calibration, from which five were chosen for limited data modeling, and four for assimilation modeling. Selection of the sites was based on availability of measured soil properties and soil water content at the site, and differences in soil texture and vegetative cover. Three of the nine study sites had a relatively dense vegetative cover of bermudagrass (*Cynodon dactylon*). Vegetative cover at the other study sites was a mix of native rangeland grasses consisting of big bluestem (*Andropogon gerardii*), little bluestem (*Schizachyrium scoparium*), switchgrass (*Panicum virgatum*) and indiangrass (*Sorghastrum nutans*) and ranged from sparse to moderate cover. Vegetative and soil characteristics for each site are listed in Table 2.1. A brief description and map of study sites pertinent to the work in Chapters 2, 3, and 4 are given in each chapter.

Remote sensing of hydrologic and meteorological data has been investigated in

Washita 92, *Washita 94* and the *Southern Great Plains 1997 (SGP97) Hydrology Experiment;* cooperative experiments conducted by the USDA, NASA, and other agencies and universities. Low and medium altitude flights over the watershed were coordinated with ground monitoring and in 1994 with Space Shuttle (Endeavor) experiments. Estimation of soil moisture and evaporative fluxes were the primary areas of research (Jackson and Schiebe, 1993). The watershed is also a study site for the Global Energy and Water Cycle Experiment (GEWEX), an effort to refine models of global water and energy fluxes, ultimately to improve predictions of regional impacts of climate change.

Data Acquisition

Several types of data sets are used in this study. The data sets were obtained during the Southern Great Plains 1997 Hydrology Experiment (SGP97). The core of SGP97 was a large-scale aircraft soil moisture mapping experiment, conducted over a one-month period from June 18 through July 16. Surface soil moisture was mapped over an area of approximately 10,000 km^2 of Oklahoma at a spatial resolution compatible with known data interpretation algorithms (800 m). Data from SGP97 are maintained at a public web site *http://daac.gsfc.nasa.gov/CAMPAIGN_ DOCS/SGP97/sgp97html/.*

Ground-Based Measurements

A substantial number of ground-based measurements were made during SGP97.

Data sets specific to this study are: daily surface and profile soil moisture values, soil physical and hydraulic properties, surface cover type, latitude and longitude coordinates, and daily meteorology. Gravimetric sampling techniques are considered the standard method for determining soil water content within 1 to 2% error (Gardner, 1965). Surface soil moisture water content samples were collected as ground-truth data for the passive microwave radiometer and used as a surrogate for microwave observations of surface soil moisture. Soil core samples were collected to characterize soil properties and for TDR moisture probe calibrations. Field experiments were conducted to measure in-situ soil water characteristics, i.e., hydraulic conductivity and soil matric potential-moisture relationships. Global positioning systems (GPS) were used to determine surface coordinates at field sample sites. Meteorological data were obtained from the *USDA-ARS Micronet* archive.

Two critical components of this study were the accurate measurement of profile soil moisture and the characterization of soil physical and hydraulic properties. Obtaining high quality data for soil moisture and soil properties from well-planned field experiments is essential for modeling the dynamics of soil water flow. Estimation of model parameters from the field is considered to be the most difficult issue concerning the use of hydrologic models (Hanson et al., 1998). Increasing the availability and accuracy of these data should improve the physical realism of RZWQM parameterizations and should lead to a better understanding of the water and energy budget, as well as soil moisture distribution measured in-situ and inferred from remotely sensed observations. Thus, considerable time and attention has been given to these areas of field research and lab analysis.

Profile Soil Water Content

During the spring of 1997, MoisturePoint[1] (Environmental Sensors, Inc., British Columbia, Canada) profiling TDR probes were installed at selected Micronet locations, in support of research objectives for the Southern Great Plains 1997 Hydrology Field Experiment (Jackson et al., 1997). Of the 42 Micronet locations, 13 were chosen as TDR soil moisture measurement sites (Fig. 1.1). The sites were selected based on preexisting instrumentation, soil physical and hydraulic properties, and location within the watershed. Each probe consisted of four 15 cm long segments, enabling measurements of θ_v down to 60 cm. At site 151 a 5-segment TDR probe was used reaching to a depth of 120 cm, in segments of 0-15, 15-30, 30-60, 60-90, and 90-120 cm. To coincide with available soil property data, readings from only the first four segments were used in this work. The TDR probes were calibrated in situ against site-specific gravimetric and bulk density data. The TDR probes were usually read once each day, depending on weather conditions and available personnel, between 0800 and 1000 hrs local time, during the June 18 - July 16, 1997 study period.

1

Use of company or trade names is for informational purposes only and does not constitute endorsement by the University of Oklahoma to the exclusion of any other product that may be suitable.

1.3 OBJECTIVES AND FORMAT OF THIS DISSERTATION

The objective of the study is to evaluate the use of simple methods to estimate profile soil moisture based on the application of remote sensing data assimilation, in combination with in-situ field data and soil water modeling. Selective experimentation, computational modeling, and assimilation of surface layer soil moisture data are used interactively to describe surface and profile soil moisture conditions at several locations over a large scale watershed.

The significance of this work is that it will provide a practical basis for applying remote sensing data assimilation to estimate profile soil water content. Determining a minimum threshold of model input data necessary to optimize soil moisture estimates is also a significant aspect of the research. Successful application of this approach should have a positive impact on associate processes such as the partitioning of available energy at the earth's surface into sensible and latent heat exchange with the atmosphere, as well as, in the partitioning of rainfall into infiltration and runoff. Practical applications of the research could include: 1) improvements in the area of agricultural irrigation scheduling and crop yield modeling, 2) improved water resource management in terms of better water use and storage, and 3) climate modeling.

A description of the content for the chapters that follow is given below. Chapters 2, 3, and 4 are related portions of this thesis which collectively form an integrative study of field research and theory in an effort to provide a simple and practical approach for better estimating the status of soil water in the root zone using remote sensing data.

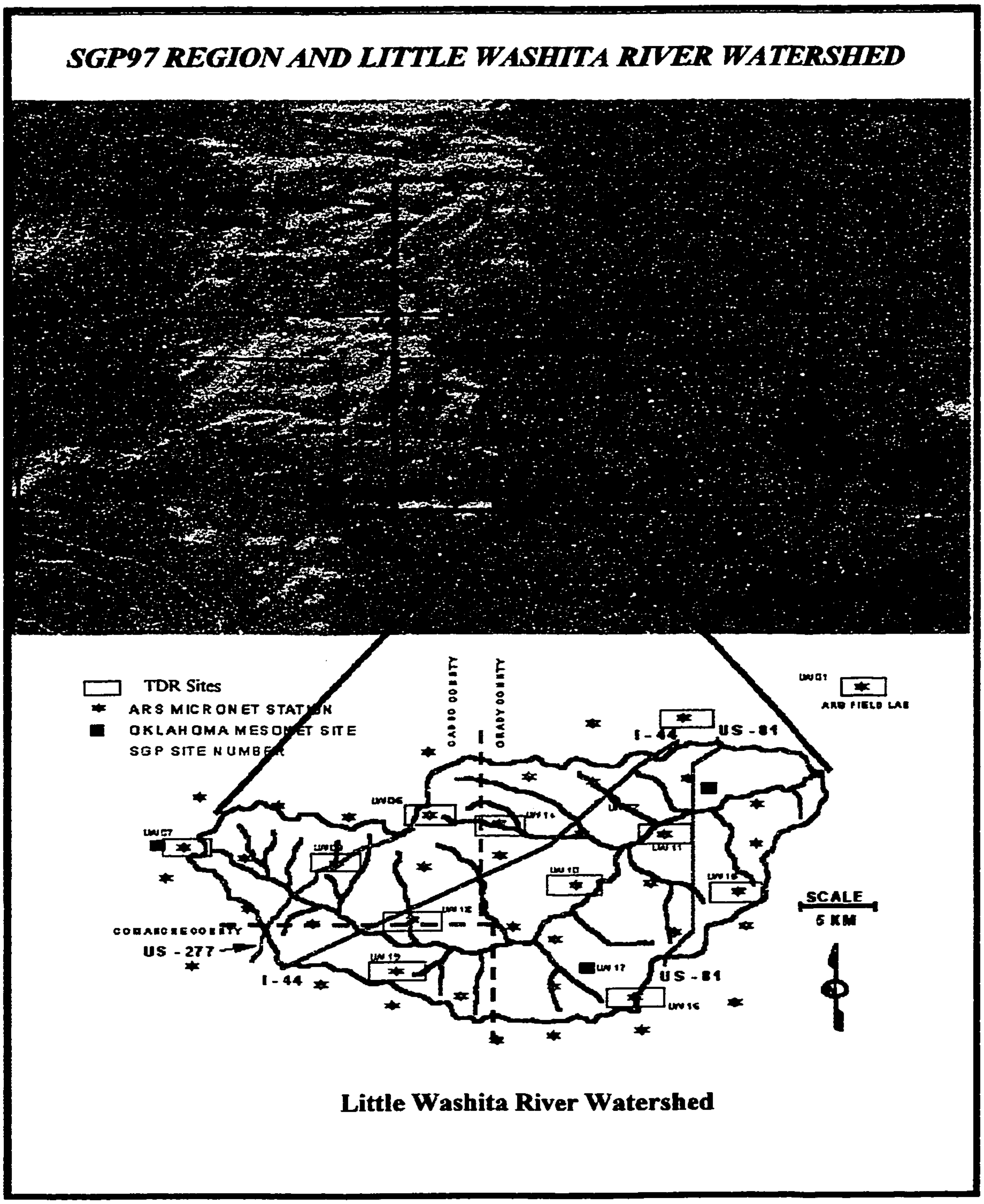
Chapter 2 describes the different types of field experiments involved with this research and establishes the validity of TDR measurements of profile soil water content based on a relatively new approach for field calibration. Three field calibration techniques are compared against the factory calibration. The field calibrated TDR probe data serve as the "true value" of soil water content, in what is defined as the root zone. The TDR data are used for comparison with model estimates during the experimental study and thus, serve as the cornerstone for this research. A complete description of the field and laboratory methods used to obtain site-specific soil characteristics is also given. The extent of experimental work conducted for this research project is emphasized in this chapter.

Chapter 3 illustrates the use of "limited" soil data information as model input since detailed information regarding soil hydraulic and physical properties necessary to adequately model the status of soil water in the root zone is usually unavailable. The use of variable levels of model input data are addressed and the results on model estimates of soil water in the profile are presented. Different modeling scenarios are used to illustrate the effective use of very limited soils input data in the RZWQM and how this is related to the application of remotely sensed surface soil moisture as model input. Results show how the use of soil hydraulic properties obtained in the field using simple techniques work as well as, or better than, those obtained from more tedious and time consuming laboratory methods. The results in this chapter are the basis for the work in Chapter 4.

In Chapter 4, the use of sequential surface soil moisture (0-5 cm) as model input for estimating soil water content in the root zone (0-60 cm) is investigated. Actual ground-truth soil sample data are used as a surrogate for the remotely sensed (microwave) surface soil moisture data. The ground truth data were used to calibrate the microwave radar sensors to obtain the final ESTAR (electronically scanned thinned array radiometer) microwave data set during the SGP97 experimental campaign. In using ground-truth data as a surrogate, the error in the surface measurement associated with the conversion algorithms is minimized. The ground samples (an average of nine samples/site/day) were collected within 1 to 10 m of TDR profile measurements, whereas the ESTAR data are at 1 km resolution. Thus, this should offer the best possible case of using surface soil moisture to estimate root zone water content from the types of data available.

Chapter 5 consolidates and summarizes the overall findings of the numerical and field experiments, discusses applications and limitations, and highlights future research considerations.

Figure 1.1. Map of the SGP97 Experimental Region and LWRW instrumentation network.



2. EXPERIMENTAL MEASUREMENTS FOR MODEL EVALUATION

2.1 INTRODUCTION

Although simulation models may provide a greater range of information that extends beyond experimental results, these models are only as good as their input data and parameters, and in how accurately they depict the fundamental physical, chemical, and biological processes involved. In some cases the analyst may have to make an educated guess as to what values to use for some model parameters. In other cases the modeling scheme may be purely synthetic, in a sense that only a conceptual or theoretical analysis is performed which is later tested for real world applications.

The purpose of this chapter is to establish that a significant amount of work and time was dedicated to this project in terms of obtaining high quality field data to be used as model input data, parameterization, calibration and evaluation. Because the focus of this work is on modeling the status of soil water in the profile, attention will be given to those methods and procedures that pertain to profile soil water measurements and for characterizing soil physical and hydraulic properties. An evaluation of field and laboratory methods is made since soil hydraulic properties determined from laboratory experiments often are non-representative of field conditions.

2.2 TDR FIELD CALIBRATION AND MEASUREMENTS OF PROFILE SOIL WATER CONTENT

Time domain reflectometry (TDR) is commonly used to measure volumetric water content in soils. It is based on the relationship between the soil dielectric constant (K) measured by TDR, and the soil volumetric water content (θ_v). Hilhorst (1998) mentions that according to a historical review by Grant et al. (1978) the technique has been in use since 1951. However, the relationship between the dielectric properties of a soil and its water content were the subject of much earlier work by Smith-Rose (1933). Based on a comprehensive laboratory study, Topp et al. (1980) developed an empirical expression relating apparent dielectric constant (K_a) and θ_v. From this general relationship an equation was derived to find θ_v from measured values of K_a:

$$\theta_v = -5.3x10^{-2} + 2.92x10^{-2}K_a - 5.5x10^{-4}K_a^2 + 4.3x10^{-6}K_a^3 \qquad [2.1]$$

The work of Topp et al. (1980), as well as earlier work by Davis and Chudobiak (1975), clearly demonstrated the potential of TDR for the measurement of soil moisture and was fundamental to future studies and many advances in TDR technology.

Many attempts have been made to improve measurements of water content obtained from dielectric data (Roth et al., 1992; Jacobsen and Schjønning, 1993; Dirksen and Dasberg, 1993; Chan and Knight, 1999; Ponizovsky et al., 1999; Yu et al., 1999). Basically these studies describe the application of various models used to relate a given soil's dielectric constant to its water content. The types of models range from complex physically based multi-phase mixing models to simple empirical relationships. Yu *et al.* (1999) give a systematic framework for evaluating the TDR response of soil using several different modeling approaches. In general, they found that soil solid fraction, porosity, and temperature have little effect on dielectric constant measurement while particle surface area was an important factor affecting water content measurement. These results are consistent with several studies in the literature (Wang and Schmugge, 1980; Roth et al., 1992; Ponizovsky et al., 1999), but inconsistent with others (Dirksen and Dasberg, 1993; Jacobsen and Schjønning, 1993; Hilhorst, 1998). Thus, the influence of soil physical properties on the dielectric properties of a soil continues to be an active area of study. There does, however, seem to be general agreement that when using a dielectric sensor, the measured dielectric data should be calibrated to the water content of the actual soil involved.

The purpose of this section was to determine if site-specific calibration of the TDR offered substantial improvement over the factory supplied calibration. The sites used in this study exhibited differences in soil texture, layering, and bulk density. It is not the intent here to develop a universal expression for determining water content from measured TDR time delay data; rather, it is to consider the possible use of a general expression for the set of data collected for this study.

TDR Theory and Soil Water Measurement

Volumetric soil water content determined by TDR involves measurement of the propagation velocity (or time delay) and attenuation of an electric step or pulse function applied along a transmission line in the soil. A time domain reflectometer generates a voltage pulse which propagates as an electromagnetic wave through the soil via a transmission line (waveguide). The propagation velocity (v) corresponds to the time it takes for a step pulse to travel a distance to the end of the transmission line and back. Velocity (v) can be expressed as,

$$v = \frac{2L}{t} \qquad [2.2]$$

where L is the linear distance traveled, and t is the measured travel time. The time interval is the variable quantity measured by the TDR technique and used to determine soil water content (Hook and Livingston, 1995). As soil water content increases, the time required to traverse the length of the transmission line also increases.

The propagation velocity is usually normalized to the speed of light and expressed in terms of K_a (Topp et al., 1980),

$$K_a = (c/v)^2 \qquad [2.3]$$

where c is the speed of light (3 x 10^8 m/s) and v is velocity as above. Based on the model of Herkelrath et al. (1991), and using the transmission line theory of Eq. [2.2] and [2.3], Hook and Livingston (1996) derived a general formula to obtain soil water content from measured travel time given as,

$$\theta_v = [(T/T_a - T_s/T_a)]/\sqrt{K_w} - 1 \qquad [2.4]$$

where they express v in terms of time intervals with T being the travel time of an electric pulse in soil and normalized with respect to the theoretical travel time of the transmission line in air (T_a). Travel time in oven-dried soil is T_s, and K_w is the dielectric constant for water equal to 80.32 (Handbook of Physics and Chemistry, 1986). Using the dielectric constant for water, Eq. [2.4] has a theoretical slope of 0.1256. An average value for T_s/T_a of 1.55 nanoseconds and an average slope of 0.1193 was obtained by Hook and Livingston (1996) and used to represent all agricultural nonclay soils.

The Environmental Sensors, Inc. (ESI) Model MP-917 TDR instrument used in this study, measures T and is referred to as measured time delay from which θ_v is calculated according to Eq. [2.5] (Hook and Livingston, 1995; 1996),

$$\theta_v = (T/T_a - 1.55)0.1256 \qquad [2.5]$$

Thus, Eq. [2.5] serves as the Model MP-917 factory calibration equation, where T/T_a is as described in Eq. [2.4] and the value of 0.1256 is the theoretical slope for the relationship between θ_v and T/T_a (Hook and Livingston, 1996).

Study Field Sites

In the spring of 1997, 13 of the 42 *Micronet* locations shown in Figure 1.1 were chosen as TDR soil moisture measurement sites to support the objectives of the Southern Great Plains 1997 Hydrology Experiment (Jackson et al., 1999). The sites were selected based on preexisting instrumentation, soil physical and hydraulic properties, and location within the watershed. Because of the variability of soil textures across the watershed, it was necessary to determine the effects of using a generalized factory-supplied calibration on the determination of soil water content from TDR time delay readings. From the 13 TDR probe sites, nine (Fig. 2.1) were chosen for calibration studies.

Soil Sample Collection and Analysis

Most devices commonly used to measure soil water content are calibrated against gravimetric determinations of soil water content (θ_g) (Gardner, 1965). Calibration procedures presented in this work are based on this standard technique. Soil-core samples were collected at three locations at each site, and within approximately 1 m of the TDR probe. Measurements of θ_g, bulk density, and texture were made at depth intervals coincident with TDR measurement intervals (TDR readings were taken just prior to soil sampling). Soil core average volumetric water content (θ_{vc}) for each depth interval was determined from the three θ_g samples based on core sample volume and soil bulk density. Samples were collected at various times to obtain a range of water contents. Table 2.1 gives bulk density values and percentage sand, silt, and clay for each site and depth interval based on soil-core lab analyses.

Instrument Features

The ESI TDR system includes a hand-held data measurement, processing, and logging unit, a connecting cable, and TDR probe (transmission line). Once the instrument is plugged into the probe and activated, the instrument then automatically interrogates the probe, processes the electronic pulses or waveforms, and displays (and/or stores) the results as numerical data. The numerical data is logged as time (in counts, an internal instrument measurement) and as volumetric water content (m^3 m^{-3}). Stored data can be exported to a computer for archive and further processing.

The TDR probes are constructed of stainless steel, epoxy, and high density plastic that vary in length and are approximately 1cm thick and 2 cm wide. The probes are a segmented device having known distances between segment endpoints. Probe design is based on TDR remote diode shorting technology (Hook et al., 1992) that enables profile measurements of θ_v in layered soils. They are installed using a probe insertion/extraction tool kit. The type of probes used in this work were one 5-segment probe with 0 -15, 15 - 30, 30 - 60, 60 - 90, and 90 - 120 cm segments, and eight 4-segment probes with 0 15, 15 - 30, 30 - 45, and 45 - 60 cm segments.

Specific features of the ESI MoisturePoint instrument pertinent to this study were: Measured time delay displayed by the unit is in nanoseconds (ns) and uncorrected. However, measured time delay is stored by the unit as 'instrument counts' which must be converted to ns and then corrected. This distinction is important to note when downloading data files and converting time delay to water content by site-specific calibration. Conversion of instrument counts to uncorrected time delay *(Tm)* in ns is obtained by multiplying counts by the instrument-specific calibration factor (UO). Corrected time delay (*Tmc*) in ns is obtained via $Tmc=Tm/B - A$, where A and B are segment-specific calibration coefficients. Values for A and B are related to segment length and geometry and are the same for a given segment depth interval and probe type, but differ segment to segment along the length of the probe. According to the manufacturer, A and B coefficients differ by only 2% and, thus, average values are used for a specific probe type (ESI, personal communication). The UO calibration factor and A and B coefficients can be obtained using the ESI Viewpoint software while connected to a probe.

Methods of Calibration

Four calibration methods were evaluated in this study to determine which provided the most accurate measurement of θ_v from TDR time delay measurements.

Method 1: The value of volumetric soil water content stored by the MP-917 data logger at the time of measurement is calculated as in Eq. [2.4] using the factory calibration,

$$\theta_v = [(Tmc/T_a - T_s/T_a)]/\sqrt{K_w} - 1 \qquad [2.6]$$

Method 2: Volumetric soil water content is calculated based on the site-specific linear regression of θ_{vc}, and corresponding *Tmc*. This approach is analogous to the standard method of field calibration for the neutron probe (van Bavel et al., 1956), where neutron count ratio would be used rather than *Tmc*. The equation is written as,

$$\theta_v = (m)\ Tmc + b \qquad [2.7]$$

where the slope (*m*) and intercept (*b*) are the site-specific regression coefficients that apply to all segments of a particular probe type.

Method 3: This method uses the factory calibration equation, but rather than assuming the factory value of 1.55 for T_s/T_a in all soils, an average site-specific T_s/T_a is determined from *Tmc* and the corresponding θ_{vc} reflecting a range of moisture values. The calculation is expressed as,

$$\theta_v = (Tmc/T_a - T_s/T_a)\ 0.1256 \qquad [2.8]$$

where,

$$T_s/T_a = Tmc - (\theta_{vc} / 0.1256) \qquad [2.9]$$

The average value for T_s/T_a is applied to all probe segments.

Method 4: A general linear regression was performed on all θ_{vc} and *Tmc* data from nine sites to give one equation for determining θ_v from time delay measurements. For our set of data the expression is,

$$\theta_v = 0.0882(Tmc) - 0.0948 \qquad [2.10]$$

Statistical Analysis

Statistics of mean error (ME), root mean square error (RMSE), coefficient of determination (r^2), and correlation coefficient (R) were adopted in this work to examine the correspondence between observed and predicted θ_v and thereby, determine which of the four methods of calibration is most accurate. The ME and RMSE statistics are defined as:

$$ME = \frac{\Sigma(P-O)}{n} \quad [2.11]$$

$$RMSE = \sqrt{\frac{\Sigma(P-O)^2}{n}} \quad [2.12]$$

where P is water content predicted by one of the calibration methods, O is the corresponding observed soil-core water content and n is the number of observations. The coefficient of determination (r^2) represents the proportion of the total variability among soil-core θ_v that is accounted for by TDR time delay (ns), whereas the correlation coefficient (R) represents a measure of the strength of the relationship between predicted θ_v and observed measurements. The z-statistic was used to determine if there was any evidence to suggest a difference in population means.

TDR Calibration Results

The results for each of the four calibration methods are discussed in detail below. Linear regression analysis for the relationship between θ_{vc} and *Tmc*, at three of the nine study sites are plotted in Fig. 2.2a-c. These sites were chosen from the nine to illustrate differences in regression analyses for three different soil types. Fig. 2.2d shows the general linear regression analysis for θ_{vc} and *Tmc* data sets from all nine sites. In Fig. 2.3a-d. we plot volumetric soil-core water content vs. TDR volumetric soil water content for each of the four methods. If no error where involved with either the sample or instrument measurement, all points would fall on the 1:1 line. It should be noted that the soil-core data used for these plots was the same as that used for the linear regression analysis. However, we also present the 1:1 relationships from an independent data set in Fig. 2.4a-d for each of the four calibration methods. Figure 2.5 shows a plot of field calibrated TDR profile data during the SGP97 experimental campaign.

Method 1

Estimates of θ_v obtained using the factory calibration (Eq. 2.6) were compared with field observations resulting in RMSE values ranging from 0.032 to 0.078 $m^3 m^{-3}$ for the nine study sites. In both the calibration data set and independent sample data, use of the factory calibration resulted in the highest ME and RMSE. Method 1 also had the widest range in both types of error analysis. The data in Figs. 2.3a and 2.4a indicate that θ_v is over estimated at higher water contents using the factory calibration of Method 1.

Method 2

Once a linear regression was performed for each of the nine sites, the site-specific linear model was used to determine θ_v from TDR time delay data at a given site. Coefficients of determination (r^2) for all site-specific analyses ranged from 0.74 to 0.87 (Table 2.2). Plots of the regression analyses in Figs. 2.2a - 2.2c show that the slope and intercept vary among soil types. This was true for all study sites. Figs. 2.3b and 2.4b show very little bias in TDR θ_v over the range of water content using Method 2. The smallest values for RMSE were obtained using Method 2 which ranged from 0.031 to 0.042 $m^3 m^{-3}$.

The results from our site-specific linear analyses at nine locations across the watershed gave an average slope of 0.10822 ± 0.27 and an average value of 1.71 ± 0.27

for *Ts/Ta* (x-intercept). Both the theoretical (0.1256) and experimental (0.1193) values for slope and the average value for *Ts/Ta* (1.55) reported by Hook and Livingston (1996) lie within the 95% confidence interval for the range of values that were obtained from the field. Findings from the field data analyses are also consistent with those of Topp and Ferre (2000) where a linear relationship between θ_v and TDR time delay was depicted by calibration data from numerous sources reported in the literature. In their work they determined the average slope to be 0.115 and a value of 1.53 for *Ts/Ta*. They suggest that fitting a linear relationship where possible presents a significant improvement over fitting a polynomial calibration curve because it has only two parameters to fit and is much easier to use. In addition, it was determined from linear regression analysis that because of the difference in the intercepts among the linear relationships, the calibration data set requires very low water content values to determine absolute water content. The work of Topp and Ferre (2000) make an important note of this as well. Of the four methods, TDR water content determined using Method 2 resulted in the highest correlation coefficient (R=0.91) and the lowest RMSE value of 0.0374 m^3 m^{-3} (Table 2.2).

<u>*Method 3*</u>

In Method 3 the average value for *Ts/Ta* in the factory equation was replaced with a site- specific value determined from soil-core moisture sample analysis. This approach was considered to determine whether legitimate values for *Ts/Ta* could be obtained in such a simple manner and if so, to what degree this might improve the measurement of soil water content. Analyses of the data show that the values obtained for *Ts/Ta* are comparable to those reported in the literature for similar soils. The data plotted in Fig.

2.3c and 2.4c show a closer fit to the 1:1 relationship than the other three methods. This suggest that, although the factory calibration equation in Method 1 may be theoretically valid, determining site-specific values for *Ts/Ta* will improve the accuracy of measurement and reduce measurement bias. The results further support the hypothesis, that knowledge of the x-intercept (*Ts/Ta*) among site-specific linear calibration methods is critical in determining absolute water content, which again emphasizes the need for very low soil water content data in the analysis procedure. The RMSE for Method 3 ranged from 0.032 to 0.057 $m^3 m^{-3}$ and the mean error was equal to 9.24E05 $m^3 m^{-3}$.

Method 4

A considerable amount of research has been aimed at finding a general equation for determining soil water content from TDR data, and thus, a generalized calibration was considered for the nine study sites in this work. The regression equation in Fig. 2.2d was derived from sample data at all nine sites and used as the general linear model in Method 4. A value of 0.77 for r^2 was determined for the range of sample data. In the calibration data set, the smallest mean difference was obtained using Method 4 (ME = 3.25E-05). In the independent data analysis, the values for RMSE for each of the three field calibration methods were quite close and ranged from 0.0307 to 0.0348 $m^3 m^{-3}$ with Method 4 having the smallest RMSE equal to 0.0307 $m^3 m^{-3}$, but also the highest mean error (Table 2.2). Although Method 2 had the smallest degree and range of error on a site-specific basis, results from the independent data set indicate that the use of Method 4 would be sufficient for similar soil types within the watershed. Thus, for this case, Method 4 would provide better measurements of soil water content than the factory calibration, especially in situations where additional TDR probes have been installed and site-specific data are not currently available to obtain a calibration using Method 2.

Summary and Conclusions

Four methods for TDR calibration were evaluated in the Little Washita River Watershed in south central Oklahoma. Our objective was to determine if site-specific linear analysis might serve as a method for improving instrument calibration, and thus the accuracy of TDR measurements. Three methods of field calibration were investigated and the results compared with a factory supplied calibration. When compared to the factory calibration, all three field calibration methods improved the measurement of soil water content, with a site-specific linear regression method providing the most accurate results. It can be concluded from this work that measured dielectric data should be calibrated to the water content of the actual soil involved for determining absolute water content, otherwise the measured soil water content should be considered in relative terms.

Based on the results of this study, Method 2 was chosen as the primary field calibration technique for determining soil water content from TDR time delay data in the LWRW. This choice was based on the fact that Method 2 consistently showed the smallest error for site-specific analysis in comparison to the other methods described (Table 2.2). However, Method 3 or 4 could also be used under certain circumstances, with either being a better alternative than the factory calibration (Method 1). Because Methods 2, 3, and 4 are all derived in a simple manner from a common set of samples, it would be easy for the researcher to decide which calibration technique works best for the soils in their study.

As a product of the work presented in this chapter, an example set of calibrated TDR profile soil moisture data is shown in Fig. 2.5 for site LW02 during the SGP97 Hydrological Experiment. The TDR data have been field calibrated according to Method 2. Also plotted are the 0-5cm surface soil moisture data that were collected during the study as ground-truth for microwave radar calibration. The surface moisture data represents an average of nine soil samples collected daily near the TDR probes. The differences in moisture content between the 0-5 cm surface layer and the 0-15 cm TDR layer can be considerable due to rainfall events during the 30-day study (Fig. 2.5). As would be expected, the surface data are more responsive and dynamic than the 0-15 cm layer, although both approach the same value during three of the events. The TDR data show that soil moisture increases with depth and that the water content for the three deepest layers is relatively constant, perhaps a consequence of an argillic horizon (Table 2.1).

The *z*-statistics (n =148) for the three field calibration methods were well below the critical value (z_{crit}= 1.960) using a significance level = 0.05 and a two-tailed test. The *z*-test for Method 1 (factory calibration) resulted in a value of 1.644 which is only slightly below the critical value. However, all *z*-statistics support the hypothesis that no evidence exits to suggest that the population means, for any one method, are different in comparison to the mean of the soil-core data.

The results of this work demonstrate that use of a simple linear relationship between soil water content and TDR time delay output, provides an easy means for obtaining site-specific field calibrations. The results show, at nine field sites with different soil physical properties, that use of a site-specific linear regression approach reduces measurement error, as well as the range of error, when compared to soil moisture values obtained using the factory calibration. It was also determined that in collecting soil moisture samples for the regression analysis, it is important that the data set include very low moisture samples in order to determine absolute water content. It should be emphasized that great care should be taken during the collection of soil samples in an effort to minimize sample error. For example, a small error in the measurement of bulk density can have considerable effects on calculating the volumetric water content. Although the techniques used in this study do not directly attempt to discern the effects of soil texture and bulk density on TDR calibration, the data presented here, in addition to that being collected at new probe sites within the watershed, should provide the data necessary to address such issues in future work.

2.3 MEASUREMENTS OF SOIL PHYSICAL AND HYDRAULIC PROPERTIES

Knowledge of the hydraulic properties of soil is essential to understanding and modeling of soil moisture dynamics. The ability of the soil in the vadose zone to conduct or retain water is a function of its hydraulic properties. The basic soil hydraulic properties and characteristic functions that govern the flow of water in soils are soil hydraulic conductivity as a function of soil water content $K(\theta)$ or matric suction $K(h)$ and soil water content as a function of matric suction $\theta(h)$, commonly referred to as the soil water characteristics curve (Hillel, 1980; Ahuja and Nielsen, 1990). These hydraulic properties depend on the pore size distribution, which is, in turn, affected by soil texture and structure (Ahuja et al., 1976; Paige and Hillel, 1993). In order to model the movement of water in the soil profile, either measurements or estimates of the hydraulic properties are required. Although measured soil hydraulic properties are preferable, RZWQM provides an option for estimating these properties and their relationships if data are not available. Techniques used in this study to measure the soil physical and hydraulic properties in the laboratory and field are described below.

Field Experiments

Soil hydraulic properties at each of the five field sites were measured *in situ* using the instantaneous profile method (Hillel, 1980). According to a comparative study by Paige and Hillel (1993), the instantaneous profile method is the most effective method for determining soil hydraulic properties *in situ*. The method involves gravimetric soil sample analysis, double-ring infiltrometry, and tensiometric data analysis. It is based on the Darcian analysis of *in-situ* tensiometric measurements during infiltration and the subsequent drainage, using the water content-matric pressure relationship (Richards et al., 1956; van Bavel et al., 1968). The soil water content-matric pressure relationship can be obtained by periodic measurement of soil water content during the drainage phase by gravimetric, neutron thermalization, TDR, or gamma-ray attenuation techniques.

The instantaneous profile method involves measuring the rate of water entering the soil surface and the changes in soil water potential with depth and over time using tensiometers. A double-ring infiltrometer with two concentric metal rings having diameters of approximately 90 cm and 50 cm, respectively, were co-located with tensiometers placed at depths of 15, 30 and 60 cm in the soil profile located just outside the inner ring. The rings were driven into the soil approximately 10 cm leaving approximately 20 cm of ring above the soil surface. The rings were completely filled with water the day before measurements began to pre-wet the soil. By pre-wetting the soil, sufficient wetting to at least a depth of 1 meter is more easily and readily obtained on the day measurements begin. On the day of measurement, water was carefully ponded in the rings with the change in water level over time observed. Once the rate of change became constant, the vertical flux of water in the profile was assumed to be at steady state. At this time the hydraulic conductivity in the zone of constant matric potential is said to be numerically equal to the flux density of water and thus a value of saturated conductivity was obtained. Tensiometric readings were taken at this time as a check on unit gradient conditions and saturated water content. The rings were then covered to minimize evaporation and protect the area from rainfall. In this data set, tensiometric data and gravimetric soil samples were obtained from each site to determine matric potential and soil water content, respectively, 4 to 6 days during the drainage phase.

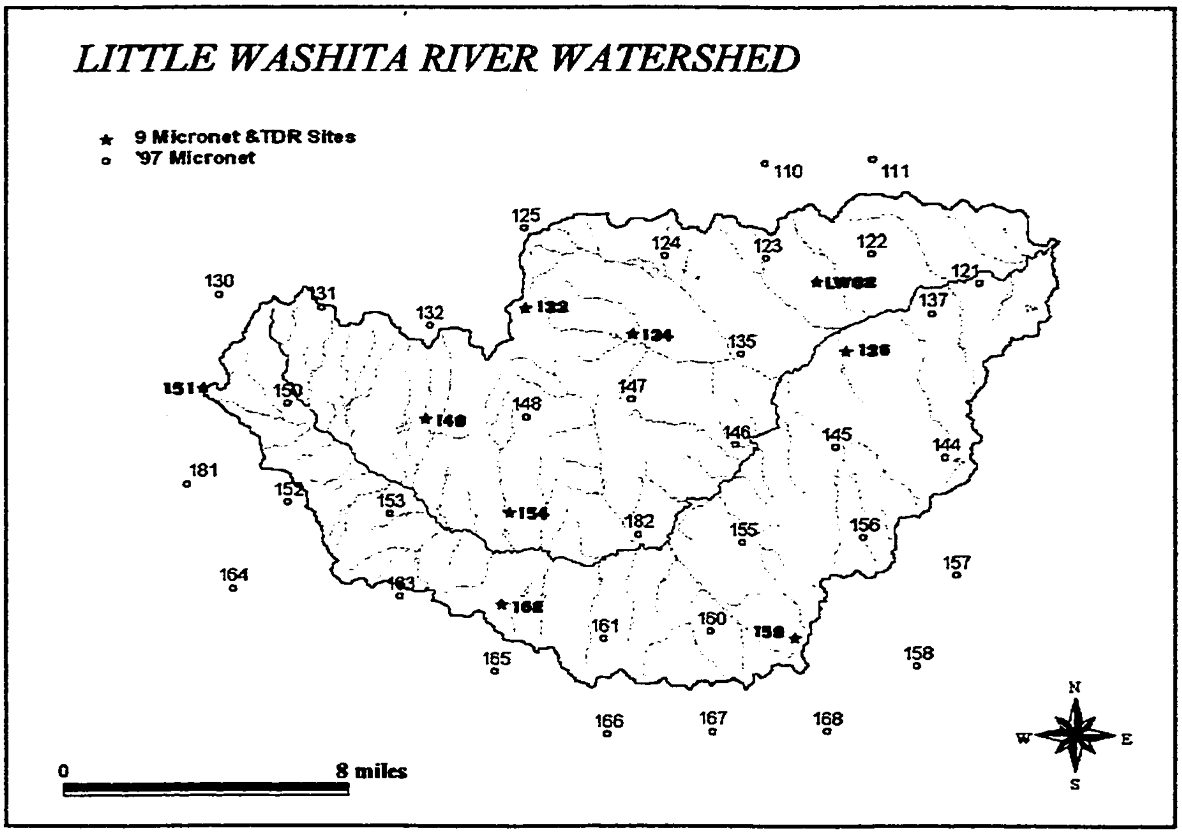
Laboratory Methods

Selected soil physical and hydraulic properties were determined at each site to a depth of at least 60 cm in 15 cm intervals. Soil cores were extracted from the site using a soil-core sampling tool having a 15 cm long barrel with a 5 cm inside diameter. Care was taken to minimize compaction during sampling. Each soil core was divided into 7.5 cm long subsamples. One subsample was used to determine soil texture using the hydrometer method (Day, 1965). The remaining subsample was used to determine the soil water characteristics using the procedure given in Ahuja et al. (1985). Bulk density and θ_v at saturation and at 1, 5, 10, 20, 33, 100, 500, 1000, and 1500 -kPa were determined for each 15 cm interval in the profile.

2.4 APPLICATIONS

Accurate measurement of profile soil water content is essential to many areas of environmental research. It is a key component to many practical considerations regarding agricultural and water resource management. In this study four calibration methods were evaluated for determining volumetric profile soil water content from time domain reflectometry (TDR) data at nine locations within the Little Washita River Watershed (LWRW) in south central Oklahoma. Comparisons were made between soil water content as determined by the factory calibration, two methods of site-specific calibration, and a general calibration technique. Values of soil water content determined by each calibration method were compared to the actual soil-core water content data taken at the time of calibration, as well as to an independent collection of soil-core samples. All field calibration methods show that it is necessary to include very low water content data in determining absolute water content. When compared to the factory calibration, all three field calibration methods improved the measurement of soil water content, with Method 2 providing the most accurate results.

Figure 2.1. Map of LWRW nine TDR sites and *Micronet* locations.



Figures 2.2 a - d.

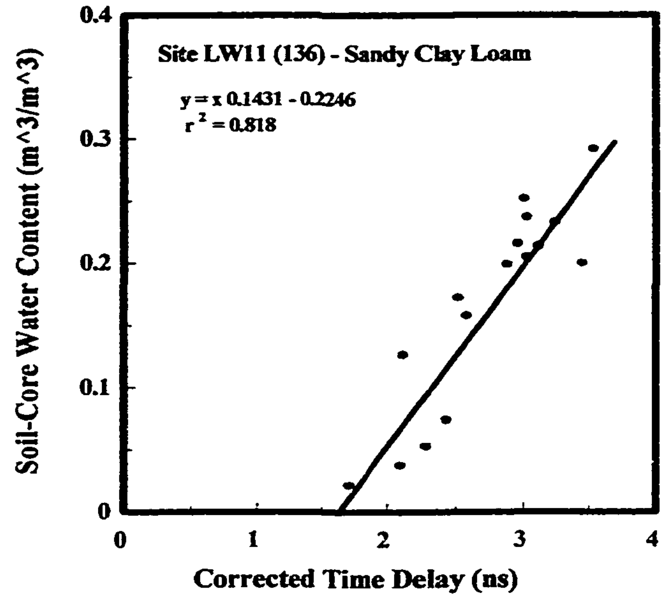


Figure 2a. Calibration data set linear regression.

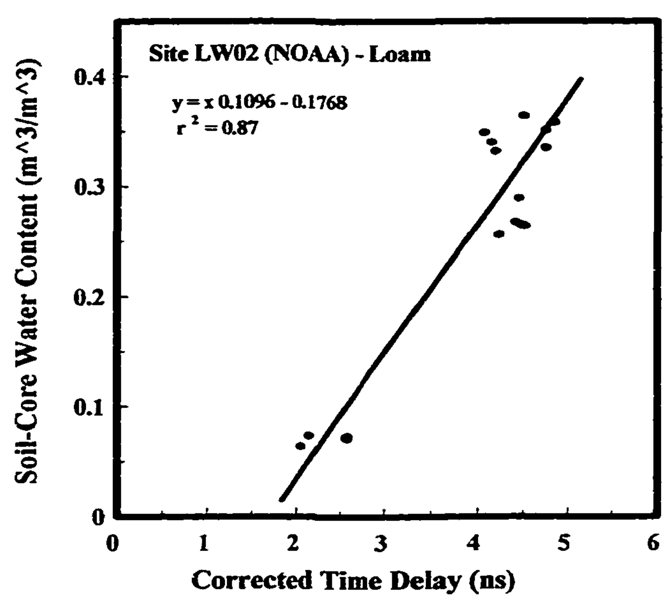


Figure 2b. Calibration data set linear regression.

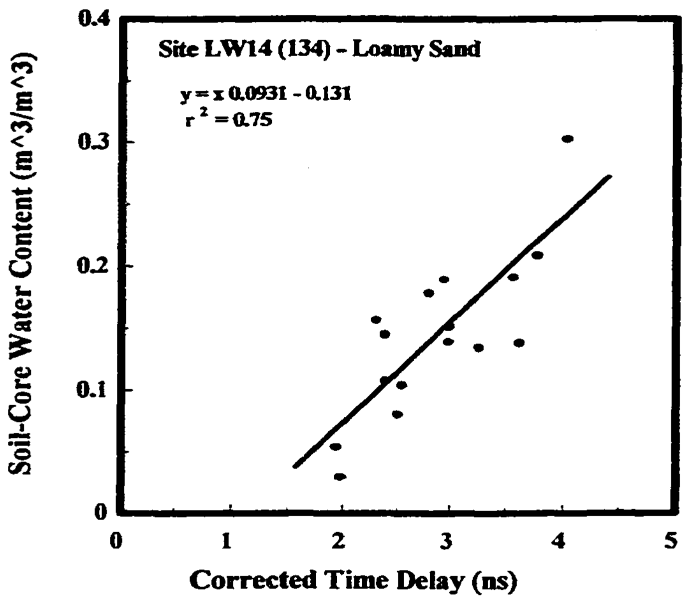


Figure 2c. Calibration data set linear regression

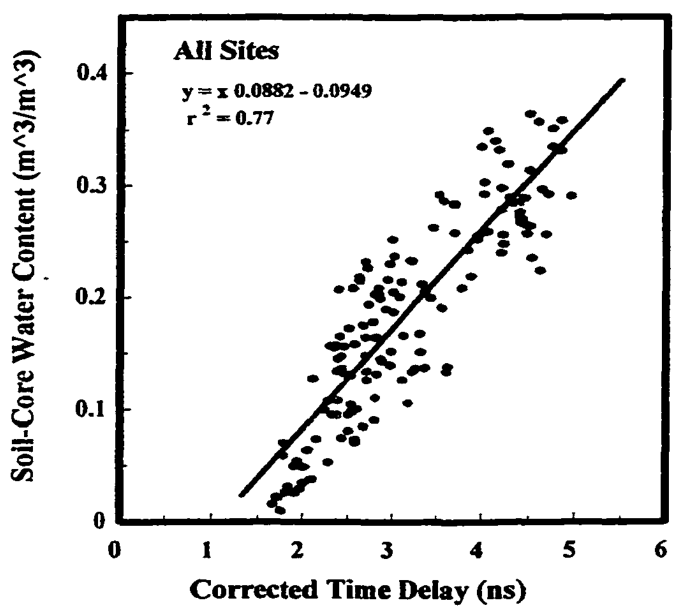


Figure 2d. Calibration data set for linear regression.

Figures 2.3 a - d.

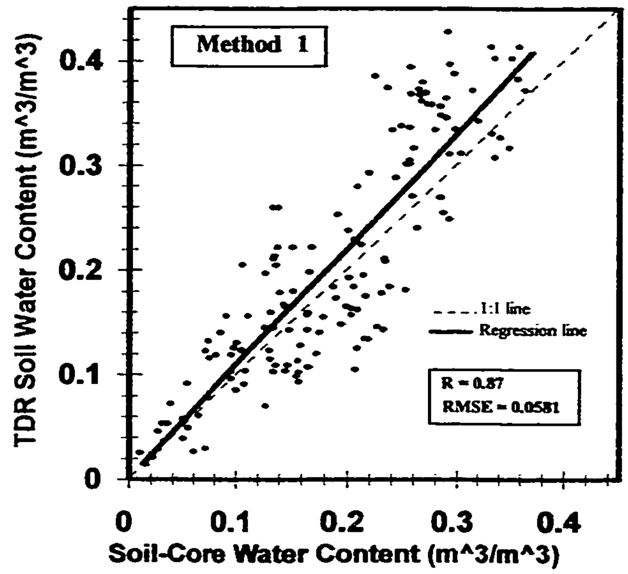


Figure 3a. Comparison of soil-core vs TDR volumetric water content at 9 sites using sample calibration data.

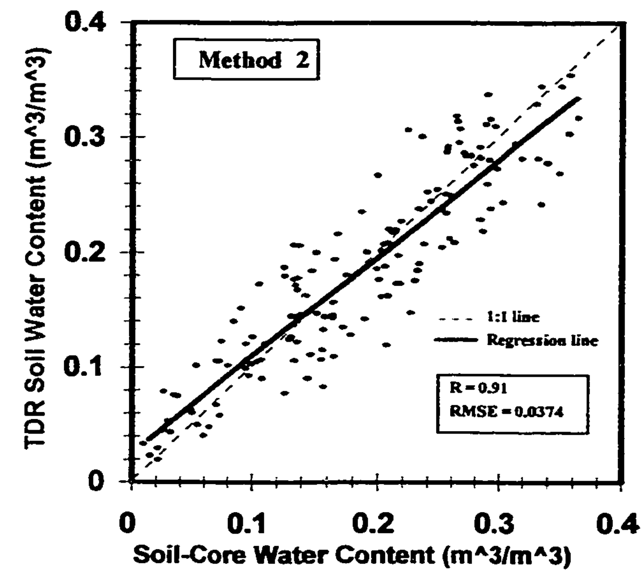


Figure 3b. Comparison of soil-core vs TDR volumetric water content at 9 sites using sample calibration data.

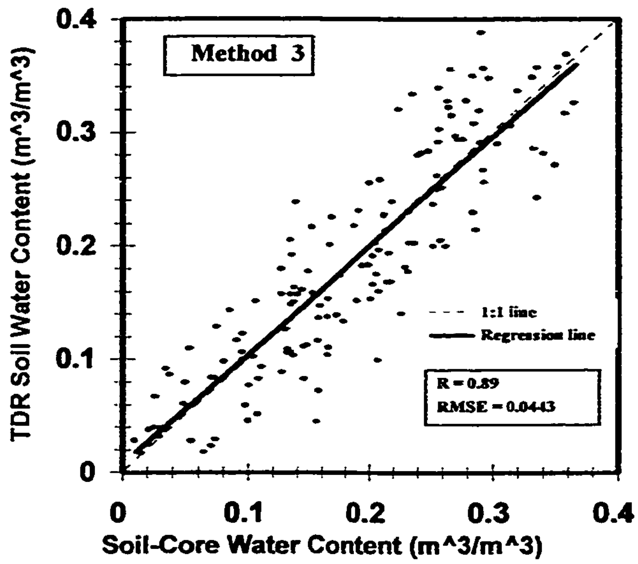


Figure 3c. Comparison of soil-core vs TDR volumetric water content at 9 sites using sample calibration data.

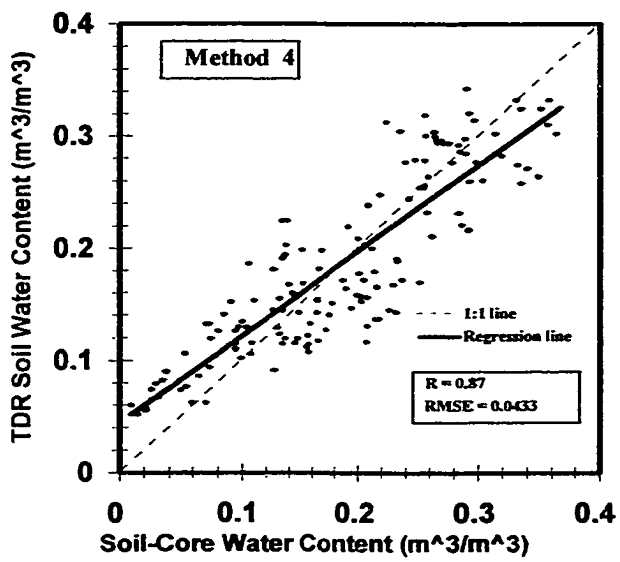


Figure 3d. Comparison of soil-core vs TDR volumetric water content at 9 sites using sample calibration data.

Figures 2.4 a - d.

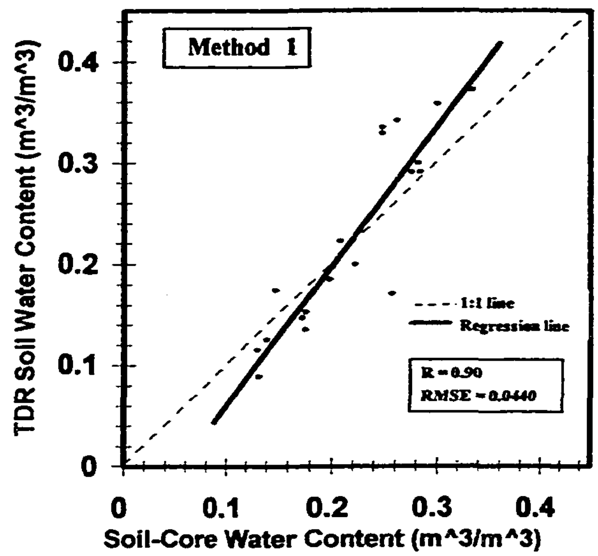


Figure 4a. Comparison of soil-core vs TDR volumetric water content at 9 sites using independent sample data.

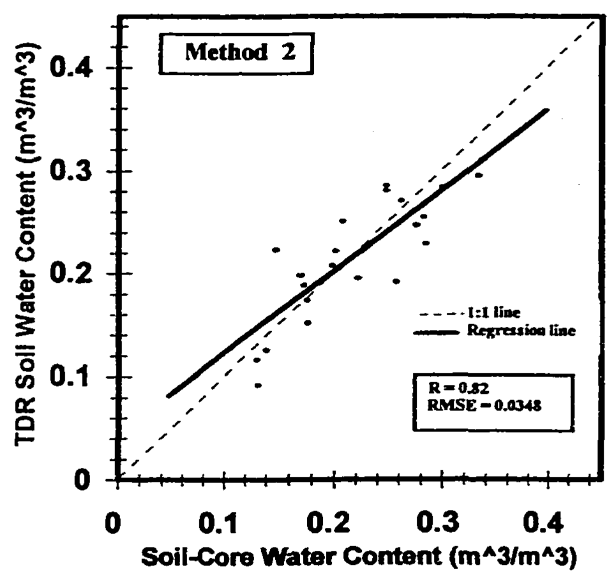


Figure 4b. Comparison of soil-core vs TDR volumetric water content at 9 sites using independent sample data.

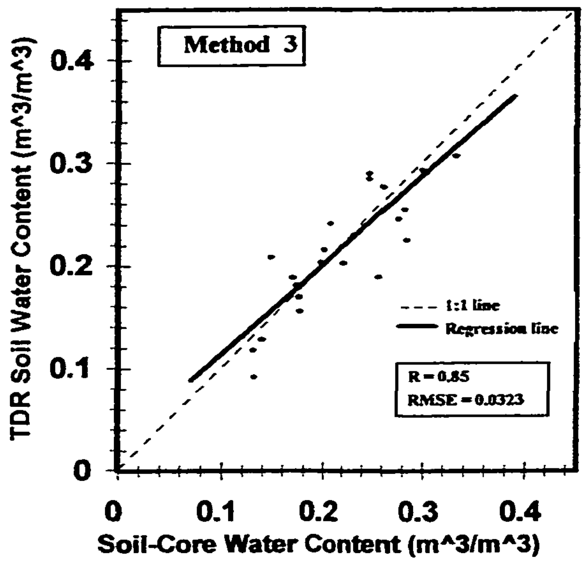


Figure 4c. Comparison of soil-core vs TDR volumetric water content at 9 sites using independent sample data.

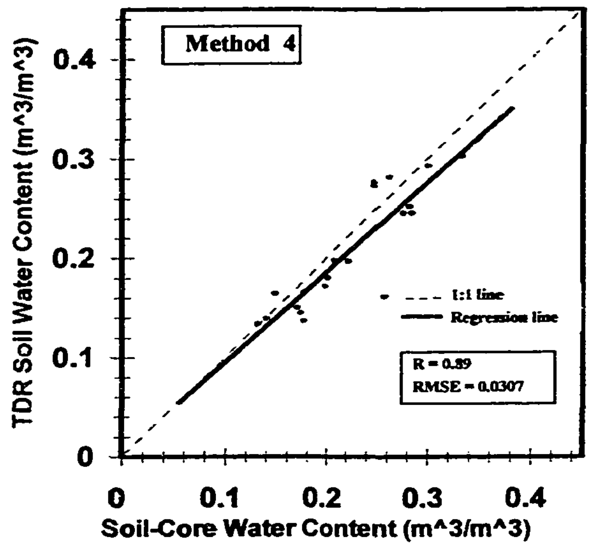


Figure 4d. Comparison of soil-core vs TDR volumetric water content at 9 sites using independent sample data.

Figure 2.5. Measured TDR profile soil water content at site LW02 during SGP97.

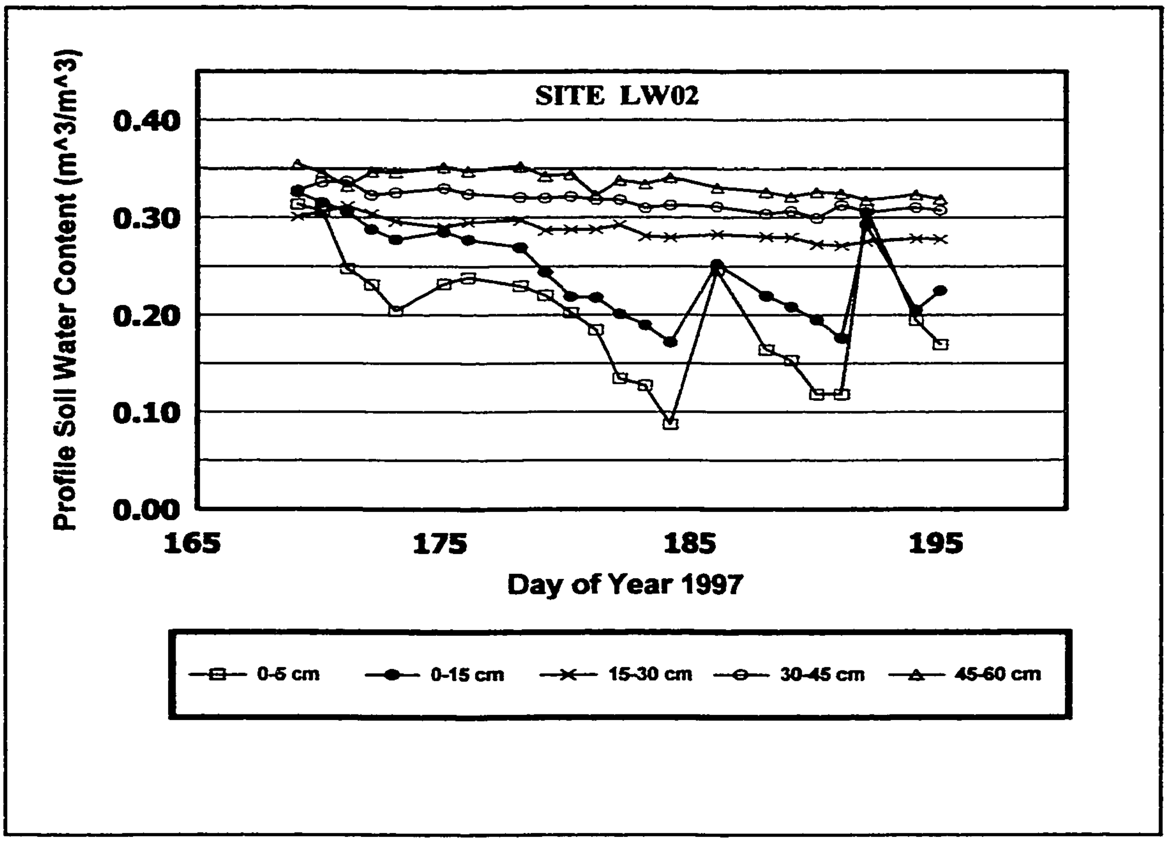


Table 2.1. Soil physical properties at nine study sites in the LWRW.

Site ID	Depth	Sand	Silt	Clay	Texture Name[1]	Bulk Density
	(cm)	----------	%	---------		-----g/cm³----
133	0-15	70.8	19.6	9.6	SL	1.41
	15-30	72.8	17.6	9.6	SL	1.43
	30-45	70.8	17.6	11.6	SL	1.45
	45-60	68.8	19.6	11.6	SL	1.38
134	0-15	77.2	17.6	5.2	LS	1.45
	15-30	79.2	15.6	5.2	LS	1.43
	30-45	81.2	11.6	7.2	LS	1.41
	45-60	79.2	13.6	7.2	LS	1.42
136	0-15	50.8	35.6	13.6	L	1.37
	15-30	54.8	25.6	19.6	SL	1.42
	30-45	52.8	26.0	21.2	SCL	1.41
	45-60	48.8	25.6	25.6	SCL	1.44
149	0-15	29.2	53.6	17.2	SiL	1.47
	15-30	25.2	53.6	21.2	SiL	1.41
	30-45	25.2	49.6	25.2	L	1.48
	45-60	25.2	47.6	27.2	CL	1.46
151	0-15	74.4	17.2	8.4	SL	1.37
	15-30	80.4	11.2	8.4	LS	1.47
	30-60	86.4	7.2	6.4	LS	1.32
	45-90	84.4	9.2	6.4	LS	1.46
154	0-15	36.8	37.6	25.6	L	1.43
	15-30	46.8	25.6	27.6	SCL	1.42
	30-45	48.8	21.6	29.2	SCL	1.44
	45-60	50.8	21.6	27.6	SCL	1.39

Table 2.1 (Cont.)

Site ID	Depth	Sand	Silt	Clay	Texture Name[¶]	Bulk Density
	(cm)	---------	%	--------		-----g/cm^3----
159	0-15	78.8	8.7	12.5	SL	1.31
	15-30	77.8	9.7	12.5	SL	1.33
	30-45	76.8	9.7	13.5	SL	1.30
	45-60	78.8	8.7	12.5	SL	1.32
162	0-15	62.4	15.2	22.4	SCL	1.33
	15-30	62.4	19.2	18.4	SL	1.38
	30-45	58.4	23.2	18.4	SL	1.33
	45-60	60.4	21.2	18.4	SL	1.35
LW02	0-15	28.4	45.2	26.4	L	1.53
	15-30	24.4	47.2	28.4	CL	1.49
	30-45	26.4	47.2	26.4	L	1.54
	45-60	26.4	53.2	20.4	SiL	1.54

[¶]Symbols used in the texture name category are as follows: S = sand(y), L = loam(y), Si = silt, C = clay.

Table 2.2. Statistical data analysis for different calibration methods.

Site ID	Calibration Method							
	Method 1		Method 2		Method 3		Method 4	
	RMSE	ME	RMSE	ME	RMSE	ME	RMSE	ME
	---------- m^3/m^3 ----------							
Site-Specific Data								
133	0.0499	-0.0351	0.0341	-6.59E-05	0.0363	-1.62E-04	0.0513	-0.0275
134	0.0510	0.0218	0.0389	-7.95E-03	0.0461	4.12E05	0.0401	0.0141
136	0.0402	-0.0172	0.0340	-2.12E-04	0.0351	-4.39E-05	0.0486	-0.0210
149	0.0696	0.0401	0.0422	-9.69E-04	0.0568	-4.7E-06	0.0425	0.0013
151	0.0317	-0.0013	0.0314	-9.84E-05	0.0317	0.0013	0.0349	0.0242
154	0.0775	0.0647	0.0399	5.16E-05	0.0427	-6.02E-05	0.0437	0.0103
159	0.0540	0.0063	0.0388	-8.26E-03	0.0537	4.7E-06	0.0396	-0.0104
162	0.0732	0.0544	0.0366	6.26E-03	0.0490	-5.3E-06	0.0433	0.0228
LW02	0.0641	0.0460	0.0405	-4.39E-05	0.0432	-4.89E-04	0.0453	-0.0022

Table 2.2 (Cont.)

Site ID	Calibration Method							
	Method 1		Method 2		Method 3		Method 4	
	RMSE	ME	RMSE	ME	RMSE	ME	RMSE	ME
	---------- m^3/m^3 ----------							
Combined Calibration Data (9 Sites)	0.0581	0.0194	0.0374	-1.22E-03	0.0443	9.24E-05	0.0433	-3.25E-05
Combined Independent Data (5 Sites)	0.0439	6.5E03	0.0349	-3.3E-03	0.0323	-4.1E-03	0.0307	-0.014

3. USE OF LIMITED SOIL DATA INFORMATION AND SOIL WATER MODELING

3.1 INTRODUCTION

An efficient means for assessing the impact of alternative agricultural management strategies on the quality of water resources and the environment is the interactive use of selective experimentation and computational modeling. For example, assessments can be made of climate change and its effect on watershed hydrology, as well as rangeland production using such an interactive approach. Once verified and evaluated, a model can be an effective research tool that provides an enhanced view of specific problem interactions than what might be afforded by direct experimentation. The recently developed Root Zone Water Quality Model (RZWQM), Version 3.2, is an example of such a tool (RZWQM Team; 1992, 1995, 1998)

The RZWQM is a comprehensive, one-dimensional model that integrates physical, biological, and chemical processes to simulate plant growth and predict the effects of agricultural management practices on the movement of water and chemicals through the root zone. The model was recently calibrated and evaluated at five Management Systems Evaluation Areas (MSEA) located in the upper Midwest of the U.S. and at two sites in Colorado (Hanson et al., 1999). Each of the studies evaluated the performance of the RZWQM for cropping and management conditions important in their respective regions (Martin and Watts, 1999; Farahani at al., 1999; Ghidey et al., 1999; Jaynes and Miller, 1999; Landa et al, 1999). An iterative approach for calibrating the model was followed in order to match the predicted and observed results for soil water, nitrogen, and plant growth. Each MSEA site had different types of data with which to parameterize the model, as well as the required 'minimum input' data set. Predictions were found to match the observed data in most cases.

The hydraulic description of the soil in the RZWQM forms the cornerstone of the model's ability to interact with all the other components of the system. The primary focus of this work was to examine how different soil hydraulic descriptions may affect model estimates of profile soil water content. In order to simulate the hydrologic responses of the model, the soil profile is divided into individual soil horizons or layers. The model requires an adequate description of the physical and hydraulic soil properties for each of these horizons. Physical soil properties include fraction of sand, silt, and clay, as well as bulk density and porosity. Levels of hydraulic soil properties accepted by the RZWQM may range from the volumetric water content at 1/3 or 1/10 bar (-33 kPa and -10 kPa, respectively) and saturated hydraulic conductivity (minimum input data), to a 'full description' of all the necessary parameters to characterize the Brooks and Corey soil-water relationships (Brooks and Corey, 1964). If only the minimum input data are available, RZWQM has a subroutine that estimates all other necessary model parameters.

The use of a minimum data set is appealing since it is seldom that a full description of a given soil's physical and hydraulic properties is readily available. Further, the RZWQM may be used in studies where it is impractical to perform the field and/or laboratory work necessary to fully describe a soil's physical and hydraulic properties. Thus, supplying the model with a minimum data set has several advantages, provided the model adequately simulates the hydrologic system and in particular, gives satisfactory estimates for profile soil water content. The minimum data set may be further reduced to serve as a 'limited input' data set, as might be the case when using limited soil survey data. Modeled output for the limited case could then be compared to simulations using more detailed input which may provide information about a threshold level of input data required to obtain estimates within an allowable range of measured values.

Often laboratory and field measurements of a given soil property do not necessarily correspond. This lack of correspondence may be due to differences in sample size, measurement and sampling procedures, differences between measurements on a disturbed soil core compared to those made *in situ* (undisturbed), or the differences may reflect spatial variability of the soil which may not be adequately captured by a point sample. Laboratory and field measured hydraulic properties may also indicate differences between layer-specific measurements and data that are more representative of 'average' profile conditions, respectively, such as the case for hydraulic conductivity values. Thus, considering the time required for certain laboratory analyses, it would be of practical significance to determine the effect of using soil hydraulic input data derived from standard laboratory analyses versus those obtained by relatively simple *in situ* techniques.

The objectives for this chapter are (1) to evaluate estimates of profile soil water content using minimum versus limited input data sets, (2) to assess the performance of the model for the minimum data set where input data were derived from either laboratory or *in situ* analyses, and (3) to evaluate the need for model calibration since calibrated model parameters are seldom transferable to other experimental conditions. In contrast to the MSEA agricultural study sites located in the upper Midwest, this study was conducted on various soil types under rangeland conditions within the Southern Great Plains of Oklahoma. Spaeth et al. (1996) stated that rangelands comprise over 60% of the land area of the 48 contiguous states, and that agricultural, industrial, recreational and municipal water supplies in many areas of the U.S. are linked directly to rangeland watershed management. Taking into consideration the increased competition for available water supplies, a model such as RZWQM could be modified and used to quantify soil water resources over large land areas, such as rangelands, to further aid in the efficient management of our nations water resources and watersheds.

3.2 MODEL OVERVIEW

The RZWQM consists of six sub-components that integrate physical, biological, and chemical processes to simulate plant growth and the movement of water, nutrients, and pesticides in the root zone (Ahuja et al., 1999). Detailed descriptions of the operation of the RZWQM and its process components can be found in Ahuja et al. (1999) and RZWQM Team (1992, 1995, 1998). Of main importance here is the physical process component that includes a number of interrelated hydrologic processes. The present research focuses on this component since it controls the simulation of infiltration and redistribution of water in the soil matrix and thus, predicts the profile soil water content.

The physically-based nature of RZWQM requires that the user provide a rather extensive amount of data to adequately parameterize and initialize the model. At a minimum, RZWQM requires the usual driving variables of meteorological data (daily minimum and maximum air temperature, solar radiation, relative humidity, wind speed, and rainfall or irrigation), coupled with specific site and soil profile descriptions (physical and hydraulic properties, soil horizons, surface residue cover, and crop specifications). To facilitate use of the model, RZWQM allows for input options where certain parameters are estimated or obtained from default value tables when measured values are not available (described below). In particular to this study, are the 'soil hydraulics data input options' where the user may chose either the 'minimum input' or 'full description' mode. For this work we have chosen the minimum input mode using different types and combinations of soil physical/hydraulic input data for a given scenario.

Infiltration of water into the soil is simulated by a modified Green-Ampt approach (Green and Ampt, 1911; Ahuja et al., 1993; 1995), whereas redistribution of water in the soil matrix is simulated by a mass-conservative numerical solution of the Richard's equation (Ahuja et al., 1999). The Green-Ampt equation for infiltration is:

$$V=K_s\frac{\tau_c+H_o+Z_{wf}}{Z_{wf}} \qquad [3.1]$$

where V = infiltration rate at any given time (cm hr-1), K_s = effective average saturated hydraulic conductivity of the wetting zone (cm hr-1), τ_c = capillary drive or suction head at the wetting front (cm), H_o = depth of surface ponding (cm), and Z_{wf} = depth of the wetting front (cm). The Richard's equation for soil water redistribution between rainfall events is:

$$\frac{\partial\theta}{\partial z}=\frac{\partial}{\partial z}[K(h,z)\frac{\partial h}{\partial z}-K(h,z)]-S(z,t) \qquad [3.2]$$

where θ = volumetric soil water content (cm3 cm^{-3}), t = time (hr), z = soil depth (cm), h = soil-water pressure head (cm), K = unsaturated hydraulic conductivity (cm hr^{-1}), and $S(z,t)$ = sink term for root water uptake (hr^{-1}). The Green-Ampt and Richards equations require hydraulic properties (saturated and unsaturated hydraulic conductivity, respectively) of the soil, but often these hydraulic properties are not known and must be estimated.

The RZWQM provides two optional approaches for estimating unknown soil hydraulic parameters used to derive the basic relationships necessary for modeling soil water flow (i.e., soil water content and unsaturated hydraulic conductivity as functions of matric suction, θ (h) and K (h)), respectively. The approaches are based on slightly modified forms of the Brooks-Corey (1964) functions which are described as Methods 1 and 2 below.

Method 1 - Hydraulic Property Estimation

RZWQM provides estimates of all hydraulic properties based on simpler and limited known soil properties of soil texture, bulk density, and 1/3 or 1/10 bar soil water content, where the θ (h) relationship is first estimated by the extended similar-media scaling technique (Warrick et al., 1977 ; Ahuja et al., 1985; 1988) using the textural-class mean values of Rawls et al. (1982). Ahuja et al. (1985) compared this method with five other approaches (largely based on the work of Rawls et al., 1982 and 1983) to estimate soil water characteristics, (θ (h) from limited data), concluding that the estimated soil water characteristic curves based on either known bulk density and two water content-suction values (i.e., 1/3 and 15 bar values) or one water content-suction value (1/3 or 1/10 bar) and bulk density gave satisfactory results. The latter model, the extended similar-media concept, is utilized by RZWQM. While this method of estimating soil-water characteristics requires reliable estimates or measures of bulk density and 1/10 or 1/3 bar water content as a minimum, the potential uncertainties in final characteristic curves due to errors in input parameters are not well understood.

Saturated hydraulic conductivity (Ks) is estimated using an empirical function (a modified form of the Kozeny-Carmen equation) describing Ks as a power function of effective porosity (φ_e). The method is based on the experimental studies of Ahuja et al. (1988), in which effective porosity is defined as saturation water content (θs) minus the 1/3 bar water content. The equation is written as,

$$Ks = 764.5\ \varphi_e^{\ 3.29} \qquad [3.3]$$

where Ks is in cm hr^{-1}, and φ_e is given in cm^3 of pores per cm^3 of bulk soil. Considering the magnitude of errors involved with field-measured Ks due to the presence of macropores and air entrapment, the proposed equation has shown promise (Ahuja and Hebson, 1992).

The unsaturated conductivity-suction relationship, K(h), is then estimated by utilizing the approximate capillary-bundle approach of Campbell (1974), given Ks and $\theta(h)$ functions. Campbell concluded that the agreement between K(h) and measured values for five soils is at least as good as with other procedures such as that by Millington and Quirk (1959).

Method 2 - Hydraulic Property Estimation

If both soil bulk density and 1/3 or 1/10 bar water content are unknown, the model utilizes a compiled list of average values (Soil Hydraulic Parameter Default Values) for all hydraulic parameters based on soil texture alone (Rawls et al., 1982). This popular method of gross estimation of hydraulic parameters based on soil texture is more applicable to large scale studies with broad textural groups where the differences in textural groups may be much larger than the errors in estimation of their hydraulic parameters (Ahuja et al., 1985). Method 2 represents the case of limited input data.

3.3 MODEL SCENARIO DESCRIPTION AND DATA INPUT

In this research, five basic scenarios were used to initialize the physical and/or hydraulic properties for each soil layer in the RZWQM and are discussed below. These scenarios where chosen based on the amount and type of input data. Five study sites (described later) were used to evaluate these scenarios. An additional scenario (RZS7) was used in an effort to match model θ_v estimates to measured θ_v by adjusting the 1/3 bar θ_v or Ks input parameters. Scenario RZS7 is essentially the same as scenario 1 (RZS1) with the exception of hydraulic parameter adjustments that are defined later in this section. The type of input format for each scenario was selected to investigate the influence of soil type, soil layering, levels of input data, and soil properties obtained from the field verses those measured in the laboratory on model estimates of profile soil water content. Soil properties measured in the field, *in situ*, were considered to be more representative of average profile values, whereas laboratory measurements provided more detailed layer descriptions, especially in the case of conductivity values. To maintain consistency in the calculation of effective porosity throughout the scenarios, all input data for texture and bulk density were taken from lab soil-core analysis. However, such data could also be obtained from different types of survey information for a given soil type, i.e., county soil surveys, Statsgo, or Miads. Also, soil samples collected in the field during infiltration and drainage experiments to measure soil water content could have been used to determine texture class and bulk density.

In scenario RZS1 the model is supplied only the soil textural-class name. According to the texture class, the model uses soil physical and hydraulic default values as input for particle size fraction, bulk density, porosity, θ_v at 1/3 bar, and Ks (Method 2 estimation technique). In scenario RZS2 the model is supplied site-specific, lab-measured particle size fraction and bulk density values for each layer, from which the model then derives soil texture and assigns the corresponding 1/3 bar θ_v default values. Ks is estimated according to Method 1 described earlier by Eq. 3.3. Porosity is calculated from measured bulk density and assumes a value of 2.65 g cm^{-3} for particle size density. Scenario RZS3 is the same as RZS2 with the exception that 1/3 bar θ_v is explicitly specified and was measured in the laboratory on soil cores. Again, hydraulic conductivity functions are calculated according to Method 1. Scenario RZS4 is the same as RZS3 but θ_v at 1/3 bar was measured *in situ* based on two-day drainage data taken at each site during infiltration experiments. In scenarios RZS1 through RZS4, soil properties were specifically described for each soil layer utilized by the model.

In scenario RZS5, the model is supplied texture name and field measured values of

θ_v at 1/3 bar and Ks. θ_v at 1/3 bar for different soil layers bar was assumed to be the water content sampled 2 days after saturated conditions. Matric potential was measured using tensiometers placed at different depths in the soil profile and served as a check for 1/3 bar conditions at the time of sampling. Ks was considered an average for the soil profile and thus, constant for all soil layers. Scenario RZS5 was included in this study since it seeks to mimic soil properties that might be derived from remotely sensed data. Scenario RZS5 also provides an alternative to using soil hydraulic data obtained from more intensive laboratory methods. In all scenarios, the model was supplied the minimum required soil, vegetation and meteorological data and was run without benefit of prior calibration.

As mentioned previously, an additional scenario (RZS7) was evaluated in this phase of modeling in an attempt to minimize the difference between modeled and measured values of θ_v by conditioning or calibrating model hydraulic input parameters. According to previous RZWQM testing in the literature, this is best accomplished by adjusting either the 1/3 bar θ_v values or Ks (Wu et al., 1999; RZWQM Team, 1998). Because the model estimates Ks from 1/3 bar θ_v, a low (RZS7) and high (RZS7b) value of 1/3 bar θ_v was selected as input at sites 133 and 154 due to the differences between soil texture at these sites. The same value for 1/3 bar θ_v in RZS7b was used in RZS7a, but Ks was manually input using a much higher value compared to the model estimate in RZS7b.

Four soil layers were specified in the model for each site except for site 151 where a 5-segment TDR probe had been installed. Each soil layer was 15 cm thick, except at site 151 where the third, fourth and fifth layers were 30 cm thick. These thicknesses were chosen to correspond to soil water content measurements made with a profiling TDR instrument (described below). Initial soil water contents required by the model were taken from TDR measurements at each study site. Daily profile soil water averages of θ_v from RZWQM output were calculated and compared to measured values.

Plant water uptake is accounted for in the RZWQM according to plant species utilizing a generic plant growth and crop production submodel. Although a number of agricultural crops are available to choose from in the model, options for rangeland vegetative species, at this time, are rather limited. The 'quick turf' management option was chosen in this study so that plant species could be selected which more closely approximate the vegetative conditions at the study sites. Where applicable, the species of grass chosen was bermudagrass. Some sites had so little vegetative cover that no plant type was specified.

3.4 STUDY FIELD SITES

Five *Micronet* sites were selected (Fig.3.1) for use in this chapter based on the availability of measured soil properties and soil water content at the site, and differences in soil texture and vegetative cover. Three of the five study sites had a relatively dense vegetative cover of bermudagrass (*Cynodon dactylon*). Vegetative cover at the other study sites consisted of a mix of big bluestem (*Andropogon gerardii*), little bluestem (*Schizachyrium scoparium*), switchgrass (*Panicum virgatum*) and indiangrass (*Sorghastrum nutans*) and ranged from sparse to moderate cover. Vegetative and soil characteristics of each site are listed in Table 2.1.

Five of the nine TDR calibration sites were selected for the research in this chapter. Each probe consisted of four 15 cm long segments, enabling measurements of θ_v down to 60 cm. At site 151 a 5-segment TDR probe was used reaching to a depth of 120 cm, in segments of 0-15, 15-30, 30-60, 60-90, and 90-120 cm. To coincide with available soil property data, readings from only the first four segments were used in this work. The TDR probes were calibrated in situ against site-specific gravimetric and bulk density data. The TDR probes were usually read once each day, depending on weather conditions and available personnel, between 0800 and 1000 hrs local time, during the June 18 - July 16, 1997 study period.

3.5 STATISTICAL METHODS

To evaluate the overall correspondence of model output to measured values of soil water content, the use of standard statistical measures of the standard deviation (s),correlation coefficient (r), coefficient of variation (r^2), root mean square error (*RMSE*), mean bias error (*MBE*) and mean relative error (*MRE*) have been calculated. *RMSE*, *MBE*, and *MRE* were calculated as:

$$RMSE = \sqrt{\frac{\Sigma(P-O)^2}{n}} \qquad [3.4]$$

$$MBE = \frac{\Sigma(P-O)}{n} \qquad [3.5]$$

$$MRE = \frac{\Sigma(P-O)100}{n} \qquad [3.6]$$

where P is water content predicted by the model, O is the observed soil water content and n is the number of observations. The correlation coefficient (r) represents a measure of the strength of the relationship between predicted θ_v and observed measurements, whereas the *MBE* and *RMSE* are indicative of bias and error, respectively.

3.6 RESULTS AND DISCUSSION

The results of this study demonstrate that average profile soil water content may be adequately modeled using very limited soils data information as input in the RZWQM, e.g., scenario RZS1 (texture name only).Considering both the *RMSE* and *MRE* statistics at all five sites (Table 3.3), RZS1 provided the best estimates of profile θ_v with statistical values ranging from 0.013 to 0.019 m^3m^{-3} and 10.32 to -1.54 %, respectively. Though not quite as good overall, the results from scenarios RZS4 and 5 were closer to measured values at some sites compared to RZS1, but also showed that use of field measured hydraulic properties as model input provided better estimates of soil water content than using properties obtained in the laboratory. Both these findings are substantial in regards to: 1) considering the amount of soils data that is usually available to the analyst and, 2) the time that can be saved by avoiding detailed laboratory analysis to determine soil water characteristics.

Figures 3.2 through 3.6 are graphical comparisons of the daily time series of total root zone θ_v at each site as measured by the TDR and as estimated using the five

RZWQM scenarios. Scenarios tested at site 133 consistently underestimated measured values over the course of the study period, except for day of year (DOY) 169 and 192 where modeled and measured values agreed (Fig. 3.2). This underestimation was largely due to faster soil drying rates exhibited by the scenarios than was indicated by the TDR measurements. Modeled θ_v reached a minimum value of about 0.10 $m^3\ m^{-3}$ on DOY 182, eight days before that shown by the measured data. The average underestimation (*MBE*, Table 3.3) is 0.01 $m^3 m^{-3}$ for RZS1, and 0.02 $m^3 m^{-3}$ for scenarios RZS2, 3 and 4. RZS5 showed the largest *MBE* at this site with a value of 0.03 $m^3\ m^{-3}$. Although the model simulations underestimated measured θ_v, the *r* and r^2 statistics (Table 3.3) indicate that all model simulations agreed well with measured values.

Model estimates of θ_v at site 136 (Fig. 3.3) closely agreed among the scenarios, but tended to overestimate measured values at the beginning and end of the modeling period. RZS1 and 2 consistently overestimated θ_v relative to RZS3 through 5. Similar to site 133, the modeling results show faster soil drying rates than that indicated by measurements. Additionally, the measured data show a minimum θ_v of about 0.10 $m^3\ m^{-3}$ occurring around DOY 190, but modeled θ_v was at least 0.02 to 0.06 $m^3\ m^{-3}$ higher for all scenarios. The *MBE* indicates overestimates of measured θ_v for all scenarios. RZS1 and 2 had the largest *MRE* at this site ($\geq$10%). RZS5 performed best overall, having the highest *r* and r^2, the lowest *MRE* and one of the lowest *RMSE*s and *MBE*s.

Site 151 was the most sandy textured site in the study. The high fraction of sand and limited rainfall contributed to the small range (0.04 $m^3\ m^{-3}$) of measured θ_v at this site (Fig. 3.4), which largely explains the rather low *r* and r^2 values. Observation of Figure 3.4

coupled with the statistical data indicates that model estimates of θ_v for RZS1 through 4 closely approximated measured values over most of the study period. Scenario RZS5 exhibited the largest overestimation of θ_v (*MBE* = 0.02 $m^3 m^{-3}$) compared to all other scenarios. The *RMSE* of RZS5 at this site was 0.03 $m^3 m^{-3}$, and the *MRE* was approximately 20%.

The modeling scenarios employed at site 154 produced similar estimates of θ_v over most of the study period (Fig. 3.5). The measured values of θ_v were underestimated by $\leq$0.02 $m^3 m^{-3}$, on average, with *MRE*s and *RMSE*s < 10% and $\leq$ 0.02 $m^3 m^{-3}$, respectively, for all scenarios. RZS4 overestimated measured θ_v on DOY 192 by about 0.08 $m^3 m^{-3}$. The other scenarios produced estimates of θ_v within ± 0.02 $m^3 m^{-3}$ of the measured value on this day.

At site LW02, scenarios RZS1 and 5 produced estimates of θ_v closely corresponding to each other, and agreeing well with measured values (Fig. 3.6). The *MRE*s for these two scenarios was < 2%, with *RMSE*s of approximately 0.01 $m^3 m^{-3}$. Scenarios RZS2, 3 and 4 also produced estimates of θ_v similar to each other. However, these estimates were lower than measured values by 0.06 $m^3 m^{-3}$, on average, leading to *MRE*s of about 20% and *RMSE*s of 0.06 $m^3 m^{-3}$. This site represents one of the most complex relative to soil layering (Table 3.1), but it is interesting to note that the Ks values used in RZS1 are much lower, in general, than those in RZS2 through 4 (Table 3.2), and are much closer in value to those used in RZS5.

Results from the adjustment of hydraulic parameters for the 0-5 and 0-15 cm surface layers at site 133 and site 154 are presented in Figures 3.7 and 3.8. The results given for the surface layers are indicative of those found at deeper depth intervals which are not shown. These sites were chosen due to their difference in texture with site 133 being a uniform sandy loam and site 154 being predominately sandy clay loam (Table 3.1). Gravimetric sample data and TDR measured data at 0-5 cm and 0-15 cm, respectively, are compared with predicted values of soil water content. The results for deeper layers were essentially the same as those for near-surface layers. RZS1 was chosen for calibration since it was a simple case of replacing default values with new values for either 1/3 bar water content and/or Ks. The method of calibration used was that of adjusting the hydraulic input data in an effort to match model results to measured values of soil water content. Several combinations of input were applied, taking into consideration the range of values representative of the texture class. Although this is not a rigorous test of calibration or optimization at this point, the results do provide certain insight. The overall effect of making any type adjustment in hydraulic parameters was a general shift in the model estimates, above or below the measured values. The shape of the graphed data basically remained the same. The results for these sets of data indicate that while the difference between predicted and measured values may be minimized by calibration and to obtain hydraulic property values, it is difficult to capture the absolute dynamic structure of the measured data.

This study also shows, as did the work of Martin and Watts (1999), that correct simulation of plant water uptake is essential for soil water prediction. This should seem obvious; however, based on the work at three sites it became apparent that not only is the choice of plant species important, but that the manner in which the model calculates the root distribution can be a significant factor as well. Perhaps further research in this area should be considered for representing various species of rangeland vegetation in the model. This would be of particular interest in areas of watershed management where rangeland production systems are more predominant than agronomic systems.

3.7 CONCLUSIONS AND APPLICATIONS

Comparison between RZWQM simulated and measured TDR soil water content values demonstrate that the model provided reasonable estimates of average soil water content at five sites within the LWRW. Experiments were conducted on several different soil types and modeled for a one-month period. Variable levels of physical and hydraulic input data were applied in the model, as well as, the use of field or laboratory measurements of soil hydraulic properties.

This phase of the study illustrates how soil type, different levels of input data, and differences in soil hydraulic parameter estimation or measurement influence the capability of the RZWQM in simulating average profile soil water content under rangeland conditions. Generally, the model provided satisfactory results, especially considering that no soil hydraulic properties were calibrated or optimized, though measured (site-specific) hydraulic properties were used in some cases. In addition, the environmental and site conditions for our experimental study were quite different from those reported in previous RZWQM evaluation and calibration studies (Hanson et al., 1998; Ma et al., 1998; Wu et al., 1999). The experimental time-scale for this work was also considerably shorter than what is normally applied to the model, in order to coincide with other studies during the

SGP97 Hydrology Experiment. It does not appear that the shorter time-scale had any appreciable effect on model results, though some studies have suggested that soil moisture predictability may be related to modeled time-scale (Schlosser and Milly, 2000).

Overall, the results from RZS1, using hydraulic properties estimated from soil texture, give the best agreement between predicted and measured soil water content. In all but one case, RMSE values for RZS1 are lower than those where detailed laboratory measured values were used as input. These results are consistent with those of Landa et al. (1999) where they used hydraulic properties estimated from soil texture and obtained close agreement between predicted and measured soil water content. This implies that the default values used in RZWQM are acceptable input for model applications when using a very limited input data set. An advantage of using this particular approach might be when applying remotely sensed surface soil moisture data to model profile soil water content when soil information is limited.

In all cases, RZS4 or 5 (field input data) showed good agreement between predicted and measured values indicating that the use of field measured 1/3 bar water content and/or Ks as hydraulic input data, may be preferable to those obtained by more detailed laboratory measurements (RZS3). This, in part, could be due to the large spatial variation in soil properties and the fact that for a given texture class, the corresponding range of property values can be quite broad; thus, the use of average profile values obtained in the field is quite adequate. Besides improving model estimates of soil water content, the input data obtained from field measurements requires much less time than laboratory analysis, is less expensive, and may be considered more representative of actual field conditions. As mentioned earlier, the data may also typify hydraulic properties obtained through the use of remotely sensed data.

Results presented here are consistent with previous studies that evaluated the capability of the RZWQM to predict soil water content, but also show that use of a limited input data set or soil hydraulic properties obtained in the field using relatively simple techniques provided the best estimates of average profile soil water content. These findings illustrate the potential application for modeling profile soil water content based on very limited soil data information and indicate the possibility of using soil hydraulic data obtained from remotely sensed observations which will be further evaluated and discussed in Chapter 4.

Table 3.1. Soil physical properties and vegetative cover type for the study sites.

Site ID	Depth	Sand	Silt	Clay	Texture Name[¶]	Bulk density[‡] Measured	Estimated	Vegetative Cover
	(cm)	------- % -------				-------g cm^{-3}-------		
133	0-15	70.8	19.6	9.6	SL	1.41	1.45	Bermudagrass
	15-30	72.8	17.6	9.6	SL	1.43	1.45	
	30-45	70.8	17.6	11.6	SL	1.45	1.45	
	45-60	68.8	19.6	11.6	SL	1.38	1.45	
136	0-15	50.8	35.6	13.6	L	1.37	1.42	Bermudagrass
	15-30	54.8	25.6	19.6	SL	1.42	1.45	
	30-45	52.8	26.6	21.2	SCL	1.41	1.60	
	45-60	48.8	25.6	25.6	SCL	1.44	1.60	
151	0-15	74.4	17.2	8.4	SL	1.37	1.45	Bermudagrass
	15-30	80.4	11.2	8.4	LS	1.47	1.49	
	30-60	86.4	7.2	6.4	LS	1.32	1.49	
	45-90	86.4	9.2	6.4	LS	1.46	1.49	
154	0-15	36.8	37.6	25.6	L	1.43	1.43	No cover
	15-30	46.8	25.6	27.6	SCL	1.42	1.60	
	30-45	48.8	21.6	29.2	SCL	1.44	1.60	
	45-60	50.8	21.6	27.6	SCL	1.39	1.60	
LW02	0-15	28.4	45.2	26.4	L	1.53	1.42	No cover
	15-30	24.4	47.2	28.4	CL	1.49	1.42	
	30-45	26.4	47.2	26.4	L	1.54	1.42	
	45-60	26.4	53.2	20.4	SiL	1.54	1.32	

[¶]Symbols used in the texture name category are as follows: S = sand(y), L = loam(y), Si = silt, C = clay.

[‡]Measured values of bulk density are used in scenarios 2, 3, and 4, and used in the model to determine Ks. Bulk density values for RZS1 and 5 are default values determined by the model from the soil texture name. However, since Ks is specified in RZS5, bulk density plays no role as it does in scenario 1.

Table 3.2. Measured and estimated soil hydraulic properties for each study site.

		Measured			Estimated by RZWQM				
		θ_v at -33 kPa		Ks [‡]	θ_v at -33 kPa[†]	Ks			
						RZS			
Site ID	Depth	Lab[¶]	In situ[§]	In situ		1	2	3	4
	cm	$m^3 m^{-3}$		$cm\ hr^{-1}$	$m^3 m^{-3}$	$cm\ hr^{-1}$			
133	00-15	0.127	0.176	29.3	0.192	2.59	11.1	22.2	13.3
	15-30	0.110	0.214	29.3	0.192	2.59	10.1	24.2	7.61
	30-45	0.086	0.149	29.3	0.192	2.59	9.24	28.3	15.1
	45-60	0.126	0.271	29.3	0.192	2.59	12.6	24.9	4.35
136	00-15	0.207	0.125	3.4	0.234	1.32	1.32	11.1	26.0
	15-30	0.197	0.181	3.4	0.192	2.59	2.59	9.92	12.0
	30-45	0.219	0.151	3.4	0.246	0.43	0.43	7.89	17.5
	45-60	0.236	0.176	3.4	0.246	0.43	0.43	5.33	11.7
151	00-15	0.093	0.199	4.8	0.192	2.59	13.2	2.6	12.2
	15-30	0.098	0.133	4.8	0.106	6.11	21.7	6.1	16.6
	30-60	0.138	0.127	4.8	0.106	6.11	36.3	6.1	30.5
	60-90	0.162	0.127	4.8	0.106	6.11	22.9	6.1	18.8
154	00-15	0.239	0.246	0.4	0.234	1.32	5.77	5.33	4.79
	15-30	0.242	0.315	0.4	0.246	0.43	5.11	5.41	1.46
	30-45	0.295	0.305	0.4	0.246	0.43	4.59	1.92	1.55
	45-60	0.332	0.347	0.4	0.246	0.43	6.00	1.27	0.88
LW02	00-15	0.263	0.314	0.15	0.234	1.32	3.21	1.84	0.52
	15-30	0.208	0.244	0.15	0.312	0.23	0.84	6.07	3.48
	30-45	0.212	0.250	0.15	0.234	1.32	2.99	4.29	2.22
	45-60	0.212	0.243	0.15	0.286	0.68	1.01	4.27	2.52

[¶]Values used in RZS3.
[§]Values used in RZS4 and 5.
[‡]Values used in RZS5.
[†]Value used in RZS1 and 2.

Table 3.3. Results from statistical analysis of the five scenarios implemented at the five study sites.

Site ID	Scenario	r^2	r	s	*RMSE*	*MBE*	*MRE*
					----- $m^3\ m^{-3}$-----		%
133	1	0.84	0.92	0.02	0.018	-0.01	-9.97
	2	0.88	0.94	0.03	0.022	-0.02	-13.54
	3	0.92	0.96	0.03	0.025	-0.02	-16.80
	4	0.87	0.93	0.03	0.020	-0.02	-12.28
	5	0.88	0.94	0.03	0.028	-0.03	-18.03
136	1	0.85	0.92	0.03	0.019	0.01	10.32
	2	0.85	0.92	0.03	0.025	0.02	15.69
	3	0.83	0.91	0.03	0.016	0.01	6.13
	4	0.84	0.92	0.03	0.014	0.00	3.27
	5	0.88	0.94	0.03	0.012	0.00	1.37
151	1	0.26	0.51	0.01	0.015	0.01	7.87
	2	0.30	0.55	0.01	0.014	0.00	1.38
	3	0.34	0.58	0.01	0.013	0.00	0.13
	4	0.32	0.57	0.01	0.013	0.00	1.08
	5	0.05	0.23	0.02	0.025	0.02	20.43
154	1	0.72	0.85	0.02	0.015	-0.01	-2.23
	2	0.79	0.89	0.03	0.024	-0.02	-7.56
	3	0.69	0.83	0.02	0.024	-0.02	-7.15
	4	0.49	0.70	0.03	0.024	0.00	-1.26
	5	0.82	0.90	0.02	0.017	-0.01	-5.00
LW02	1	0.51	0.71	0.02	0.014	0.00	-1.54
	2	0.51	0.71	0.04	0.064	-0.06	-21.11
	3	0.71	0.84	0.04	0.063	-0.06	-20.97
	4	0.77	0.88	0.04	0.052	-0.05	-17.20
	5	0.63	0.80	0.01	0.011	0.00	1.16

$MBE = n^{-1}\sum(E - x)$
$MRE = n^{-1}[\sum(E - x)/x][100]$
$RMSE = [n^{-1}\sum(E - x)^2]^{0.5}$
s = standard deviation

$\bar{x}$ = mean of measured value
r = correlation coefficient
r^2 = coefficient of determination

Figure 3.1. Map of five LWRW "limited data" modeling sites and *Micronet* locations.

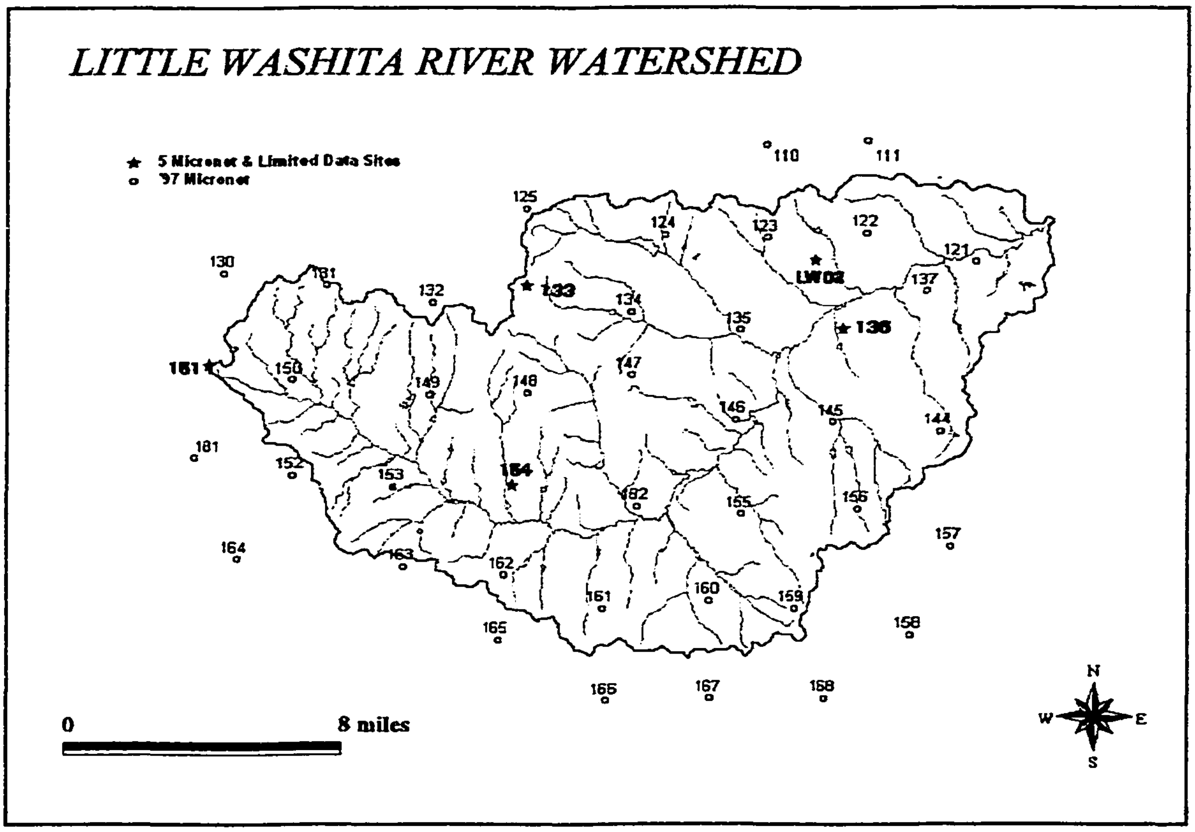


Figure 3.2. Modeled and measured average profile soil water content at Site 133.

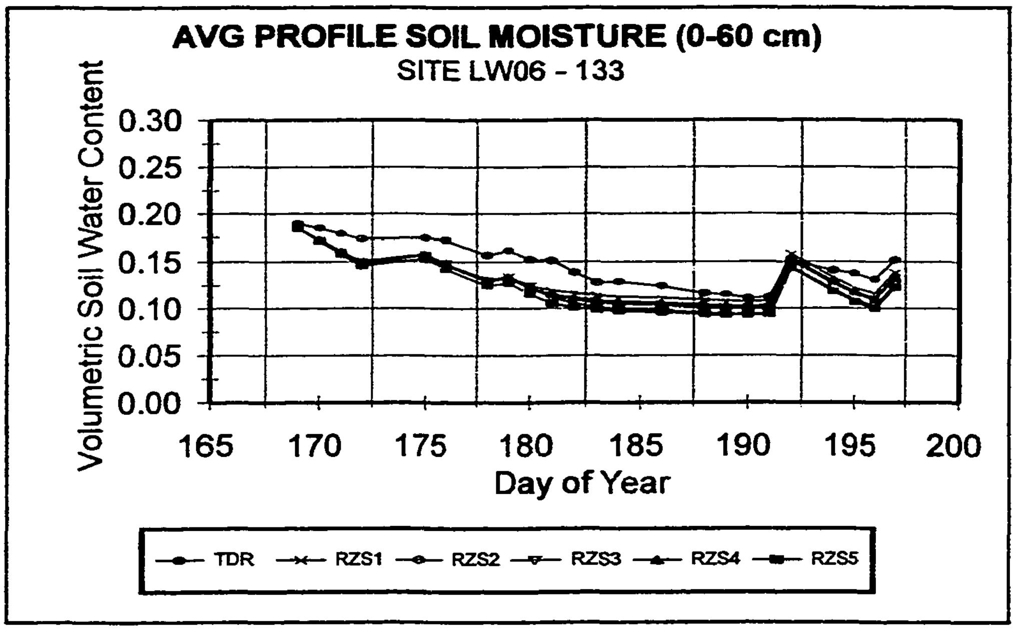


Figure 3.3. Modeled and measured average profile soil water content at Site 136.

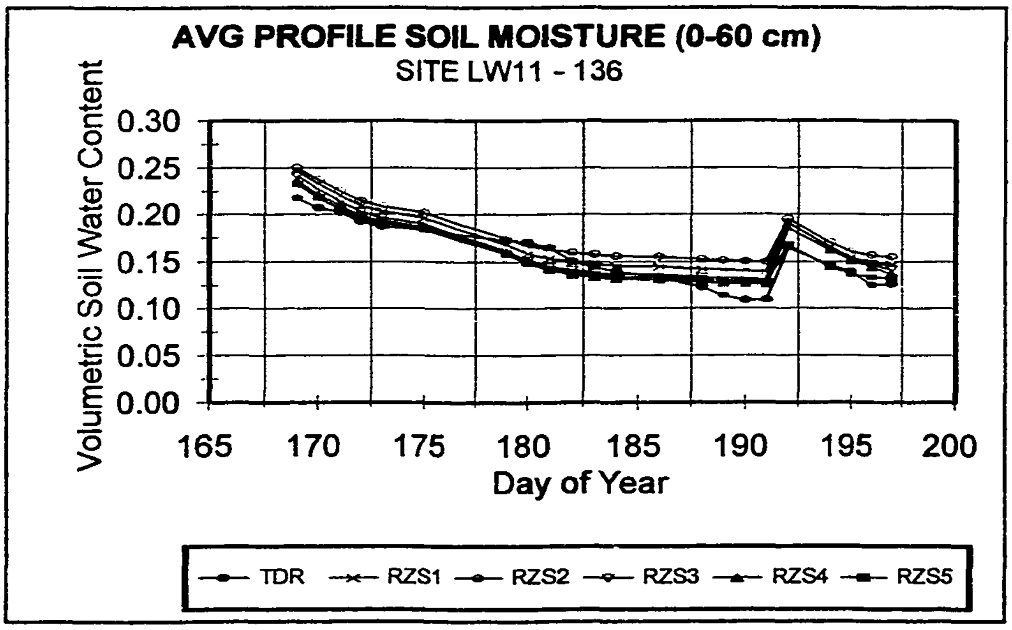


Figure 3.4. Modeled and measured average profile soil water content at Site 151.

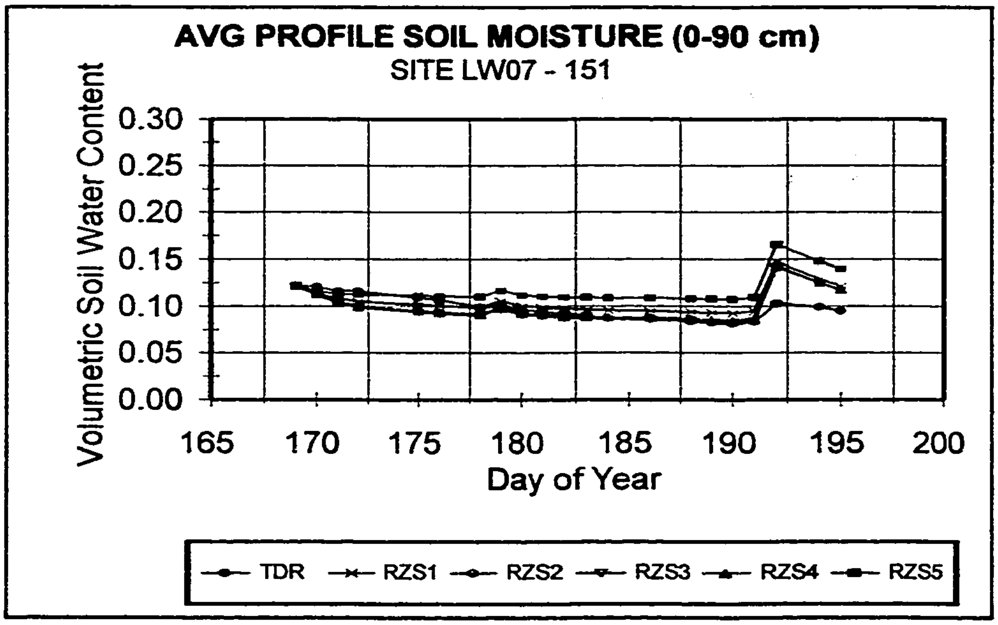


Figure 3.5. Modeled and measured average profile soil water content at Site 154.

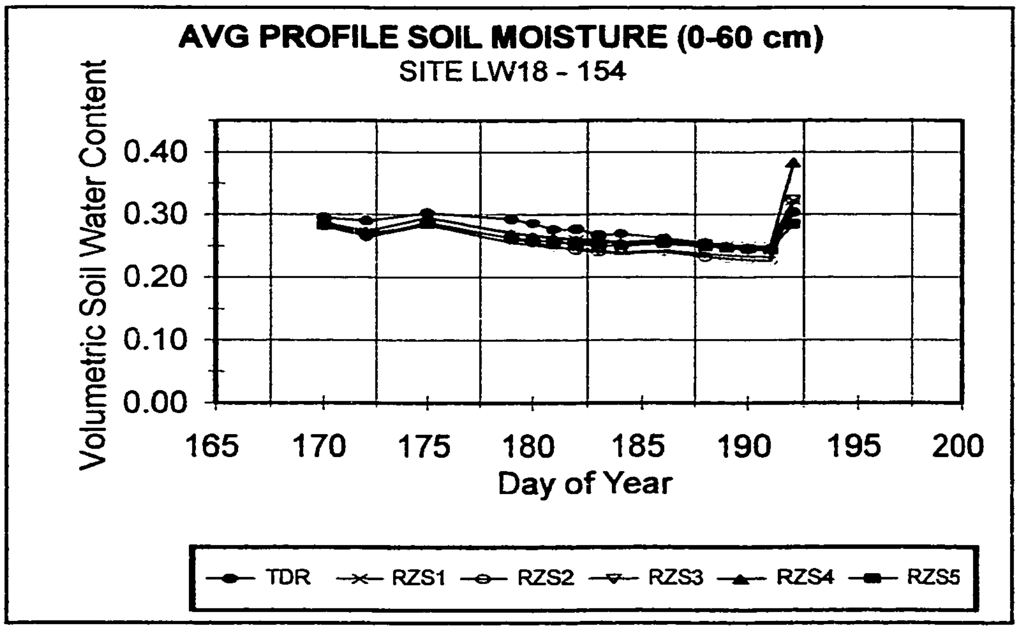


Figure 3.6. Modeled and measured average profile soil water content at Site LW02.

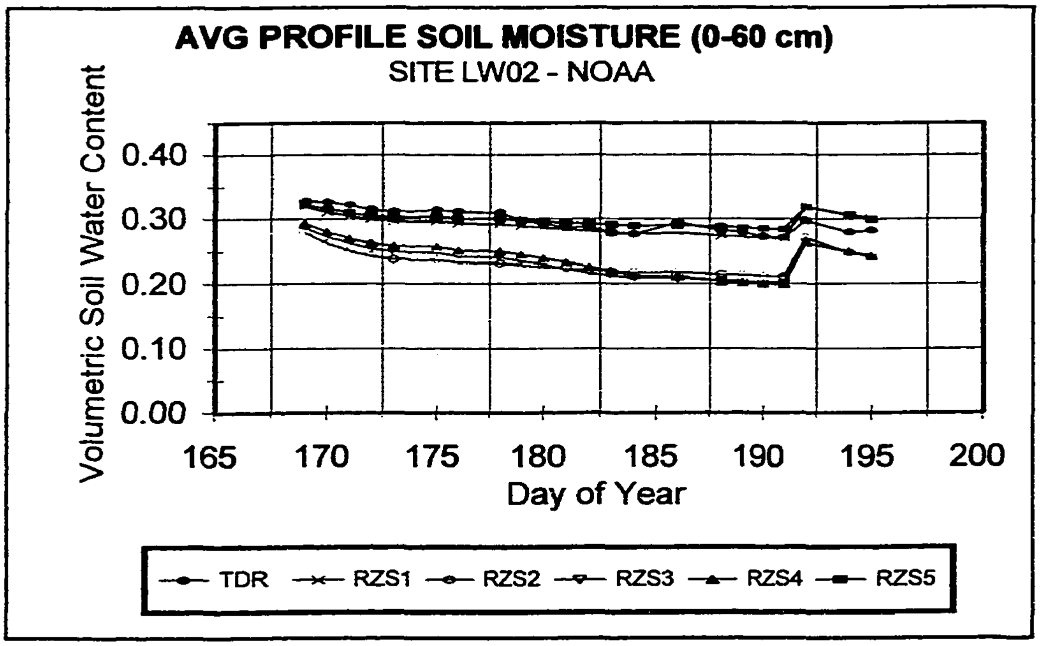


Figure 3.7a. Calibration results at Site 133 for the 0-5 cm layer.

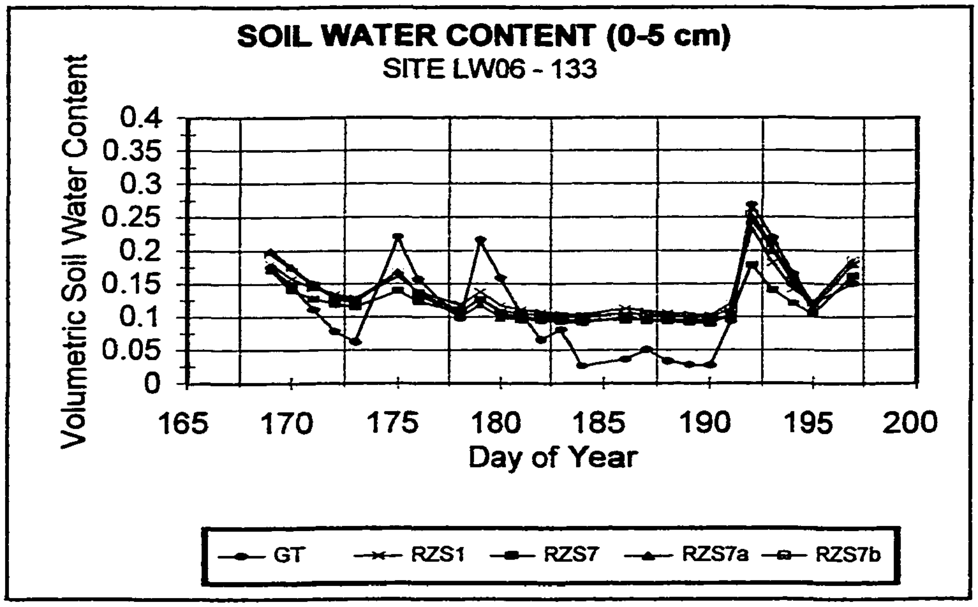


Figure 3.7b. Calibration results at Site 133 for the 0-15 cm layer.

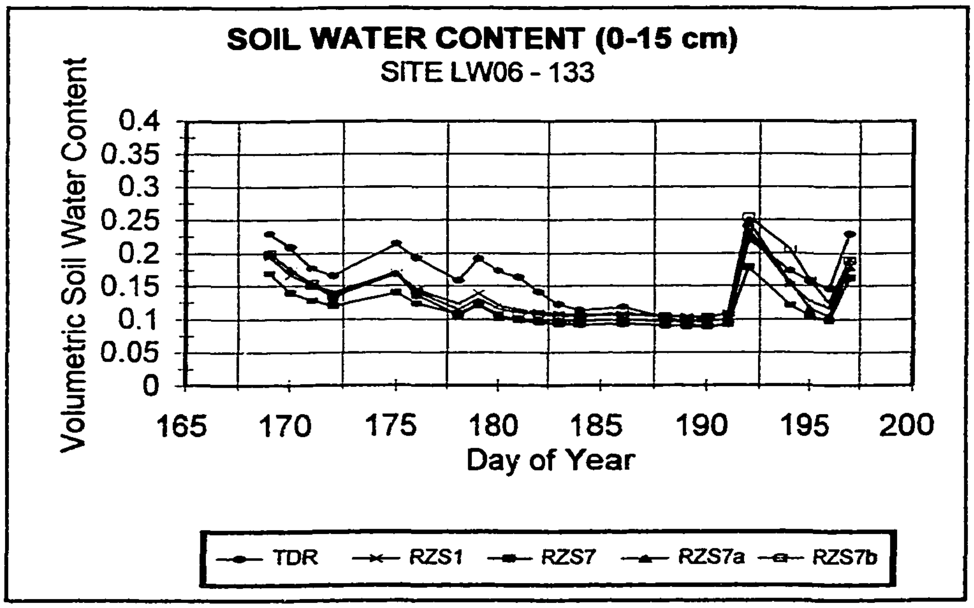


Figure 3.8a. Calibration results at Site 154 for the 0-5 cm layer.

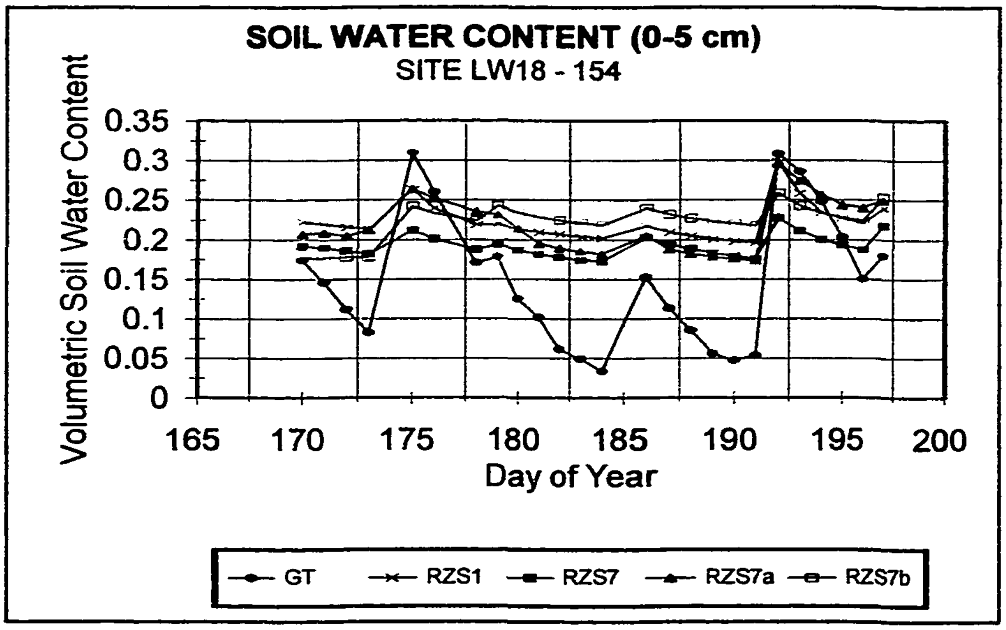
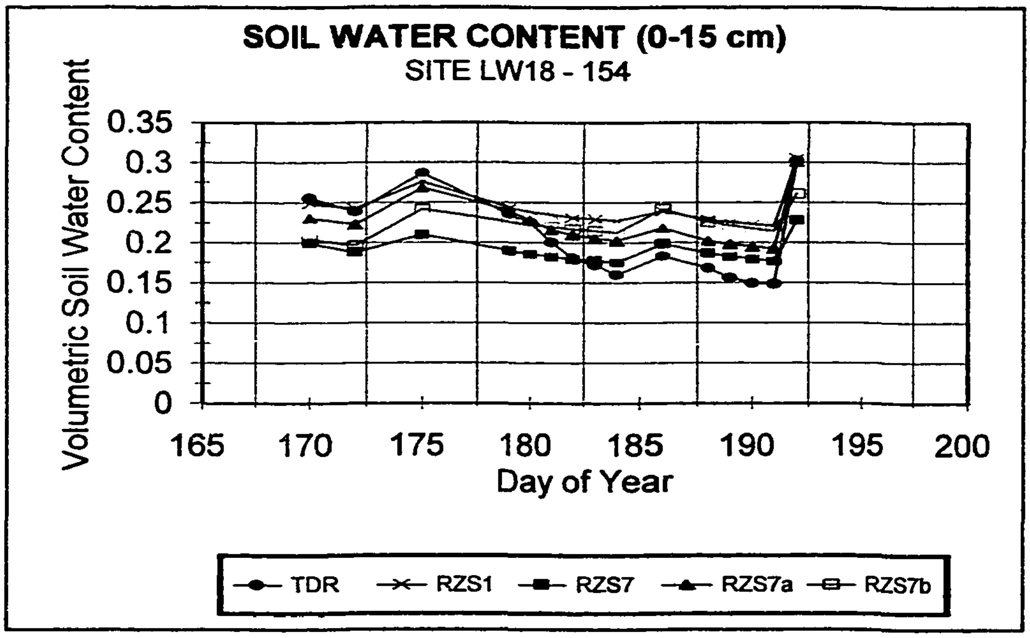


Figure 3.8b. Calibration results at Site 154 for the 0-15 cm layer.



4. ASSIMILATION OF SURFACE SOIL WATER CONTENT TO ESTIMATE PROFILE SOIL WATER CONTENT: A FIELD AND MODELING EXPERIMENTAL ANALYSIS

4.1 INTRODUCTION

The status of soil water content in the root zone is a key parameter to many aspects of agricultural, hydrological, and meteorological research. In agriculture, accurate knowledge of soil moisture conditions is essential for proper water resource management, irrigation scheduling, crop production, and chemical monitoring (Hanson et al., 1998; Ma et al., 1998; Hanson et al., 1999). In other aspects of research, soil moisture plays a significant role in the partitioning of available energy at the earth's surface into sensible and latent heat exchange with the atmosphere as well as in the partitioning of rainfall into infiltration and runoff (Chaubey et al., 1999; Silberstein et al., 1999; Western et al., 1999).

Traditionally, soil moisture has been measured at the point scale. Such point measurements do not always represent the spatial distribution since there is a limited area that can be accurately monitored with sufficient temporal resolution. Thus, during the course of the past three decades, a considerable amount of research has been dedicated to the development of remote sensing techniques that would provide spatial and temporal estimates of soil moisture over large regions. Many of these studies have successfully demonstrated the use of passive microwave remote sensors to obtain soil moisture mapping information (Jackson et al., 1982; Engman and Gurney, 1991; Jackson and Schmugge, 1989; Jackson et al., 1999). Though much progress has been made, these developments have been limited in that they characterize soil moisture in a rather shallow layer, variously estimated between 2 and 20 cm deep (Schmugge et al., 1974, 1977, 1980; Jackson and Schmugge, 1989). Jackson (1993) gives a comprehensive review of measuring surface soil moisture using passive microwave remote sensing, discussing the unique advantages that microwave remote sensing offers over other spectral regions, as well as some of the limitations involved with the measurement.

In the recent past, research investigations became increasingly focused on different strategies for estimating profile soil moisture from surface soil moisture observations (Jackson, 1986; Kostov and Jackson, 1993; Entekhabi et al., 1994). As a result of the research conducted as part of the AgRISTARS Soil Moisture project in the early 1980's, Jackson (1986) described how research up to that point in time had dealt with how remotely sensed data could be used to estimate soil moisture within the framework of existing soil water modeling approaches. As an alternative to these approaches he suggested that new models should be developed that would take advantage of the type of information that remotely sensed soil moisture provides. His is one of the earliest references that introduce the concept of integrating remotely sensed data and soil water modeling to estimate profile soil moisture and soil water properties from surface layer measurements (Jackson, 1986). Of particular significance to this work, which will be addressed later, was the suggestion of having surface soil moisture serve as the upper boundary layer condition in soil water models.

In later work, Jackson (1993) describes in much greater detail four basic approaches that can be used to expand surface soil moisture estimates to include profile soil moisture estimation. The approaches are: 1) statistical extrapolation of the surface observation; 2) integration of surface observations in a profile water budget model; 3) inversion of radiative transfer methods; and 4) the parametric profile model method. Kostov and Jackson (1993) present a comprehensive review of these basic approaches and others for estimating profile soil moisture using remotely sensed surface moisture data. They concluded that the most promising approach to the problem of profile soil moisture estimation was the integration of remote sensing and computational modeling. An illustration of this concept was the theoretical method developed by Entekhabi et al. (1994) for solving the inverse problem for soil moisture by sequential assimilation of remotely sensed data. Although their methodology consisted of a synthetic data analysis, it serves as an outstanding contribution to this area of research from which numerous investigations have followed.

Due to the earlier works of Jackson and Schmugge (1989) and Entekhabi et. al. (1994), current research emphasis has focused on the assimilation of remotely sensed surface soil moisture data into different types of hydrologic models. Data assimilation is a term that is most commonly associated with the atmospheric sciences. Applications of data assimilation arose from the meteorological custom of constructing daily weather maps which show how environmental variables such as pressure and wind velocity vary spatially (Daley, 1991). Analysis using data assimilation provides time-dependent spatially distributed estimates that can be updated whenever new data become available. The application of different data assimilation techniques has become a relatively new and challenging area of investigation concerning the integration of remote sensing and soil water modeling (Calvet et al., 1998; Houser et al., 1998; Wigneron et al., 1999; Hoeben and Troch, 2000; Walker et al., 2001).

To estimate profile soil water content from a time series of observed surface soil moisture, it is necessary to assimilate surface soil moisture data into a physical model. Calvet et al., (1998) applied an assimilation scheme to analyze the field capacity and total soil water content from surface data using the Interactions between Soil, Biosphere, and Atmosphere model (ISBA). They were able to retrieve total soil water content by inverting the ISBA, knowing the atmospheric forcing and precipitation, and having four or five surface soil moisture observations. The study was conducted at one site, for one soil type, and at the point scale. Houser et al. (1998) investigated the feasibility of updating the Topmodel-based Land-Atmosphere Transfer Scheme (TOPLATS) using several alternative assimilation techniques. These different techniques are briefly described in a later section of this paper. They found that several supplemental observations are essential for implementation of soil moisture data assimilation, the most important being atmospheric forcing. They also state that regular remotely sensed soil moisture observations are required, but these must be supplemented by in situ surface and root zone data across the operational domain to specify error correlations, to calibrate parameters, and to validate the model-calculated fields. In their work, many model parameters were not observed and had to be estimated. Measured data consisted of a rather limited set of field data using measured profile water content at two sites and an average of three soil samples at each site for surface measurements. Wigneron et al. (1999, 1999) used data sets representing one site and soil type, and the ISBA model in an effort to better define the requirements for the use of remotely sensed microwave measurements of surface soil moisture. They concluded that once the model has been calibrated for specific soil and vegetation characteristics, ISBA can be used successfully for the data assimilation process, regardless of atmospheric forcing. Their results appear to contradict those of Houser et al. (1998).

In a recent study by Li and Islam (1999), a method is proposed for soil moisture profile estimation by sequential assimilation of surface layer soil moisture using a four-layer land surface model. They evaluated the relative merits of daily assimilation of microwave measurements of surface soil moisture and measurements of rainfall for the estimation of profile soil moisture. Based on the results from one site, they found that in the absence of any measurement error, daily assimilation of surface soil moisture predicts the soil moisture profile and the partitioning of surface fluxes better than the model prediction alone. They also mention that their results should be viewed as tentative and that additional experiments are needed with actual measurements of surface soil moisture from remote sensing rather than the use of surrogate data to confirm and extend the findings of their research. In current studies by Hoeben and Troch (2000) and by Walker et al. (2001), data assimilation is evaluated based on the Kalman filter technique for active and passive microwave data, respectively. Descriptions and reviews of data assimilation procedures are provided in both papers which are complimented by well illustrated theoretical background information. Both studies show the Kalman filter assimilation scheme to be the most appropriate method for accurate profile soil moisture retrieval. However, both investigations were performed in a desktop environment using synthetic data. They recommended that use of the methodology be tested in real world applications.

Lack of adequate field measurements to support the conceptual research is a common factor among previous data assimilation studies. This continues to be an issue of concern to many research analysts which is most often due to the time, labor, and cost involved with obtaining reliable and accurate field data. A key element of this work is the combined use of an extensive set of quality field measurements and a detailed process-based model. The goal of this research was to further evaluate the application of remote sensing data assimilation and soil water modeling in estimating root zone soil water content and soil hydraulic properties. The intention of this study is that the results be of practical significance. The results of the work are based on the interactive use of good quality experimental field work, computational modeling, and the technique of direct insertion data assimilation. The recently developed Root Zone Water Quality Model (RZWQM), Version 3.2, as described below, was used in modeling profile soil water content.

4.2 MODELING SCENARIOS AND ASSIMILATION TECHNIQUES

Scenario Descriptions

A total of four different modeling scenarios were used to estimate profile soil water content. According to the results in Chapter 3, RZWQM provides a good estimate of average soil water content in the root zone using only soil textural-class name as input when compared to results from scenarios representing more detailed data input. Considering that the amount of soil data information available as model input is usually limited, especially where the use of remotely sensed data are applicable, this would seem to be the most practical scenario and approach to pursue. Thus, the scenarios used here are based on this concept and are described as follows: 1) RZS1, where a minimum or limited set of data serve as model input. In this case, the model is supplied only the soil textural-class name for each soil layer. According to the texture class, the model uses soil physical and hydraulic default values as input for particle size fraction, bulk density, porosity, θ_v at 1/3 bar (-33 kPa), and saturated hydraulic conductivity (Ks); 2) RZS10, where model input is the same as for RZS1 and surface soil moisture is sequentially assimilated; 3) RZS11, is the same as RZS10 except that the default values for 1/3 bar soil water content for each soil layer are replaced by a single value obtained from surface field data that represent surface moisture conditions 2-days after a sufficient rainfall. The use of 2-day drainage data in the field to represent 1/3 bar water content values has been investigated by Ahuja et al. (1993) and Mattikalli et al. (1998); 4) RZS12, is the same as RZS10 with plant uptake being accounted for when applicable. Scenario RZS10 represents the simple case of using data assimilation only, whereas RZS11 not only uses data assimilation but also soil properties derived from surface layer drainage information.

Data Assimilation Techniques

Remote sensing near-surface soil moisture observations have been used for updating hydrologic models by data assimilation to minimize the effects of errors in the model physics and input data (model parameters and meteorological data). The main objective for this approach is to improve estimates of evapotranspiration, infiltration, and runoff, and/or for estimating the status of soil water in the root zone. The feasibility of several assimilation schemes have been reported in Houser et al. (1998) and more recently in Walker et al. (2001). The types of alternative assimilation techniques investigated were: 1) direct insertion; 2) statistical correction; 3) Newtonian nudging; 4) statistical interpolation; and 5) the Kalman filter statistical scheme. For a detailed description of these techniques, the reader is referred to both publications. Perhaps the most common of these in use today are the direct insertion and Kalman filter techniques (Walker et al., 2001). In the work of Walker et al. (2001), they make a comparison between the direct insertion and Kalman techniques, for a synthetic case, and conclude that the Kalman filter is superior to direct insertion though there are potential problems in using the Kalman filter such as the necessity for repeat coverage frequency and a linear soil physical model. Their results provide an excellent state-of-affairs review and a thorough assessment of the most popular techniques currently available. However, due to a very limited number of publications on the evaluation of different assimilation schemes, as well as supporting field data, it is perhaps rather premature to make any final assessment at this time.

This work does not attempt to make any assessment of assimilation schemes and due to current model constraints, employs the technique of direct insertion. Direct insertion assimilation insures an instantaneous update of the model estimate with the measured soil moisture value. Thus, the work in this chapter focuses on the daily assimilation of surface layer soil moisture (0-5 cm) into the RZWQM for estimating profile soil water content (0-60 cm). Currently the model is designed to accept profile soil water content (θ_v) values to initialize the model and therefore does not have the capability to automatically update surface θ_v conditions based on daily remotely sensed observations.

To accommodate the data assimilation scheme, measured surface layer soil moisture values were input manually whenever new data were available, which was daily except when rainfall occurred or when airborne operations were canceled . Thus, the model was run one day at a time with the final profile estimates for that simulation period carried forward to reinitialize the model on the following day, in conjunction with measured surface input data. When measured surface data were not available, model estimated values were also carried forward. Modeled soil layers were at depth intervals of: 0-5, 0-15, 15-30, 30-45, and 45-60 cm to coincide with surface gravimetric or TDR probe measurements.

4.3 STUDY FIELD SITES

Four *Micronet* sites were selected (Fig.4.1) for use in this study based on the availability of measured soil properties and soil water content at the site, and differences in soil texture and vegetative cover. Two of the four study sites had a relatively dense vegetative cover of bermudagrass (*Cynodon dactylon*). Vegetative cover at the other study sites consisted of a mix of big bluestem (*Andropogon gerardii*), little bluestem (*Schizachyrium scoparium*), switchgrass (*Panicum virgatum*) and indiangrass (*Sorghastrum nutans*) and ranged from sparse to slightly moderate cover. Soil characteristics of each of the sites are given in Table 4.1.

As described in an earlier chapter, profiling TDR probes were installed at 13 selected *Micronet* locations with each probe consisted of four 15 cm long segments, enabling measurements of θ_v to a depth of 60 cm. Four of the locations were selected for the research in this chapter based on preexisting instrumentation, soil physical and hydraulic properties, and location within the watershed. Again, the TDR probes were calibrated in situ against site-specific gravimetric and bulk density data as described in Chapter 2. The TDR probes were usually read once each day, depending on weather conditions and available personnel, between 0800 and 1000 hrs local time, during the June 18 - July 16, 1997 study period.

4.4 DATA DESCRIPTIONS

Meteorological Data

A meteorological network (*Micronet*) of 45 stations is distributed across the watershed on a 5 km spacing (Fig. 4.1). Forty two of these stations continuously measure a basic suite of meteorological data: rainfall, incoming solar radiation, air temperature, relative humidity, and soil temperature at three depths. At three stations, windspeed and wind direction at two heights and barometric pressure are also recorded in addition to the basic suite of data. The meteorological data are measured every five minutes and reported every 15 minutes to a central archiving facility via radio telemetry. The data are quality controlled and final output is written in both 5-minute and daily summary files. Meteorological data from selected sites were used to determine break point precipitation required by the model, and to supply the required model inputs to calculate evapotranspiration.

Remote Sensing Data

Remote sensing was a critical component in the SGP97 Hydrology Experiment where data were collected over a one-month period from June 18 - July17. Primary investigations utilizing remote sensing involved vegetation mapping, soil moisture mapping, water vapor profiling, and estimating evapotranspiration. For the purpose of this study, only the soil moisture remote sensing data will be used and in particular, only the data obtained during actual field sampling. Multi-temporal airborne microwave data were collected using the Electronically Scanned Thinned Array Radiometer (ESTAR). The ESTAR instrument is a synthetic aperture, passive microwave radiometer operating at a center frequency of 1.413 GHz (21 cm wavelength) an bandwidth of 20 MHz (L-band). It has been well established that the soil moisture sampling depth is on the order of a few tenths of the wavelength in the soil, which translates to a depth of approximately 5 cm. Surface soil moisture was mapped at a spatial resolution of 800 m. To date, this instrument is the most efficient surface soil moisture mapping device available (Jackson et al., 1999)

During SGP97 gravimetric surface soil moisture samples were collected daily from a number of selected field sites to serve as 'ground truth' for verification of the ESTAR microwave radiometer soil moisture algorithm. A standardized tool was used to extract a sample of the 0-5 cm soil layer. After the retrieval of all samples they were weighed in their 'wet' state and placed in the oven for drying (105°C). The next day, approximately 22 hours later, the oven-dry samples were weighed again. Sample sites for SGP97 were classified as either 'full' or 'profile' sites. Sites with full sampling generally involved two transects separated by 400 m with a sample every 100 m resulting in 14 samples per site that covered an area of approximately 1 km^2. Profile sites, in reference to TDR locations, consisted of nine samples collected over a 20 m by 20 m grid near a TDR probe *Micronet* site. The four sites used in this study were selected as profile sample sites during the SGP97 experiment. Surface soil moisture values used for data assimilation were the average value obtained from the nine gravimetric samples. The values were converted to volumetric soil water content based on measured bulk density at the site.

Soil Physical and Hydraulic Data

Although the methods for determining of soil physical and hydraulic properties have been described elsewhere in this thesis, it is important to revisit this discussion as it pertains to the alternative methods proposed in this chapter. As mention previously, knowledge of the physical and hydraulic properties of soil is essential to modeling soil water flow. The basic soil hydraulic properties and characteristic functions that govern the flow of water in soils are soil hydraulic conductivity as a function of soil water content K (θ) or matric suction K (h) and soil water content as a function of matric suction θ (h), commonly referred to as the soil water characteristics curve (Hillel, 1980; Ahuja and Nielsen, 1990). It has been widely recognized that hydraulic properties of field soil are best measured *in situ* (Ahuja et al., 1976; Young et al., 1999; Zou et al., 2001). Of particular relevance, is knowledge of these parameters at matric pressures between 0 and approximately -300 kPa where the flow of water is most significant. However, in many cases this type of information is not generally available as discussed in Chapter 3.

Therefore, RZWQM provides estimates of all hydraulic properties based on simpler and limited known soil properties of soil texture, bulk density, and 1/3 or 1/10 bar soil water content, where the θ (h) relationship is first estimated by the extended similar-media scaling technique (Warrick et al., 1977 ; Ahuja et al., 1985) using the textural-class mean values of Rawls et al. (1982). Ahuja et al. (1985) compared this method with five other approaches (largely based on the work of Rawls et al., 1982 and 1983) to estimate soil water characteristics, (θ (h) from limited data), concluding that the estimated soil water characteristic curves based on either known bulk density and two water content-suction values (i.e., 1/3 and 15 bar values) or one water content-suction value (1/3 or 1/10 bar) and bulk density gave satisfactory results. The results in Chapter 3 further established the use of limited data in soil water modeling.

Knowing soil water content at 1/3 bar is not only important to RZWQM estimation techniques, but to other types of water retention models and infiltration capacity models as well (Campbell, 1974; van Genuchten, 1980; Vereecken, 1988). Thus, in addition to other methods describe in this section, a value for this parameter was obtained from surface soil data (0-5 cm) based on 2-days drainage after a sufficient rainfall and was used as hydraulic model input. Characterization of this hydraulic property based on 2-days drainage in the field is related to the concept of field capacity and studies involving steady-state infiltration and in-situ soil water characteristics (Ahuja et al., 1993; Mattikalli et al., 1998; Zou et al., 2001). Obtaining a value for this property from surface soil moisture data (e.g., remote sensing observations), which proves to be useful in modeling profile soil water content, would be of considerable benefit to large scale applications.

Laboratory methods were used to obtain soil physical and hydraulic properties for each site to a depth of 60 cm in 15 cm intervals. Soil hydraulic properties at each of the four field sites were measured *in situ* using the instantaneous profile method (Hillel, 1980). The field procedures used in this study involved gravimetric soil sample analysis, double-ring infiltrometry, and tensiometric data analysis and have been described in detail in earlier chapters.

4.5 STATISTICAL METHODS

To evaluate the overall correspondence of model output to measured values, we use the standard statistical measures of the correlation coefficient (*R*), mean bias error (*MBE*), and root mean square error (*RMSE*).The *MBE* and *RMSE* statistics are defined as:

$$MBE = \frac{\Sigma(P-O)}{n} \qquad [4.1]$$

$$RMSE = \sqrt{\frac{\Sigma(P-O)^2}{n}} \qquad [4.2]$$

where *P* is water content predicted by the model, *O* is the observed soil water content and n is the number of observations. The correlation coefficient (R) represents a measure of the strength of the relationship between predicted θ_v and observed measurements, whereas the *MBE* and *RMSE* are indicative of bias and error, respectively.

4.6 RESULTS OF DATA ASSIMILATION

Before discussing the results some clarification on the site names should be given, as well as, the order in which the data are presented. The four study sites are identified as LW02, LW18-154, LW11-136, and LW06-133. Each site name actually serves as two types of identification. Hyphenation separates the SGP97 experimental site name, which is shown first, from the permanent USDA-ARS *Micronet* station number. Both are provided here as an initial cross-reference to accommodate the reader and their association with projects on the watershed.. Hereafter, the sites are referred to as LW02, 154, 136, and 133 (Fig. 4.1). Figures 4.2a through 4.9e are grouped according to field site such that measured and modeled profile soil moisture time series data are shown first (i.e., 4.2a-e), followed by statistical comparisons of the data for that site (4.3a-e). The order in which the data pertaining to each site appears is LW02, 154, 136 and 133. Sites LW02 and 154 are finer textured soils having much higher clay contents than sites 136 or 133, especially in the top 30 cm (Table 4.1). Also, the vegetative cover at LW02 and 154 was very sparse, thus plant water uptake was not considered a factor and scenario RZS12 was not modeled for these two sites.

Estimates of Profile Soil Water Content

Figures 4.2a through 4.2e compare measured profile soil water content and model estimates for scenarios RZS1, RZS10, and RZS11 at site LW02. As shown in Chapter 3, the results of RZS1 provide a good average estimate of profile soil water content to a depth of 60 cm. This in part, is due to an overestimation in some layers while underestimating the water content for other layers. As also shown in Chapter 3, generally any attempt at calibration or conditioning of model hydraulic parameters (e.g., conductivity) to match model estimates to measured values, results in only shifting the modeled curve up or down. In other words, any change in the actual dynamic nature of the modeled curve is not accomplished by adjusting the hydraulic parameters. In Figures 4.2a and 4.2b (0-5 and 0-15 cm, respectively), data assimilation of surface soil moisture (RZS10 and RZS11) has a considerable effect on model estimates. This is also evident, to some extent, in the 15-30 cm layer (Figure 4.2c). In the 0-5 and 0-15 cm layers, data assimilation causes the model output to more closely approximate the actual value and dynamics of the measured data. Statistical data in Table 4.2 indicate less error in the estimate of soil moisture in the 0-5 and 15-30 cm layers for scenario RZS10 (RMSE= 0.024 and 0.034 m^3/m^3, respectively) compared to RZS1 without assimilation (RMSE= 0.053 and 0.051 m^3/m^3, respectively). Graphs of modeled verses measured soil water content at 0-5 and 0-15 cm depth intervals (Fig. 4.3a and b) show the highest correlation between RZS10 (0-5 cm) and RZ11 (0-15 cm) and measured data, with R values equal to 0.96 and 0.86, respectively (Table 4.2). Although the dynamic response of modeled output has been improved in the 0-15 cm layer by assimilation, soil water content is slightly underestimated by both RZS10 and RZS11 compared to RZS1. This may be due to a small amount of plant water uptake that was not accounted for during simulation and is not apparent from an analysis of RZS1 alone. Because scenarios RSZ10 and RZS11 show very similar results in the top 15 cm, use of the 1/3 bar hydraulic property value obtained from surface 2-day drainage data appears to be representative of the texture class for this depth interval, which the data in Table 4.2 support. However, because the results from scenario RZS11 below this depth show considerable deviation from the measured data and both RZS1 and RZS10 model results for at least two depth intervals, use of this hydraulic property as an average for the profile for this site does not seem plausible (Table 4.2). Below a depth of 30 cm the results from RZS10 or RZS11 show no significant improvement in soil moisture estimates using data assimilation. Graphs of modeled verses measured values for the three lowest layers (Fig. 4.3c, d, and e) are difficult to statistically interpret due to near constant soil moisture conditions. Though this condition restricts the statistical analysis to some extent, it could possibly be used in an alternate manner to estimate subsurface moisture conditions and perhaps derive hydraulic properties. For example, at sites where measured profile data show that moisture content becomes relatively constant at a certain depth, the difference between model estimates in the upper soil layers (improved by data assimilation) and average water content in the complete profile may better represent the average status of water content for the remaining lower depth intervals in question.

The simulated results given in Figures 4.4a-e and 4.5a-d for site 154 are similar to those at LW02 with the exception that better estimates of soil water content for the 0-15 cm soil layer are obtained with data assimilation at this site. Apparently the assumption of negligible plant water uptake at 154 is perhaps more appropriate than at LW02. Again, the results show that the fluctuations in measured water content in the 0-5 and 0-15 cm soil layers are simulated much more effectively using surface data assimilation (Fig. 4.4a and b), and that for these layers modeled values agree well with measured values (Fig. 4.5a and b). In the 0-5 cm an R value of 0.96 was obtained for scenario RZS10, while an R value of 0.98 was determined for the 0-15 cm layer using scenario RZS11. Though less evident in the 15-30 cm layer, some improvement in predictions due to assimilation are indicated by RZS10 which has the smallest RMSE value (0.028 m^3/m^3) and the highest R value (0.66) (Table 4.2). Again, using the 1/3 bar θ_v value from 2-day field drainage data at this site as a hydraulic input parameter appears limited to a depth of 30 cm. However, as in the case for site LW02, the narrow range of soil moisture values in the lower two depth intervals make the statistical interpretation difficult as indicated by the data shown in Figures 4.5d and 4.5e.

Influence of Plant Water Uptake

Data assimilation at sites 136 and 133 presented additional challenges other than the manual update of sequential surface soil moisture on a daily basis. Due to a dense pasture of bermudagrass at both locations it was necessary to take into account daily plant water uptake. The significance of plant water uptake has been described in detail in Chapter 3. Under normal and continuous simulation, plant water uptake is determined by a generic crop model component within RZWQM. Thus, for scenario RZS1 the 'turf grass' submodel was chosen with bermudagrass selected as the plant species. However, in the case of data assimilation and daily manual reinitialization, RZWQM at this time cannot account for the presence of a crop due to several reasons, the most important being the sequence in which the protocol of daily numerical schemes are executed in relation to the time of planting. This problem can eventually be overcome by rewriting this portion of the model, but until that time a reasonable approximation must be made. The approximation consist of running scenario RZS1 with and without plant uptake and subtracting this difference, on a daily basis, from the results of RZS10 to produce the final values of soil moisture for scenario RZS12, data assimilation with plant water uptake. Though not exact, this method should provide a fair assessment of plant uptake considering that the level of input data for each scenario is the same, with daily assimilation of surface soil moisture being the only difference.

The results of data assimilation using 1/3 bar θ_v obtained from 2-day surface drainage (RZS11) for sites 136 and 133 were consistent with those at LW02 and 154. These results are not presented here in an effort to simplify the graphics while emphasizing the effects of data assimilation and plant water uptake at these sites. However, it is important to note that the results for RZS11 at sites 136 and 133, again showed that it is possible to obtain 1/3 bar θ_v from 2-day surface drainage data to serve as model input. The depth of application, as for sites LW02 and 154, was approximately 30 cm for site 136. However, because the soil texture at site 133 is uniform to a depth of 60 cm and the surface 2-day soil moisture value was very close to the model 1/3 bar default value (Table 4.1), the results for scenarios RZS10 and RZS11 were essentially the same throughout the profile. Thus, because the soil texture of the profile is uniform with depth, the 1/3 bar θ_v value obtained from surface data may be used to represent the profile. The implications of uniform soil texture at site 133 are discussed later in this section.

In Figures 4.6a-e modeled and measured values of soil moisture at different depth intervals are plotted against time for site 136. Model results for RZS1 are consistent with simulations at previous sites that show a minimum response to rainfall in the upper soil layers compared to measured data, though average water content for the profile (0-60 cm) over time is reasonably estimated (RMSE= 0.02 m^3/m^3, Table 3.3) With data assimilation, model estimates are improved in the 0-5 cm layer by both RZS10 and RZS12 as indicated by the lower MBE and RMSE values given in Table 4.2. Any effect due to plant water uptake appears to be negligible or accounted for by the model through losses due to surface evaporation. In Figure 4.6b (0-15 cm) the effects of plant uptake are much more pronounced. Model estimates are improved considerably by data assimilation and accounting for plant water uptake, especially after day 180. Based on the data plotted in Figure 4.7b for modeled verses measured values, there is a strong linear relationship between the data for scenarios RZS10 and RZS12, with correlation coefficients equal to 0.96 and 0.93 (Table 4.2), respectively. The adjustment due to plant water uptake has essentially shifted the regression line for RZS10 closer to the 1:1 line. Accounting for plant uptake reduces the error in model estimates by about 5%. Results at lower depths in the profile show that data assimilation has no significant effect unless plant water uptake is ignored, thereby transferring the amount of water available for plant uptake to deeper layers resulting in a considerable overestimation of soil water content in these layers (Fig. 4.6c-e.).

The results for site 133 may provide the best example for illustrating the effects of data assimilation and plant water uptake on model estimates of profile soil water content.

Of the four study sites, this is the only site where the soil texture (sandy loam) is uniform to a depth of 60 cm (Table 4.1). However, due to slight differences in bulk density among the depth intervals, the corresponding hydraulic properties differ due to the change in porosity. The differences in the 1/3 bar hydraulic property between model default values, surface 2-day drainage data, and values measured *in situ* are shown in Table1. This provides a good example for the case of using limited data (RZS1) where the value for 1/3 bar θ_v is derived from texture name alone and, at this site, assigned the same default value for each layer in the profile. Though not great, there are differences between 1/3 bar θ_v values measured *in situ* and model default values however, the differences are not large enough to have a significant effect on model predictions as discussed in Chapter 3. Thus, although hydraulic input data sets may show consistency and be considered valid, this does not necessarily translate into accurate estimates of profile soil water content on a layered basis as the results show in Figures 4.8a-e for scenario RZS1. Consequently, the differences between modeled and measured values may be more related to errors in rainfall input or the partitioning of rainfall into runoff and infiltration. Several recent studies suggest this as being a possibility as well (Houser et al., 1998; Li and Islam, 1999; Walker et al., 2001).

The results for site 133 agree with those at previous sites in that model predictions of soil water content to a depth of 30 cm show improvement using data assimilation while accounting for plant water uptake, but in contrast to other sites, closely matches the results of RZS1 below this depth (Fig. 4.8a-e). The highest degree of correlation between modeled and measured values in the top 30 cm was calculated for RZS12 as shown in

Table 4.2. Below this depth there is only a slight difference between the results for scenarios RZS1 and RZS12, with RZS1 having slightly higher R values (Table 4.2). The close agreement between the results for RZS1 and RZS12 at the lower depth interval is attributable to similar and constant 1/3 bar θ_v values being used throughout the profile. These results suggest that because of uniform soil texture, the 1/3 bar θ_v value, based on two days of drainage near the surface, is perhaps characteristic of the profile. Although model estimates throughout the profile do not exactly match measured values, only a slight adjustment in the 1/3 bar v θ_v value would be necessary to minimize the difference. Because data assimilation improves the models' ability to capture near-surface soil moisture dynamics and based on the results of Chapter 3 where any adjustment of the 1/3 bar θ_v value shifts the position of the curve, it stands to reason that once the data assimilation scheme has been applied, and accounting for plant water uptake if applicable, that the 1/3 bar θ_v value could then be adjusted to achieve the best match between modeled and measured profile soil water content. Using this means of optimization should provide a new estimate of the 1/3 bar hydraulic parameter for each layer that should not only improve average profile soil moisture estimates, but individual layer predictions as well. This approach should be appropriate for all sites and is the subject of future work at these and five additional field sites.

Large Scale Applications

The main objective of this chapter was to evaluate the use of surface soil moisture data assimilation in a soil water model to estimate profile soil water content at a point, using what is considered an optimum set of measured field data. The use of actual surface sample data (0-5 cm) rather than remotely sensed microwave data in the assimilation scheme is an example of this type of data set. Use of the surface sample data as a surrogate for microwave measurements practically eliminates any issues of scale and insures that the complete set of measurements remain in close proximity (e.g., rainfall and TDR), thereby minimizing the effects of spatial variability. Thus, if the current results do not demonstrate any potential benefits from the research approach applied at this scale, using the best set of data available, then what confidence would be provided at larger scales? Because the results presented thus far do suggest potential benefits by using this approach, and are consistent with several aspects of current research in this area, a conceptual example of how this approach may be applied across the entire watershed is now considered. To actually apply this concept at the watershed scale it would be necessary to have a distributed hydrologic model, with GIS interface, that is capable of automated data assimilation. RZWQM may have this capability in the future, but at present a set of data meeting the required level of point-scale input is presented to illustrate its potential use for estimating root zone soil water content at the watershed scale using passive microwave observations. It should be noted that the concept of representative elementary area (REA), as described by Wood (1995), has been applied to the data sets, which suggest an area of 1 km^2 as being the critical spatial scale in the analysis of infiltration parameters, derived from soil classification data, on the LWRW. To further support the plausibility for using this type data set and approach are the recent findings of Young et al. (1999) where they reported that field-scale water movement studies can provide a more global interpretation of profile characteristics than rescaling laboratory results of individual soil samples.

As discussed earlier, the LWRW is equipped with a network of *Micronet* stations where rainfall measurements are recorded. These point-scale measurements have been used to create a map of rainfall distribution that would serve as model input for one rainfall event. Unfortunately, due to the untimely replacement of raingauge equipment during the SGP97 experimental campaign, the complete suite of gauges were not operational during the first half of the 30-day SGP97 study. Only 19 gauges were functioning at the beginning of the study, with additional gauges coming on-line periodically. To illustrate the degree of error or loss of information attributed to the difference in measurement points, a GIS spatial interpolation scheme (nearest neighbor) was performed on the data set and is presented in Figures 4.10a-c. A map of rainfall distribution across the watershed, based on measurement at 42 locations, is shown in Figure 4.10a, with a map of the same rainfall event using 19 measurement points given in Figure 4.10b. There is considerable difference between the spatial patterns that is quantitatively mapped in Figure 4.10c. According to the information in Figure 4.10c, the difference in rainfall amounts ranges from approximately -40 to 85 mm. Thus, during the first half of SGP97, when several significant rainfall events occurred on the watershed, any analysis involving the spatial distribution of rainfall should take this into consideration, as in the case of input for a distributed hydrologic model. This effect may be exacerbated by the convective nature of storms prevalent during the summer months as indicated by the distribution patterns in Figure 4.10a. However, based on the results of this study for soil moisture profile estimation at a point, errors attributed to rainfall input data may be ameliorated to some degree by use of surface soil moisture data assimilation. This has also been reported by Li and Islam (1999) where their results show that, in the absence of precipitation measurements, estimates of profile soil moisture and the partitioning of surface fluxes are considerably improved due to sequential assimilation of surface soil moisture with climatological mean precipitation. A good analysis of the uncertainty in model parameters due to input error from rainfall data is given in a recent paper by Chaubey et al. (1999).

An example of remotely sensed surface soil moisture data that could serve as daily assimilation input for estimating profile soil water content in the watershed is shown in Figure 4.11a. The data represent the type of soil moisture mapping product derived from SGP97 ESTAR brightness temperature. In Figure 4.11b, ESTAR data were acquired 2-days after a significant rainfall event, which under more uniform rainfall conditions, may also serve as 1/3 bar θ_v values as in the case for the point-scale model. Considering the complete set of ESTAR data available during SGP97, it is possible that a combined map of ESTAR 2-day drainage data for the watershed, based on different storms and locations, could be produced that would effectively represent the 1/3 bar hydraulic property across the watershed. However, based on point-scale results, these values should only be applied to a depth of 30 cm, except where soil texture is uniform with depth.

A map of soil texture is shown in Figure 4.11c that was inferred from the 1/3 bar θ_v data in Figure 4.11b. The texture map in Figure 4.11c was obtained in a very simple manner by assigning the soil moisture values in Figure 4.11b a texture name according to default values used in RZWQM that relate 1/3 bar θ_v to soil texture (Rawls and Brakensiek, 1989). Though not exact and very preliminary, the basic patterns in textural differences agree with those from county survey data given in Allen and Naney (1991). A much more rigorous approach for inferring soil texture types using passive microwave remote sensing was recently described by Chang and Islam (2000). Their approach is based on recent developments in Artificial Neural Network (ANN) and the temporal patterns of surface soil moisture redistribution with time. The ESTAR data set for SGP97 and supporting field observations, certainly provide an excellent opportunity to further examine the innovative approach of Chang and Islam (2000).

Overall, Figures 4.10a through 4.11c are shown here to typify the minimum set of required data necessary to run a model such as RZWQM in a spatially distributed format. As the results from this chapter and those in Chapter 3 demonstrate, the model provides good estimates of profile soil moisture using the necessary meteorological input, data assimilation of surface soil moisture (Fig. 4.11a), 1/3 bar θ_v (Fig. 4.11b), and soil texture name (Fig. 4.11c). Thus, application of the model in a spatially distributed format is anticipated using similar but more exact data sets to evaluate the use of surface soil moisture data assimilation for profile soil moisture estimation at the watershed scale. As mentioned earlier, application of this methodology will require a GIS-based distributed hydrologic model which incorporates data assimilation and spatially variable meteorological data and surface parameters into model formulations.

4.7 CONCLUSIONS AND APPLICATIONS

In this chapter, an extensive set of field data has been used in combination with direct insertion data assimilation and soil water modeling to estimate root zone soil water content at a point in the field, something which is uncommon in the literature. The modeling approach was based on the use of limited soil data information since in practical terms, this is usually the case. Model estimates were made at four field sites located in the Little Washita River Watershed for various soil types and vegetative conditions. Walker et al. (2001) reported in a recent study that only a few studies have assimilated near-surface soil moisture data into a hydrologic model with the objective to improve predictions of evapotranspiration or runoff, or to estimate profile soil moisture for a one-dimensional soil column using synthetic data, and a very short update interval. One of the unique aspects of the work in this paper is use of field data rather than synthetic.

These results provide further evaluation of the merits of surface soil moisture data assimilation for soil moisture profile estimation based on comparisons between model estimates and measured surface and TDR profile data to a depth of 60 cm. Surface soil moisture sample data was obtained during the SGP97 large scale hydrology experiment from June 18 - July 16, 1997 and used as a surrogate for microwave moisture data. In this study, a manual method of direct insertion data assimilation was used to replace (update) daily model estimates with observed data for the 0-5 cm soil layer. The Root Zone Water Quality Model (RZWQM) was used for estimating profile soil water content. The model has recently undergone a comprehensive evaluation through a cooperative effort with MSEA (Management Systems Evaluation Areas) involving water quality projects in five

Midwestern States (Hanson et al., 1999). Hence, this is an initial test of RZWQM in the Southern Great Plains and for using a data assimilation scheme.

Data assimilation of surface soil moisture improved model estimates to a depth of 15 cm at all sites and at three sites to a depth of 30 cm. Improvements were most pronounced in the 0-5 cm layer. At two sites where vegetation was dense, the results showed that plant water uptake must also be adequately modeled when applying a data assimilation scheme otherwise, the amount of water available for plant uptake is transferred to deeper layers resulting in a considerable overestimation of soil water content at these depths. Of particular significance with data assimilation, is that model estimates more closely matched the measured dynamic fluctuations of soil moisture in the top 30 cm in response to rainfall events. This may indicate that data assimilation of surface soil moisture tends to compensate for any errors that might be due to rainfall measurements or the partitioning of rainfall into runoff and infiltration. There was no significant improvement in soil water estimates below the 30 cm depth. However, considering that the model predicts the 0-60 cm average soil water content with minimum error, it is conceivable that a closer account of water content at deeper layers (30-60 cm) could be determined by finding the difference between assimilated estimates in the top 30 cm and total 60 cm estimates. An alternative approach would be, once data assimilation has been applied, adjustment of a selected model hydraulic parameter (i.e., 1/3 bar θ_v or Ks) could be made at deeper depths in order to match modeled θ_v to measured values, also providing a new estimate of the hydraulic property.

Based on the results of this study a value representing the soil water content at 1/3 bar, which is related to texture class, may be obtained from surface soil moisture 2-day field drainage data after a sufficient wetting of the profile. This value of 1/3 bar θ_v may then be used as hydraulic input data for the model to a depth of 15 cm. Although the case presented here shows that use of the 1/3 bar value obtained in this manner may also improve soil water estimates to a depth of 30 cm at some sites, the results should be considered tentative until testing at additional sites has been completed. The results also indicate that use of this value as an average for the profile may only be applicable where soil texture is uniform with depth. However, further evaluation for this condition is also recommended.

The acquisition of 2-day remotely sensed observations for this study is also related to another area of research regarding the frequency of data assimilation. Several studies have suggested certain criteria for determining the optimum or minimum frequency of soil surface assimilation (Calvet et al., 1998;Li and Islam, 1999; Walker et al., 2001). According to the literature this range is on the order of hours to several days. Though the objective of this study does not address the frequency of assimilation, it would be very difficult to reach the same conclusions if the frequency of assimilation/observation had been reduced to a 2 or 3 day interval. Thus, to acquire the type of soils data needed to initialize the RZWQM, daily observations, as a minimum, were critical to this study.

Results presented in this study should be viewed as a basic step towards better understanding the relative merits of surface soil moisture data assimilation in soil water modeling to estimate root zone soil water content based on field and modeling experimental analyses. Much further work is necessary to make a complete assessment of the methodology involved in this investigation. One aspect of the research would be to extend the spatial scale of application using a GIS-based distributed hydrologic model, as discussed earlier. The results of this research, based on the use of various types of field data, serve to support much of the theoretical and synthetic work found in the literature today. Though the four field sites chosen for this work represent a cross-section of soil types in the LWRW, extending this type investigation to an additional five sites or more should certainly provide interesting challenges in future studies.

Table 4.1. Soil physical and hydraulic properties at four assimilation field study sites in the LWRW.

Site ID	Depth	Measured in Laboratory: Sand	Silt	Clay	Texture Name[¶]	Bulk Density	Water Content at -33 kPa: Model Default	Double-Ring In situ	Surface 2-Day Drainage
	(cm)	---------- % ---------				-----g/cm³----	----------- m³/m³ ---------		
LW02	0-15	28.4	45.2	26.4	L	1.53	0.234	0.314	0.248
	15-30	24.4	47.2	28.4	CL	1.49	0.312	0.244	0.248
	30-45	26.4	47.2	26.4	L	1.54	0.234	0.250	0.248
	45-60	26.4	53.2	20.4	SiL	1.54	0.286	0.243	0.248
LW18-154	0-15	36.8	37.6	25.6	L	1.43	0.234	0.246	0.248
	15-30	46.8	25.6	27.6	SCL	1.42	0.246	0.315	0.248
	30-45	48.8	21.6	29.2	SCL	1.44	0.246	0.305	0.248
	45-60	50.8	21.6	27.6	SCL	1.39	0.246	0.347	0.248
LW11-126	0-15	50.8	35.6	13.6	L	1.37	0.234	0.125	0.210
	15-30	54.8	25.6	19.6	SL	1.42	0.192	0.181	0.210
	30-45	52.8	26.0	21.2	SCL	1.41	0.246	0.151	0.210
	45-60	48.8	25.6	25.6	SCL	1.44	0.246	0.176	0.210
LW06-133	0-15	70.8	19.6	9.6	SL	1.41	0.192	0.176	0.164
	15-30	72.8	17.6	9.6	SL	1.43	0.192	0.214	0.164
	30-45	70.8	17.6	11.6	SL	1.45	0.192	0.149	0.164
	45-60	68.8	19.6	11.6	SL	1.38	0.192	0.271	0.164

¶Symbols used in the texture name category are as follows: S = sand(y), L = loam(y), Si = silt, C = clay.

Table 4.2. Statistical data analysis for assimilation at four field sites on the LWRW.

Site/Scenario	Depth of Layer (cm)				
	Layer 0-5	Layer 0-15	Layer 15-30	Layer 30-45	Layer 45-60
LW02-NOAA					
RZS1					
Mean Bias ($m^3 m^{-3}$)	0.025	-0.003	0.048	-0.051	0.001
RMS Error ($m^3 m^{-3}$)	0.053	0.036	0.051	0.053	0.042
Correlation Coefficient	0.759	0.689	0.341	0.577	0.544
RZS10					
Mean Bias ($m^3 m^{-3}$)	-0.009	-0.030	0.024	-0.064	-0.030
RMS Error ($m^3 m^{-3}$)	0.024	0.042	0.034	0.065	0.033
Correlation Coefficient	0.962	0.779	0.230	0.608	0.516
RZS11					
Mean Bias ($m^3 m^{-3}$)	0.002	-0.027	-0.037	-0.055	-0.072
RMS Error ($m^3 m^{-3}$)	0.023	0.037	0.041	0.057	0.074
Correlation Coefficient	0.929	0.858	0.498	0.695	0.506

Table 4.2. (Continued)

Site/Scenario	Depth of Layer (cm)				
	Layer 0-5	Layer 0-15	Layer 15-30	Layer 30-45	Layer 45-60
LW18-154					
RZS1					
Mean Bias ($m^3\,m^{-3}$)	0.075	0.038	0.033	-0.039	-0.057
RMS Error ($m^3\,m^{-3}$)	0.097	0.048	0.043	0.042	0.060
Correlation Coefficient	0.910	0.901	0.522	0.534	0.342
RZS10					
Mean Bias ($m^3\,m^{-3}$)	0.020	-0.013	0.015	-0.052	-0.070
RMS Error ($m^3\,m^{-3}$)	0.037	0.016	0.028	0.056	0.073
Correlation Coefficient	0.962	0.977	0.660	0.612	0.324
RZS11					
Mean Bias ($m^3\,m^{-3}$)	0.036	-0.012	-0.011	-0.079	-0.096
RMS Error ($m^3\,m^{-3}$)	0.049	0.016	0.030	0.083	0.100
Correlation Coefficient	0.958	0.978	0.610	0.556	0.361

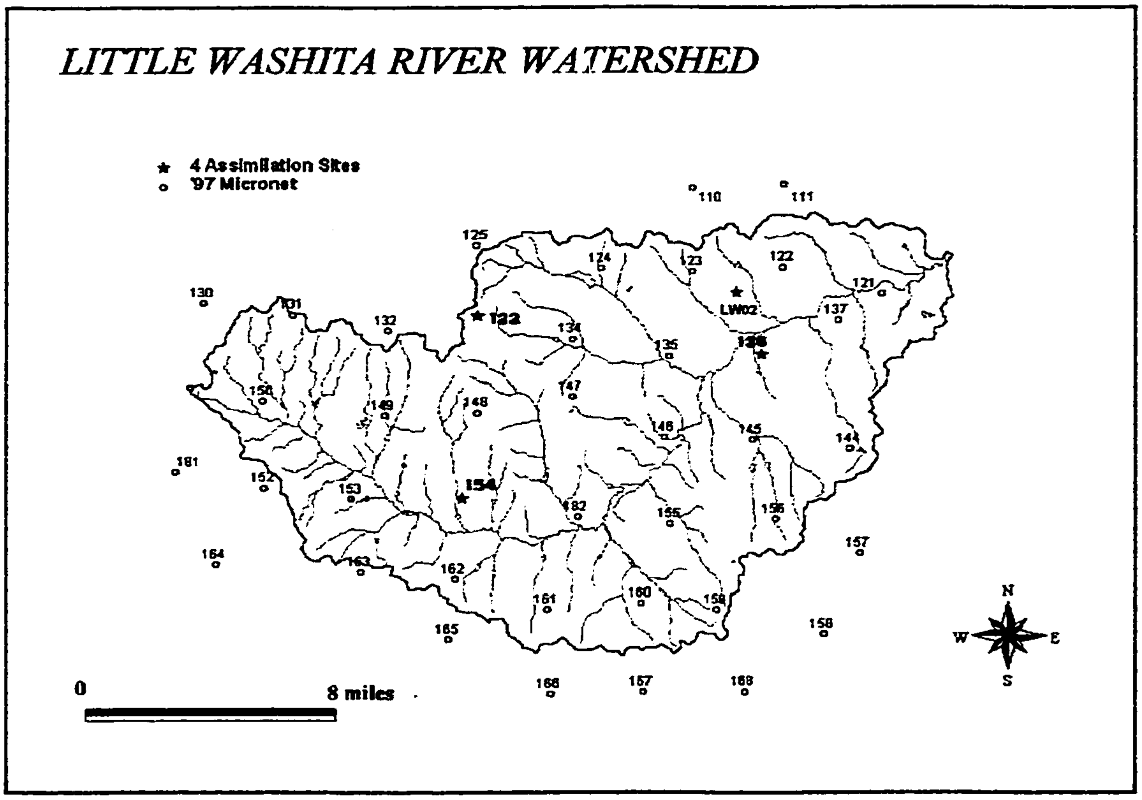
Table 4.2. (Continued)

Site/Scenario	Depth of Layer (cm)				
	Layer 0-5	Layer 0-15	Layer 15-30	Layer 30-45	Layer 45-60
LW11-136					
RZS1					
Mean Bias ($m^3 m^{-3}$)	0.020	0.083	0.004	0.008	-0.036
RMS Error ($m^3 m^{-3}$)	0.039	0.086	0.015	0.028	0.044
Correlation Coefficient	0.922	0.894	0.907	0.767	0.792
RZS10					
Mean Bias ($m^3 m^{-3}$)	0.010	0.092	0.057	0.115	0.025
RMS Error ($m^3 m^{-3}$)	0.022	0.093	0.068	0.091	0.053
Correlation Coefficient	0.966	0.961	0.118	0.640	0.677
RZS12					
Mean Bias ($m^3 m^{-3}$)	-0.019	0.039	-0.013	-0.006	-0.051
RMS Error ($m^3 m^{-3}$)	0.032	0.046	0.023	0.032	0.058
Correlation Coefficient	0.911	0.934	0.854	0.664	0.694

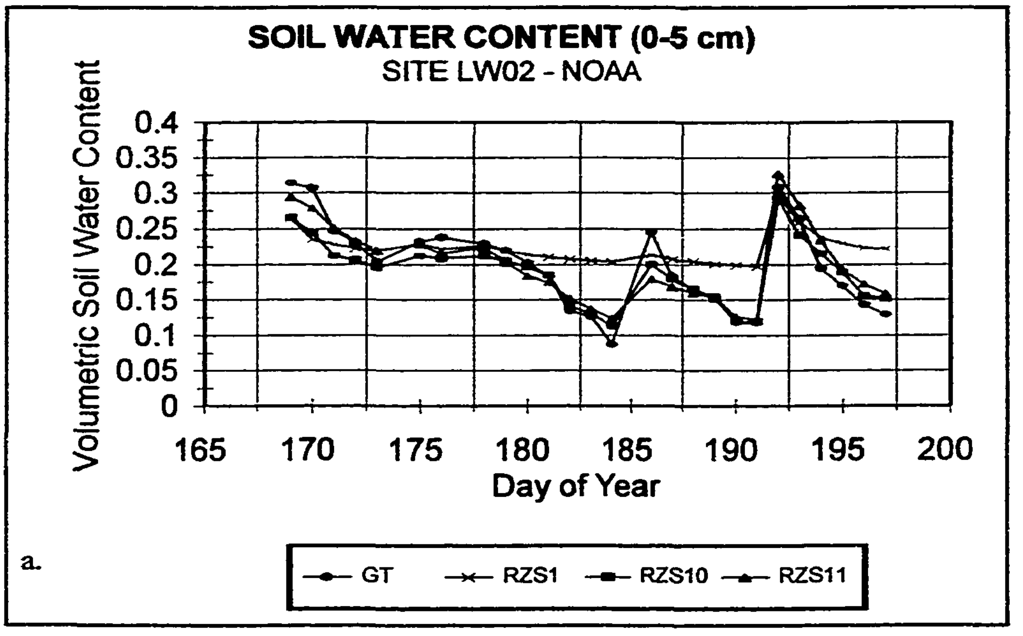
Table 4.2. (Continued)

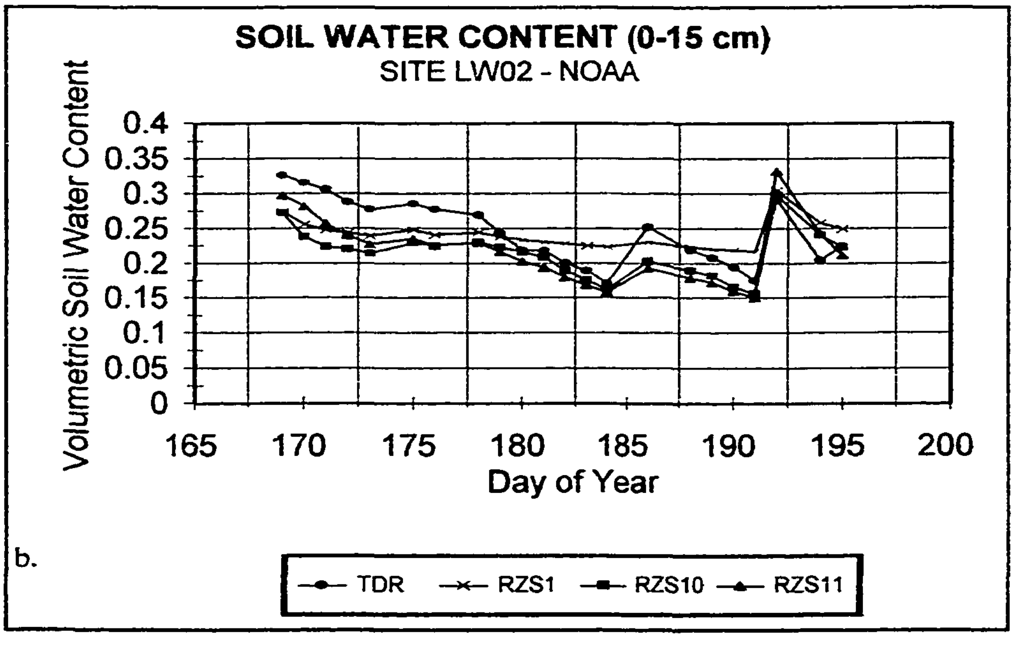
Site/Scenario	Depth of Layer (cm)				
	Layer 0-5	Layer 0-15	Layer 15-30	Layer 30-45	Layer 45-60
LW06-133					
RZS1					
Mean Bias ($m^3 m^{-3}$)	0.020	-0.023	0.010	-0.040	-0.007
RMS Error ($m^3 m^{-3}$)	0.051	0.032	0.016	0.040	0.009
Correlation Coefficient	0.826	0.869	0.830	0.859	0.967
RZS10					
Mean Bias ($m^3 m^{-3}$)	0.030	0.019	0.077	0.074	0.053
RMS Error ($m^3 m^{-3}$)	0.040	0.034	0.083	0.054	0.062
Correlation Coefficient	0.928	0.749	0.073	0.648	0.755
RZS12					
Mean Bias ($m^3 m^{-3}$)	-0.006	-0.038	0.003	-0.043	-0.011
RMS Error ($m^3 m^{-3}$)	0.027	0.044	0.016	0.046	0.014
Correlation Coefficient	0.934	0.881	0.824	0.800	0.946

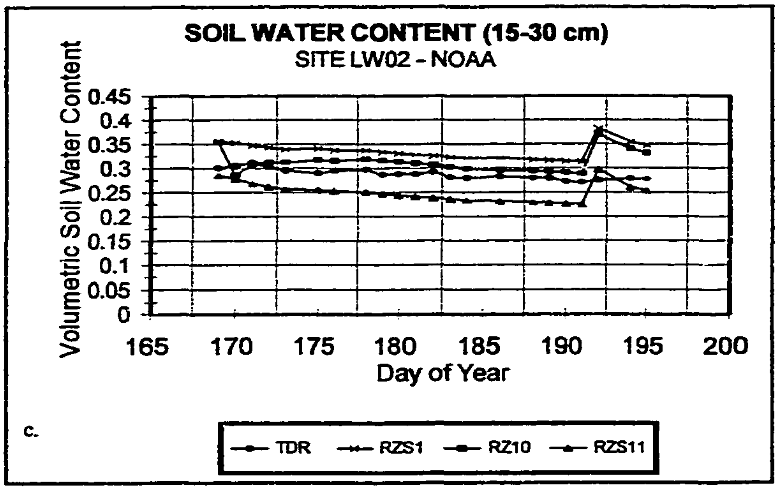
Figure 4.1. Map of LWRW 4 "data assimilation" modeling sites and *Micronet* locations.

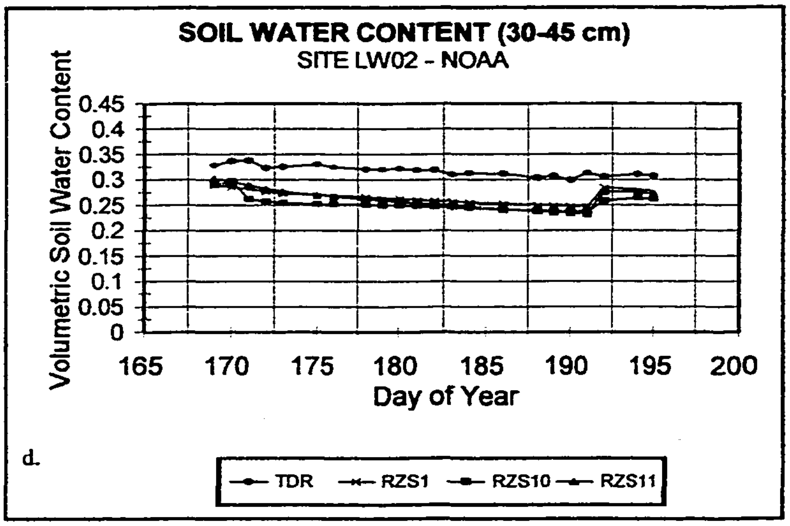


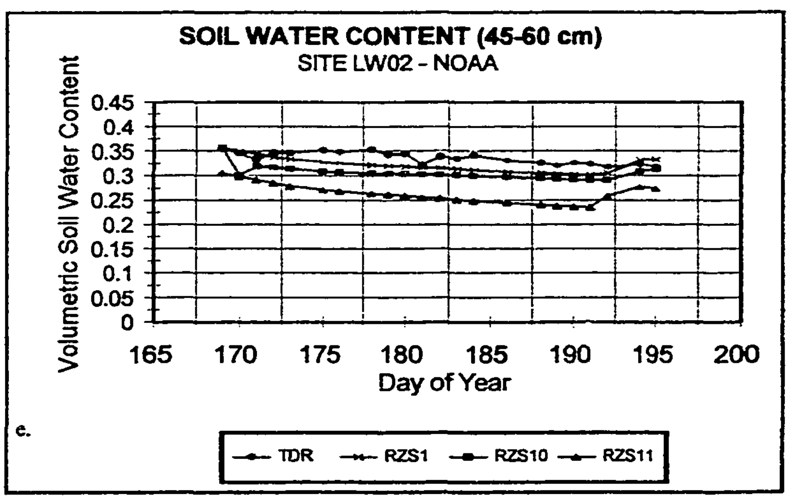
Figures 4.2a-e. Site LW02 profile soil moisture time series data for measured (GT or TDR), limited data (RZS1), assimilation only (RZS10), and assimilation with RS 1/3 bar property (RZS11).



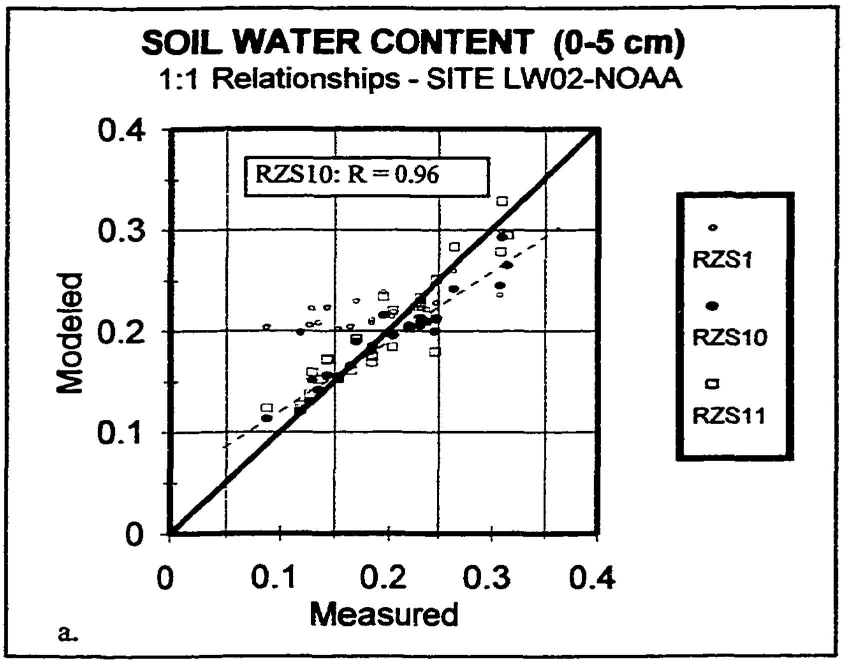



SOIL WATER CONTENT (15-30 cm)
SITE LW02 - NOAA
Volumetric Soil Water Content
0.45
0.4
0.35
0.3
0.25
0.2
0.15
0.1
0.05
0
165
170
175
180
185
190
195
200
Day of Year
c.
TDR
RZS1
RZ10
RZS11

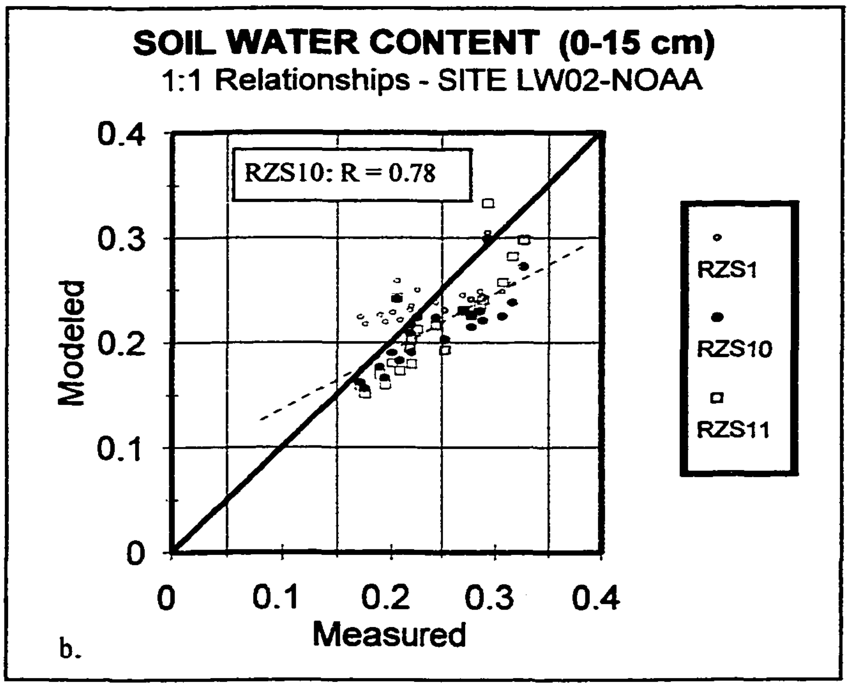

SOIL WATER CONTENT (30-45 cm)
SITE LW02 - NOAA
Volumetric Soil Water Content
0.45
0.4
0.35
0.3
0.25
0.2
0.15
0.1
0.05
0
165
170
175
180
185
190
195
200
Day of Year
d.
TDR
RZS1
RZS10
RZS11


SOIL WATER CONTENT (45-60 cm)
SITE LW02 - NOAA
Volumetric Soil Water Content
0.45
0.4
0.35
0.3
0.25
0.2
0.15
0.1
0.05
0
165
170
175
180
185
190
195
200
Day of Year
e.
TDR
RZS1
RZS10
RZS11

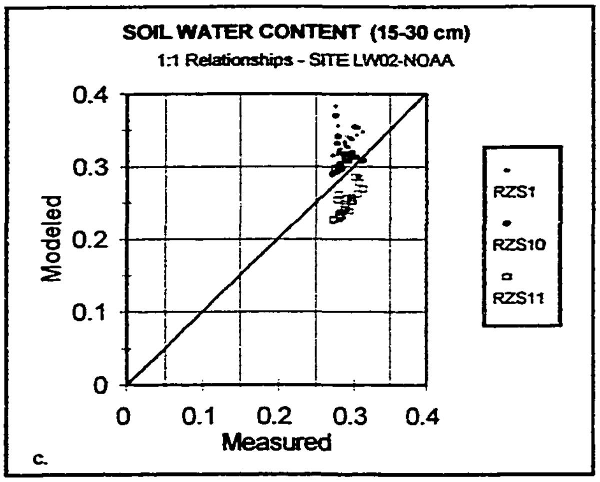
Figures 4.3a-e. Site LW02 modeled vs measured 1:1 data for different soil layers with best fit correlation in graph text box.

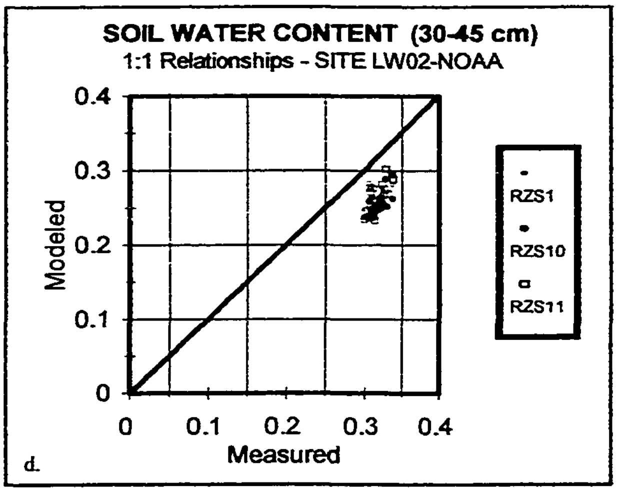


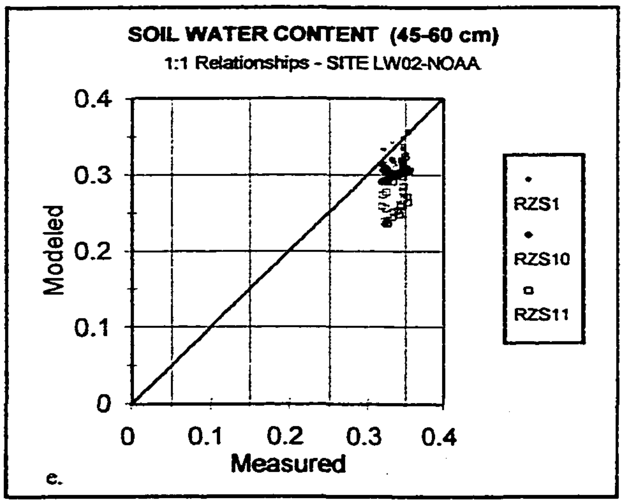
a.



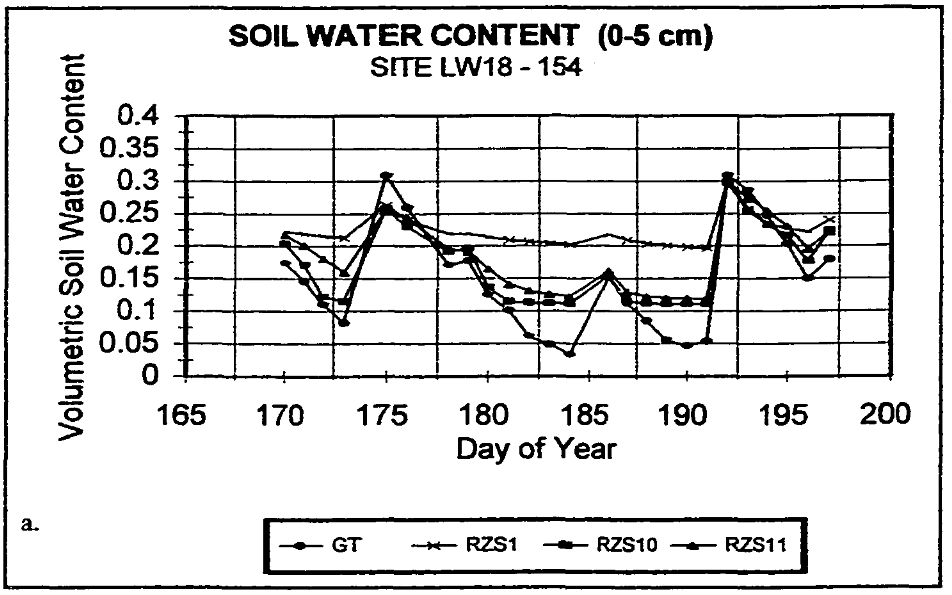
b.


SOIL WATER CONTENT (15-30 cm)
1:1 Relationships - SITE LW02-NOAA
Modeled
Measured
0
0.1
0.2
0.3
0.4
RZS1
RZS10
RZS11
c.

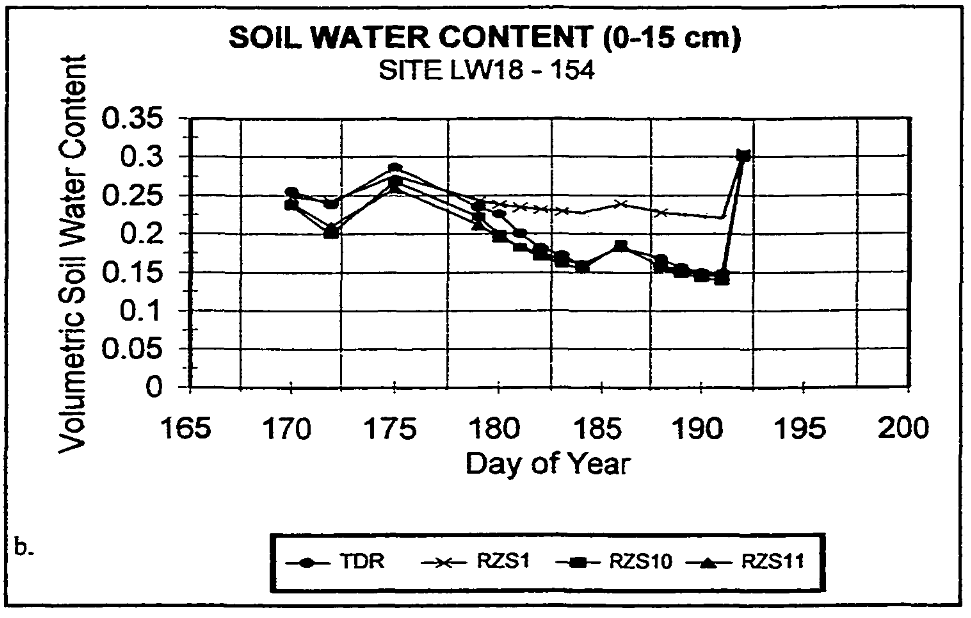

SOIL WATER CONTENT (30-45 cm)
1:1 Relationships - SITE LW02-NOAA
Modeled
Measured
0
0.1
0.2
0.3
0.4
RZS1
RZS10
RZS11
d.


SOIL WATER CONTENT (45-60 cm)
1:1 Relationships - SITE LW02-NOAA
Modeled
Measured
0
0.1
0.2
0.3
0.4
RZS1
RZS10
RZS11
e.

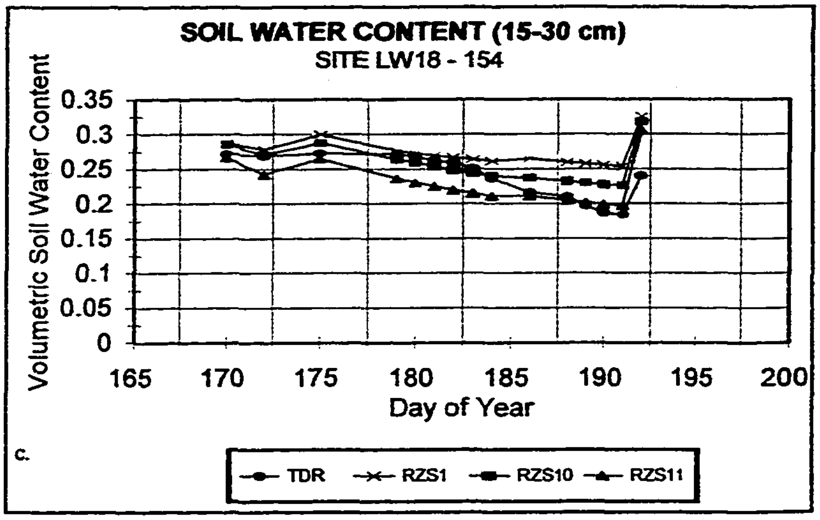
Figures 4.4a-e. Site 154 profile soil moisture time series data for measured (GT or TDR), limited data (RZS1), assimilation only (RZS10), and assimilation with RS 1/3 bar property (RZS11).

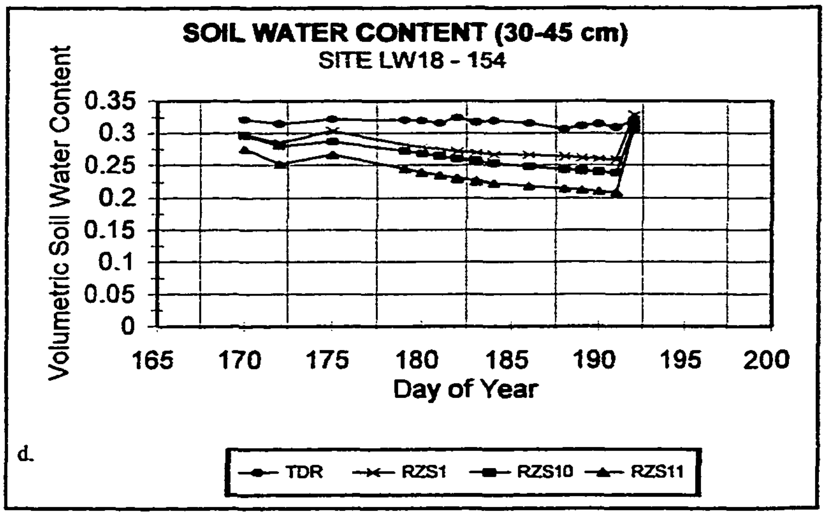


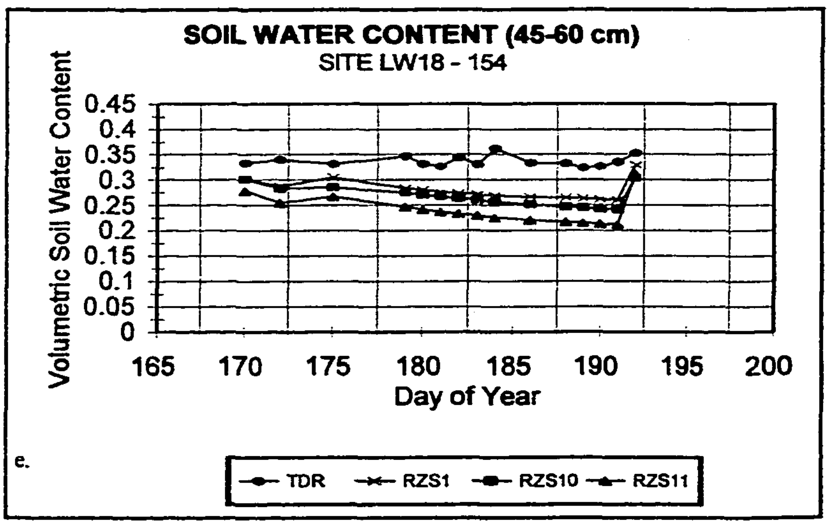
a.



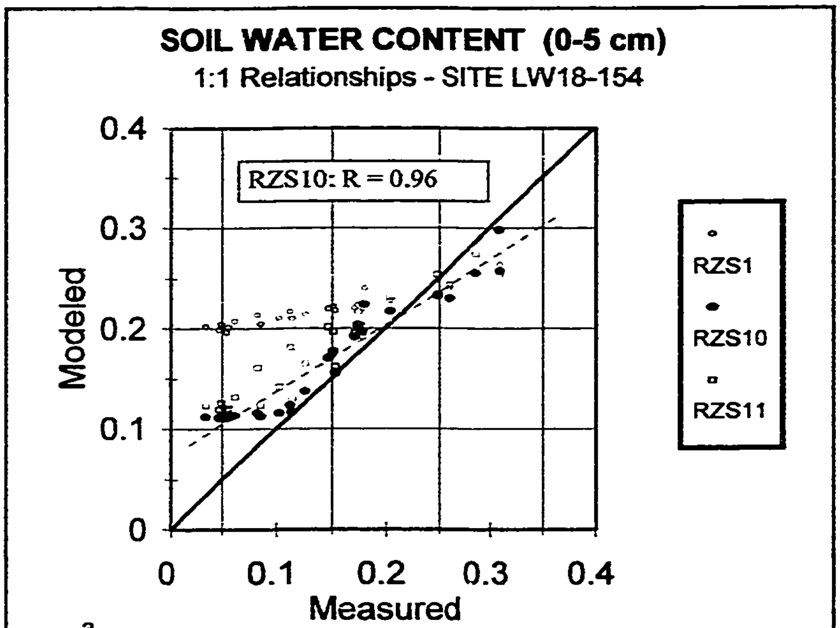
b.


SOIL WATER CONTENT (15-30 cm)
SITE LW18 - 154
Volumetric Soil Water Content
0.35
0.3
0.25
0.2
0.15
0.1
0.05
0
165
170
175
180
185
190
195
200
Day of Year
c.
TDR
RZS1
RZS10
RZS11

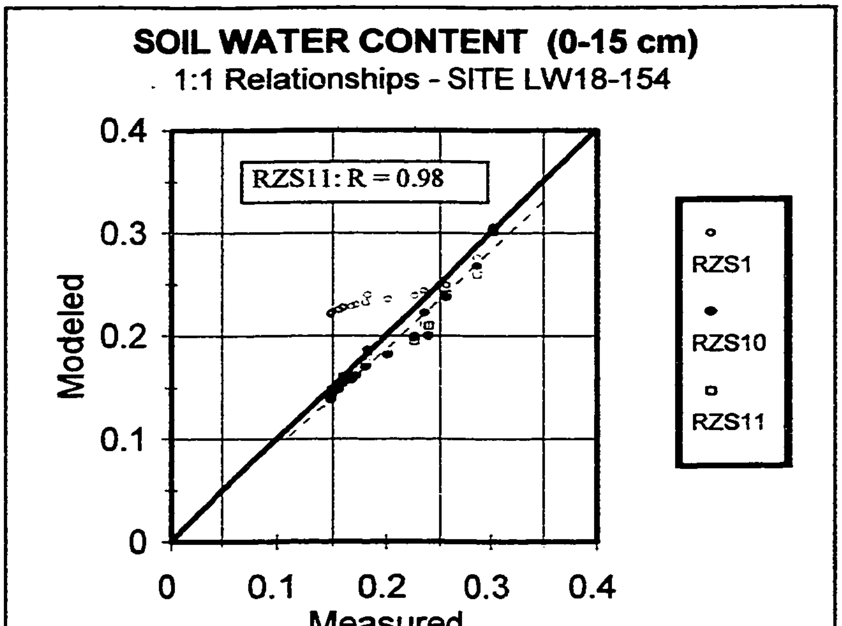

SOIL WATER CONTENT (30-45 cm)
SITE LW18 - 154
Volumetric Soil Water Content
0.35
0.3
0.25
0.2
0.15
0.1
0.05
0
165
170
175
180
185
190
195
200
Day of Year
d.
TDR
RZS1
RZS10
RZS11


SOIL WATER CONTENT (45-60 cm)
SITE LW18 - 154
Volumetric Soil Water Content
0.45
0.4
0.35
0.3
0.25
0.2
0.15
0.1
0.05
0
165
170
175
180
185
190
195
200
Day of Year
e.
TDR
RZS1
RZS10
RZS11

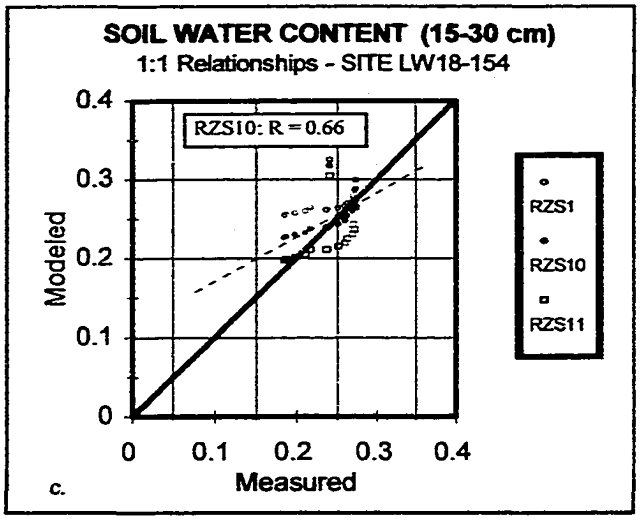
Figures 4.5a-e. Site 154 modeled vs measured 1:1 θ_v data for different soil layers with best fit correlation in graph text box.

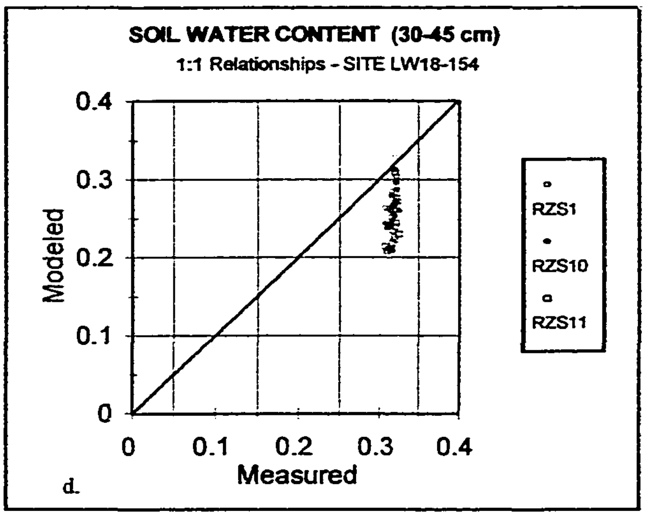


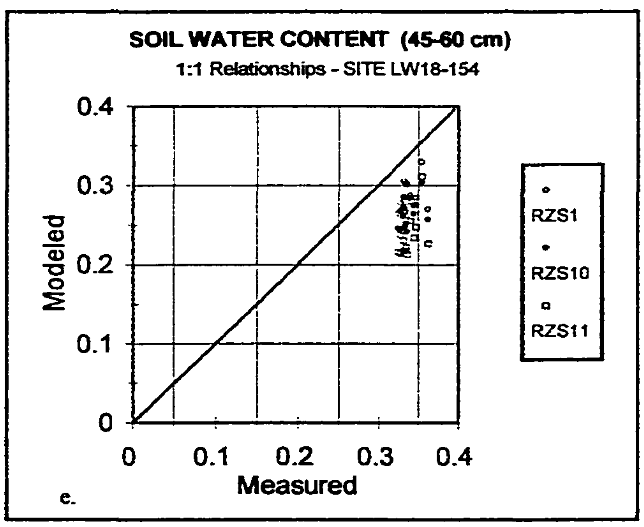
a.



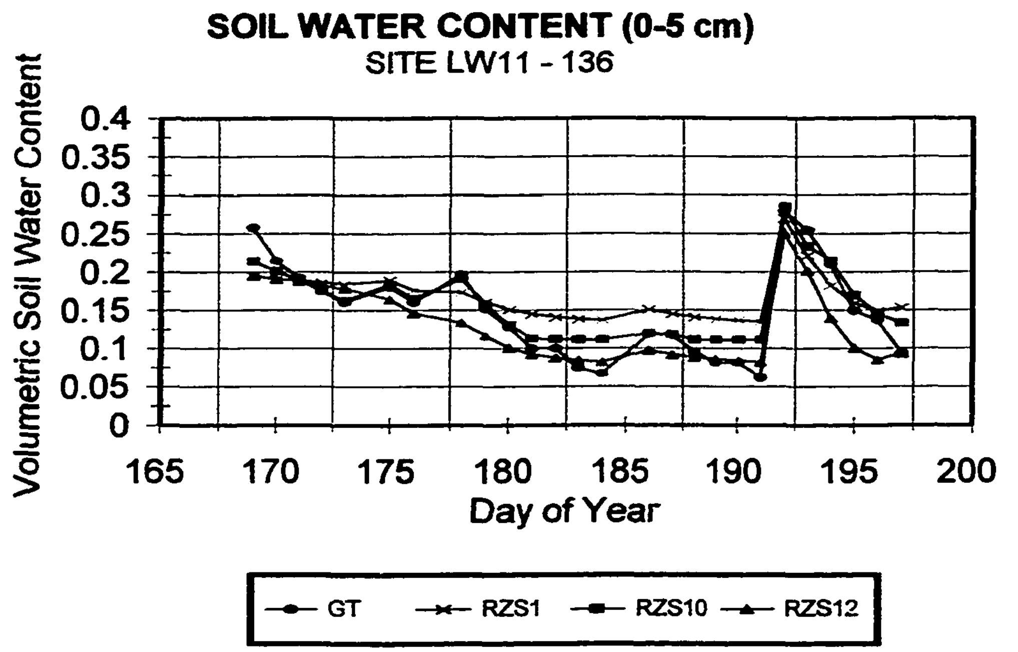
b.


SOIL WATER CONTENT (15-30 cm)
1:1 Relationships - SITE LW18-154
RZS10: R = 0.66
Modeled
Measured
0.4
0.3
0.2
0.1
0
0.1
0.2
0.3
0.4
RZS1
RZS10
RZS11
c.

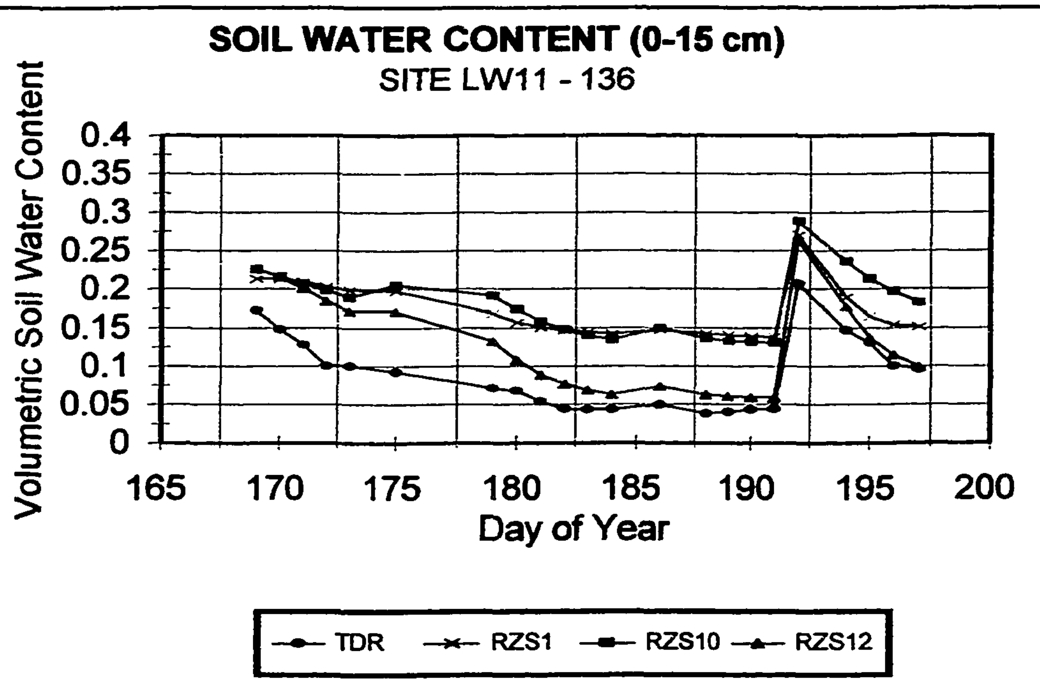

SOIL WATER CONTENT (30-45 cm)
1:1 Relationships - SITE LW18-154
Modeled
Measured
0.4
0.3
0.2
0.1
0
0.1
0.2
0.3
0.4
RZS1
RZS10
RZS11
d.


SOIL WATER CONTENT (45-60 cm)
1:1 Relationships - SITE LW18-154
Modeled
Measured
0.4
0.3
0.2
0.1
0
0.1
0.2
0.3
0.4
RZS1
RZS10
RZS11
e.

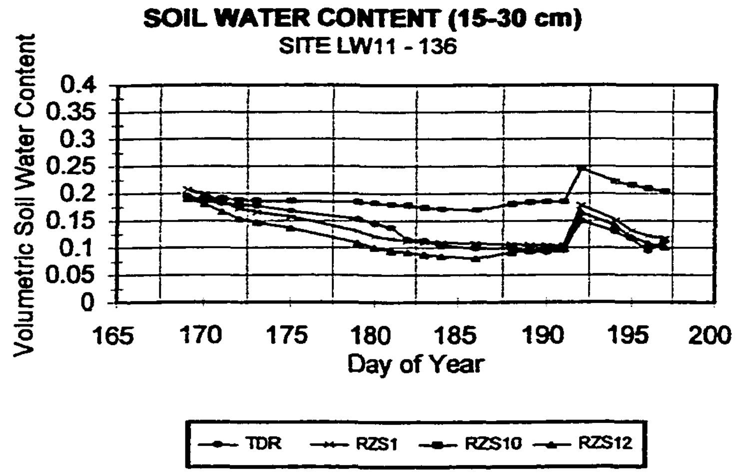
Figures 4.6a-e. Site 136 profile soil moisture time series data for measured (GT or TDR), limited data (RZS1), assimilation only (RZS10), and assimilation with plant uptake (RZS12).



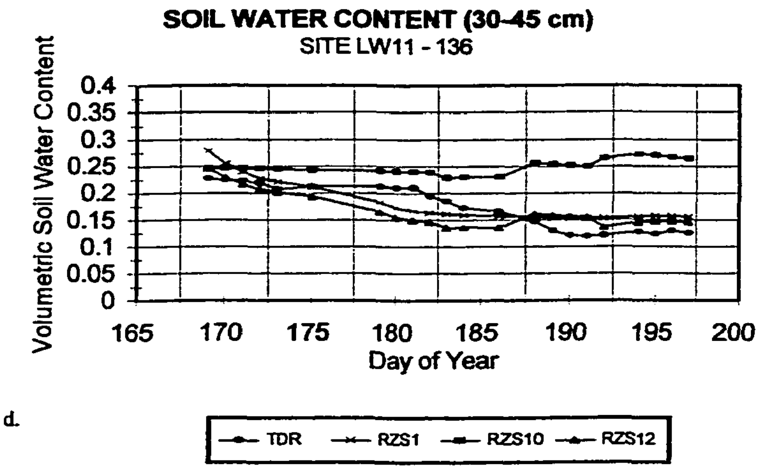
a.



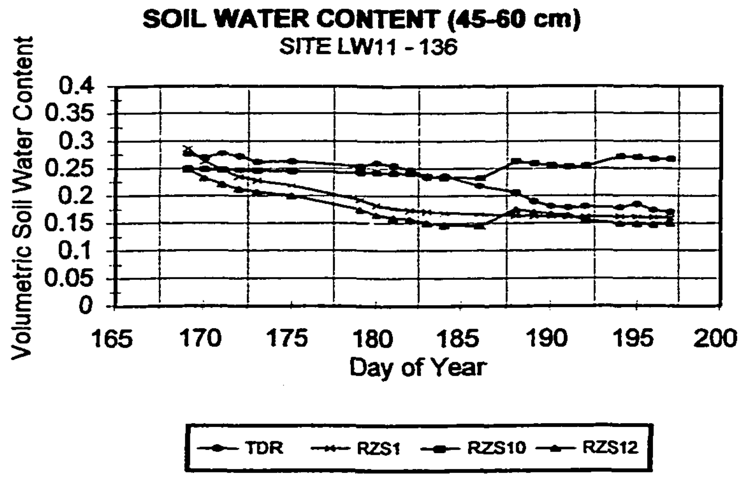
b.


SOIL WATER CONTENT (15-30 cm)
SITE LW11 - 136
Volumetric Soil Water Content
0.4
0.35
0.3
0.25
0.2
0.15
0.1
0.05
0
165
170
175
180
185
190
195
200
Day of Year
TDR
RZS1
RZS10
RZS12

c.

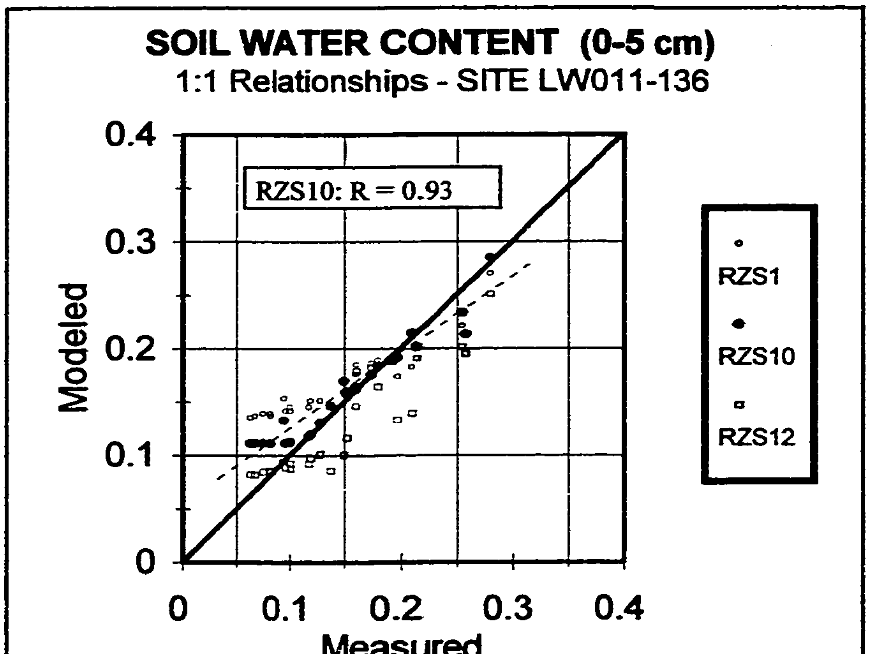

SOIL WATER CONTENT (30-45 cm)
SITE LW11 - 136
Volumetric Soil Water Content
0.4
0.35
0.3
0.25
0.2
0.15
0.1
0.05
0
165
170
175
180
185
190
195
200
Day of Year
TDR
RZS1
RZS10
RZS12

d.

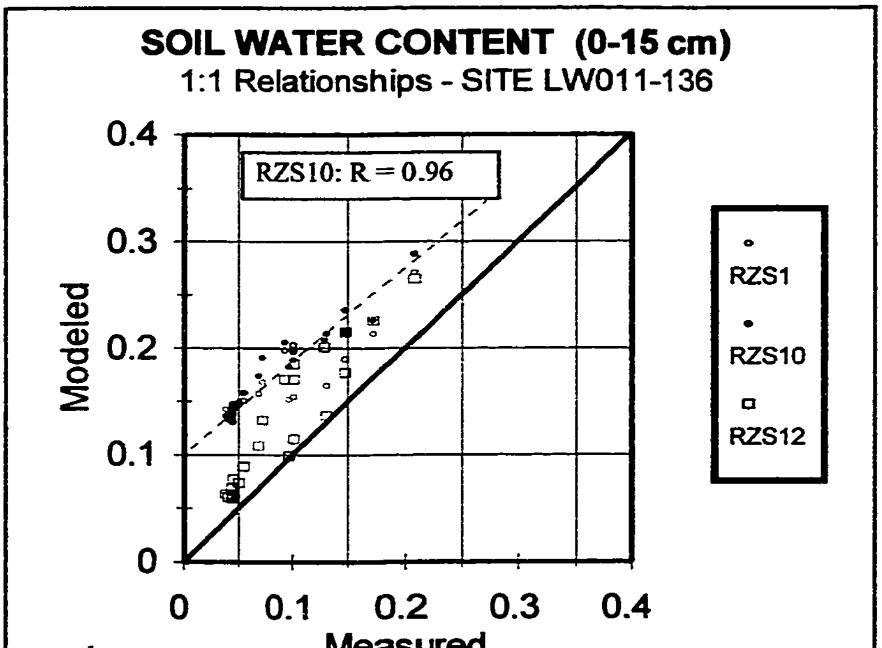

SOIL WATER CONTENT (45-60 cm)
SITE LW11 - 136
Volumetric Soil Water Content
0.4
0.35
0.3
0.25
0.2
0.15
0.1
0.05
0
165
170
175
180
185
190
195
200
Day of Year
TDR
RZS1
RZS10
RZS12

e.

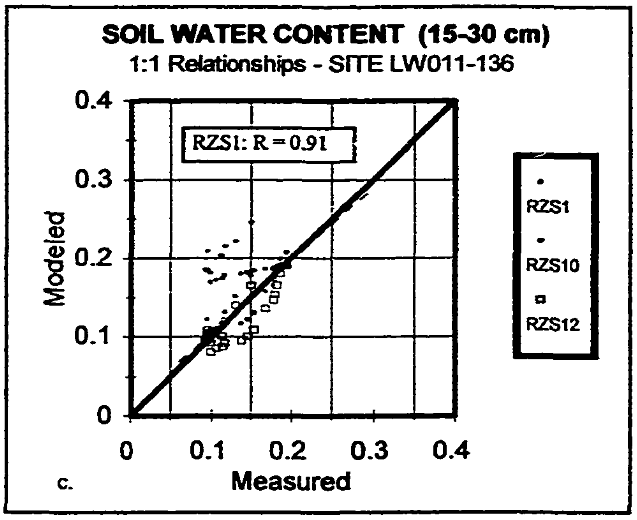
Figure 4.7a-e. Site 136 modeled vs measured 1:1 θ_v data for different soil layers with best fit correlation in graph text box.

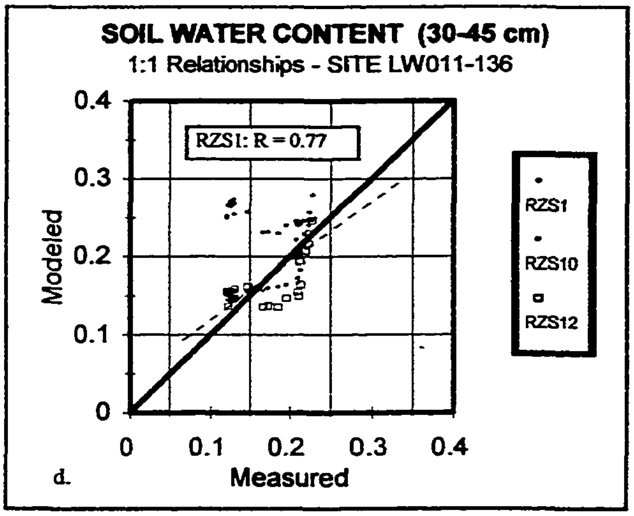


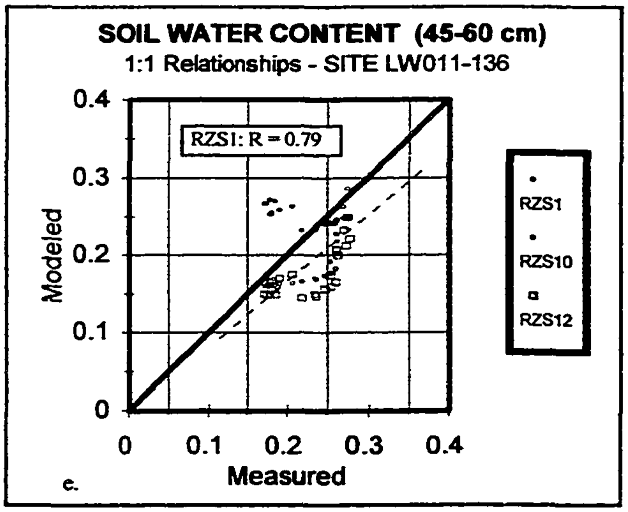
a.



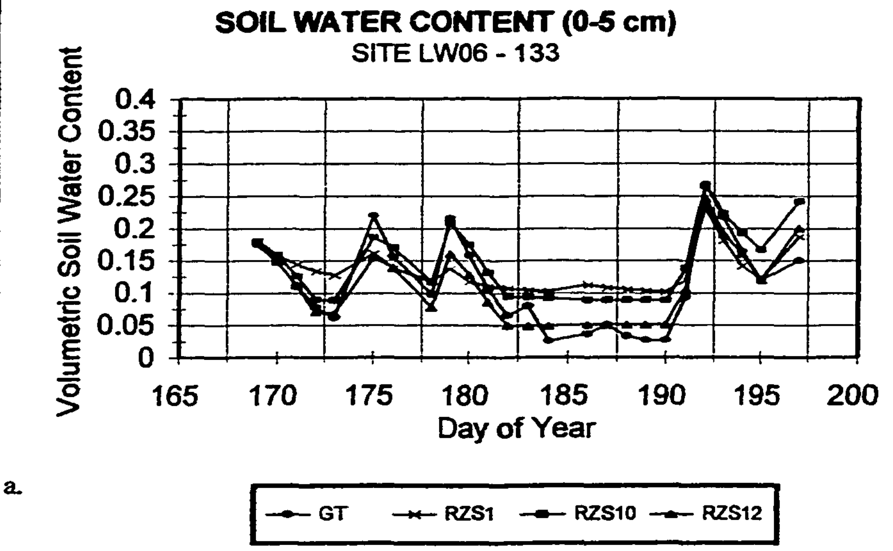
b.


SOIL WATER CONTENT (15-30 cm)
1:1 Relationships - SITE LW011-136
RZS1: R = 0.91
Modeled
Measured
0
0.1
0.2
0.3
0.4
RZS1
RZS10
RZS12
c.

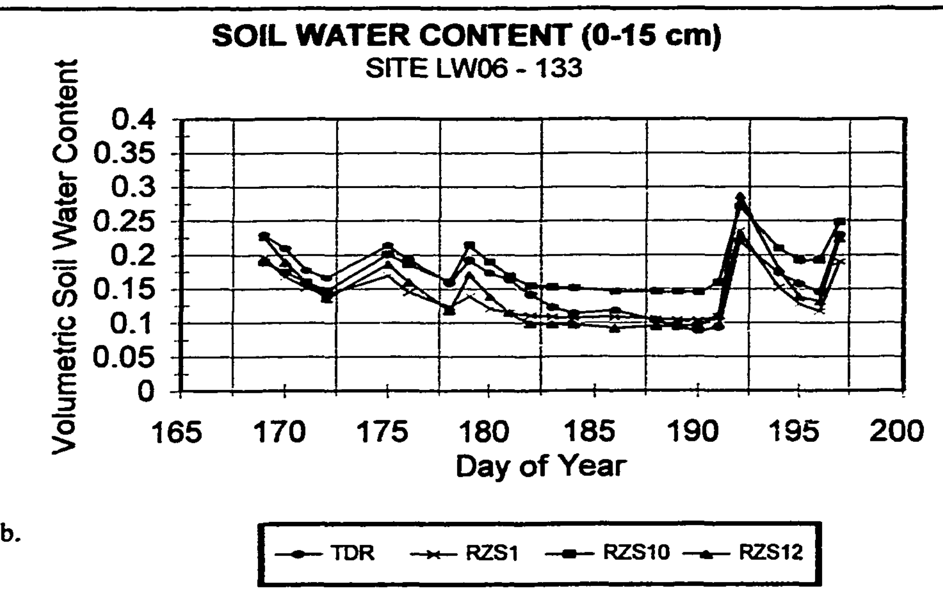

SOIL WATER CONTENT (30-45 cm)
1:1 Relationships - SITE LW011-136
RZS1: R = 0.77
Modeled
Measured
0
0.1
0.2
0.3
0.4
RZS1
RZS10
RZS12
d.


SOIL WATER CONTENT (45-60 cm)
1:1 Relationships - SITE LW011-136
RZS1: R = 0.79
Modeled
Measured
0
0.1
0.2
0.3
0.4
RZS1
RZS10
RZS12
e.

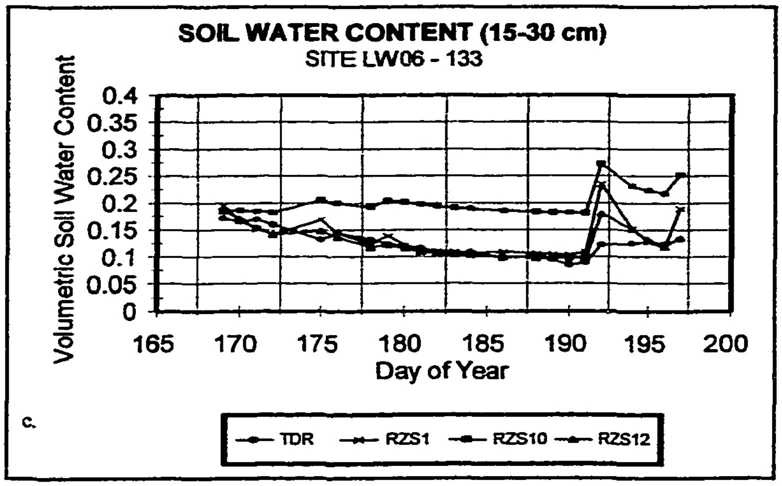
Figures 4.8a-e. Site 133 profile soil moisture time series data for measured (GT or TDR), limited data (RZS1), assimilation only (RZS10), and assimilation with plant uptake (RZS12).

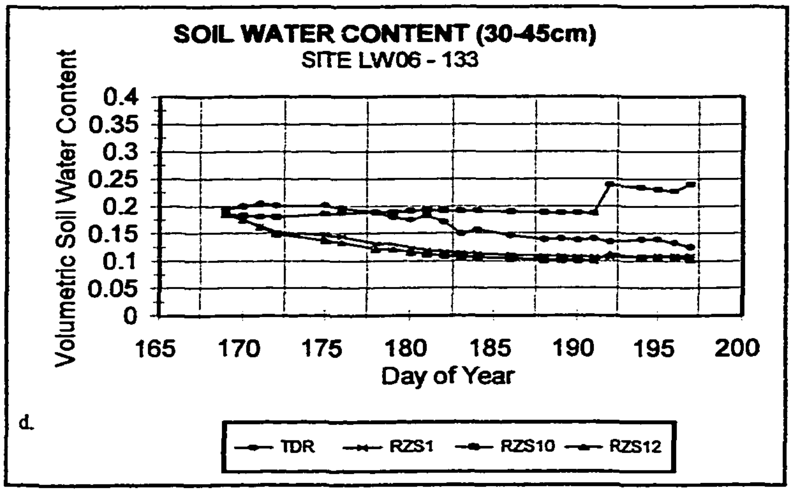


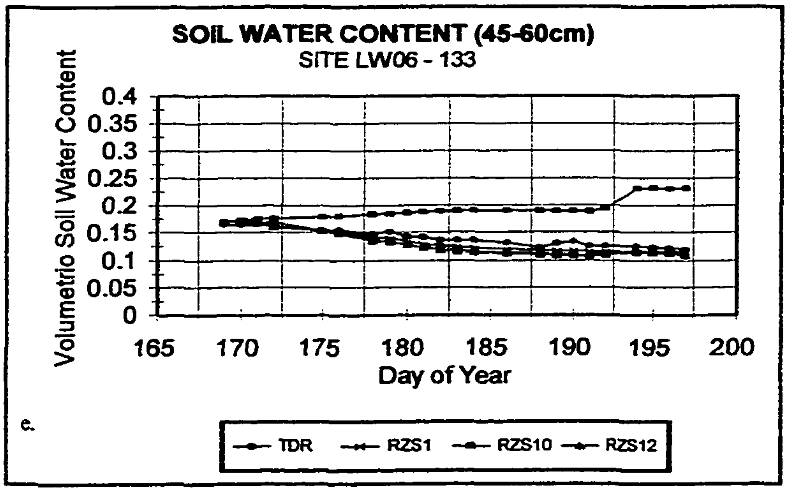
a.



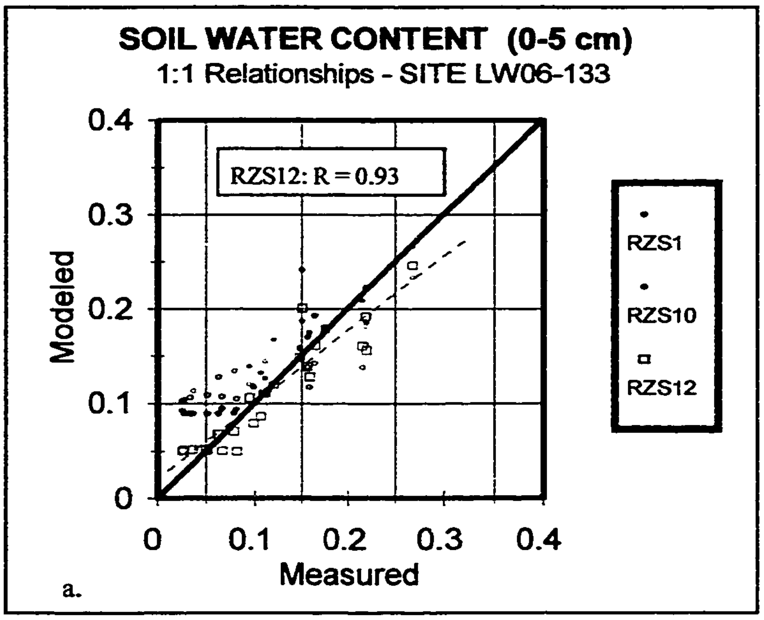
b.

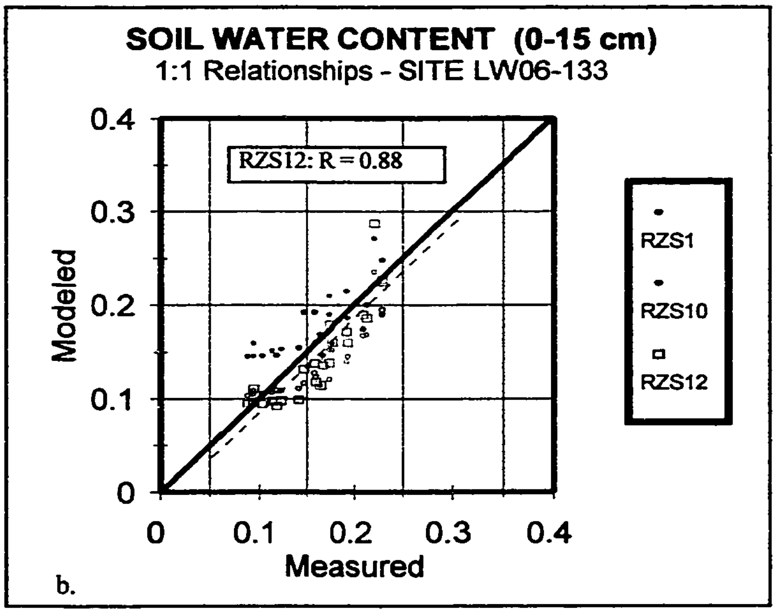

SOIL WATER CONTENT (15-30 cm)
SITE LW06 - 133
Volumetric Soil Water Content
0.4
0.35
0.3
0.25
0.2
0.15
0.1
0.05
0
165 170 175 180 185 190 195 200
Day of Year
c.
TDR RZS1 RZS10 RZS12

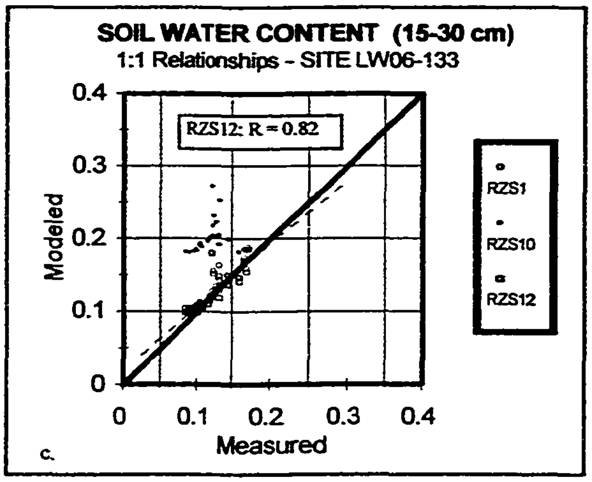

SOIL WATER CONTENT (30-45cm)
SITE LW06 - 133
Volumetric Soil Water Content
0.4
0.35
0.3
0.25
0.2
0.15
0.1
0.05
0
165 170 175 180 185 190 195 200
Day of Year
d.
TDR RZS1 RZS10 RZS12

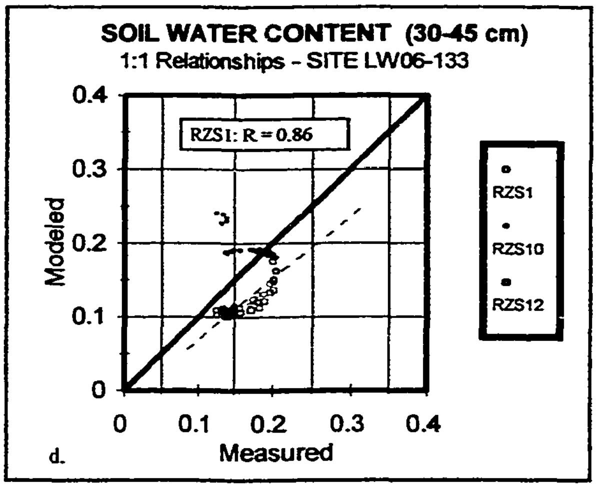

SOIL WATER CONTENT (45-60cm)
SITE LW06 - 133
Volumetric Soil Water Content
0.4
0.35
0.3
0.25
0.2
0.15
0.1
0.05
0
165 170 175 180 185 190 195 200
Day of Year
e.
TDR RZS1 RZS10 RZS12

Figures 4.9a-e. Site 133 modeled vs measured 1:1 θ_v data for different soil layers with best fit correlation in graph text box.






SOIL WATER CONTENT (15-30 cm)
1:1 Relationships - SITE LW06-133
RZS12: R = 0.82
Modeled
Measured
RZS1
RZS10
RZS12
c.


SOIL WATER CONTENT (30-45 cm)
1:1 Relationships - SITE LW06-133
RZS1: R = 0.86
Modeled
Measured
RZS1
RZS10
RZS12
d.

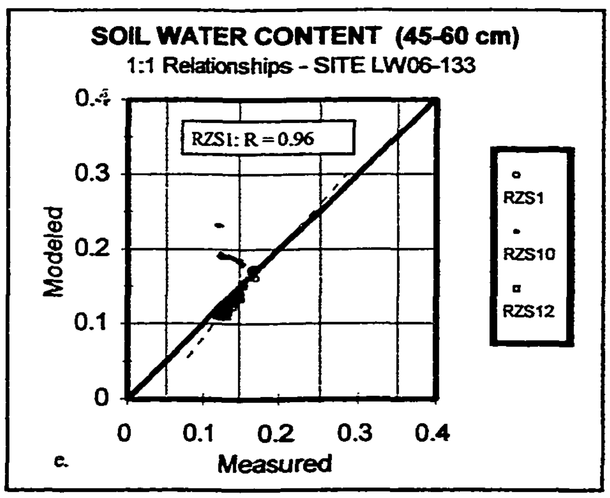

SOIL WATER CONTENT (45-60 cm)
1:1 Relationships - SITE LW06-133
RZS1: R = 0.96
Modeled
Measured
RZS1
RZS10
RZS12
e.

Figure 4.10a. Map showing 42 Micronet rainfall measurements (mm) during SGP'97, on July 10, with 1 km interpolation scheme using ArcView GIS spatial analyst.

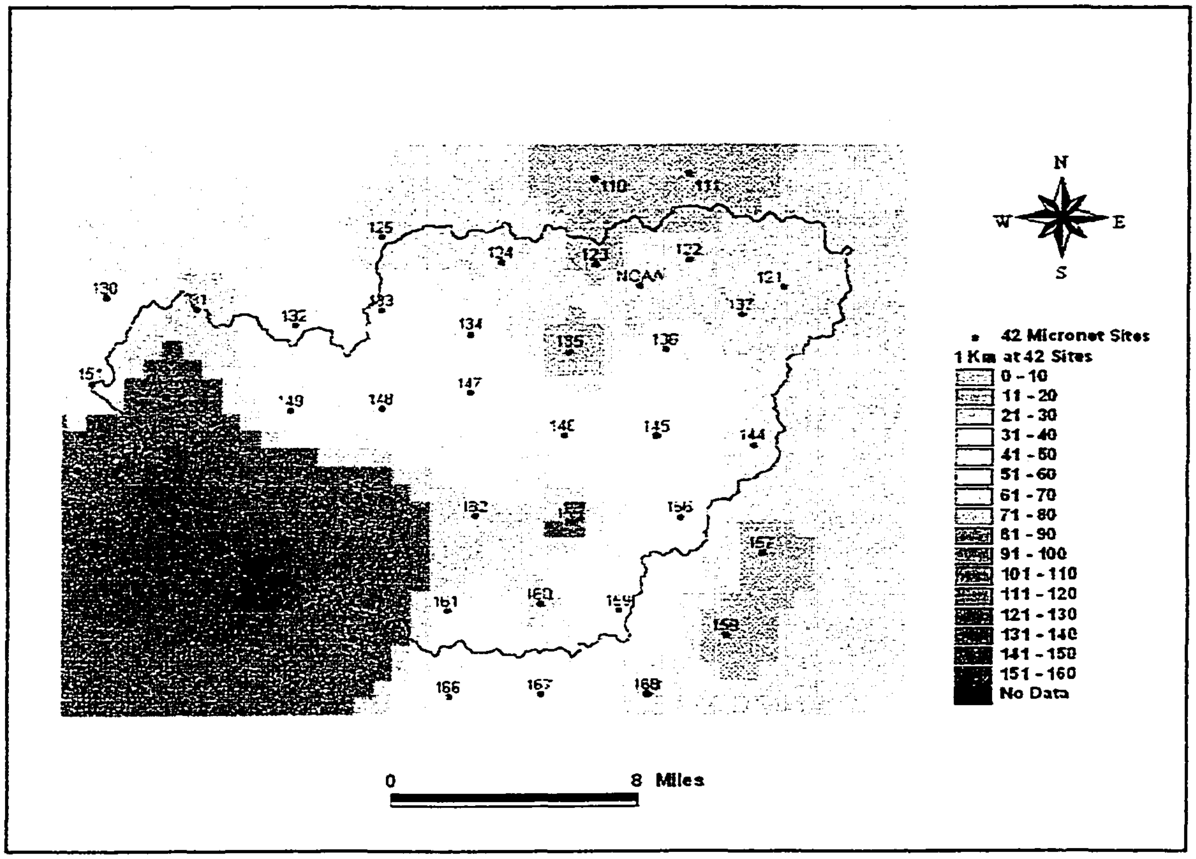


Figure 4.10b. Map showing 19 Micronet rainfall measurements (mm) during SGP'97, on July 10, with 1 km interpolation scheme using ArcView GIS spatial analyst.

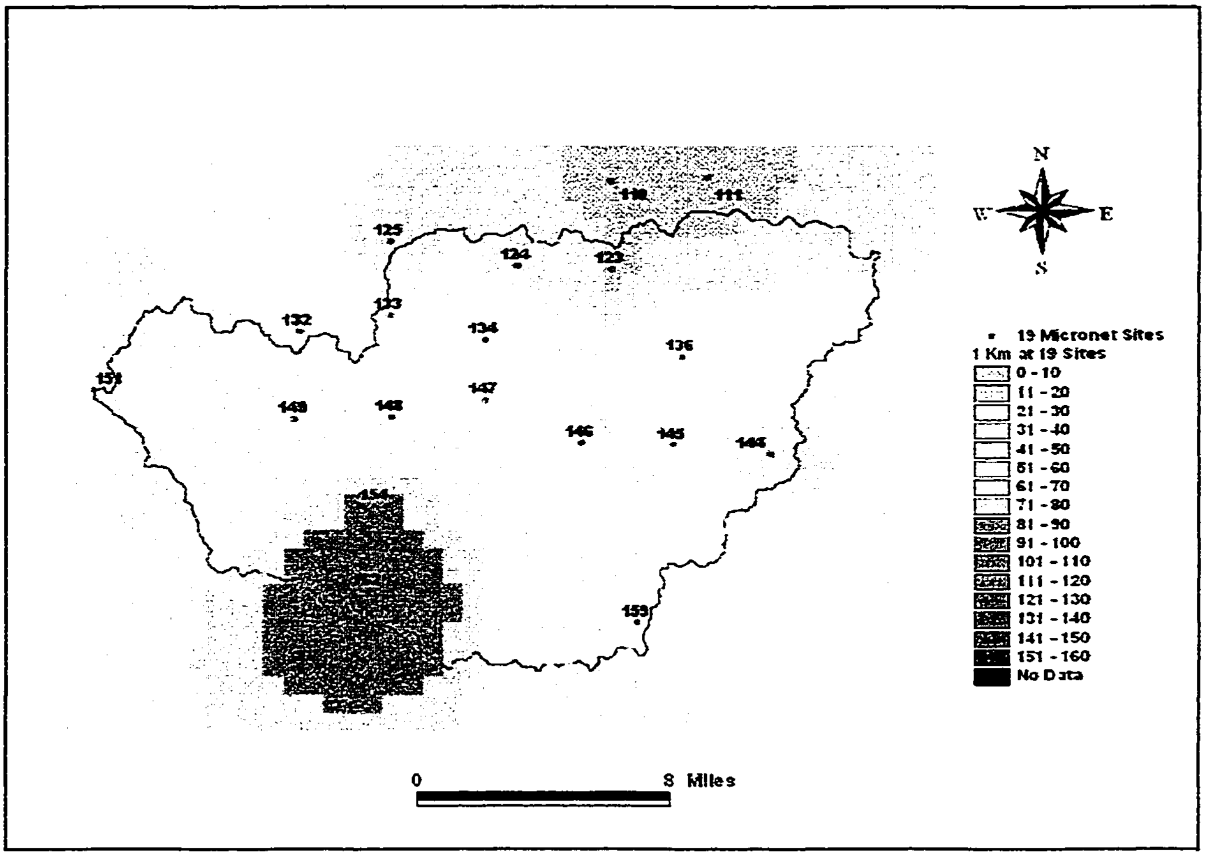


Figure 4.10c. Map showing the difference (loss of information) between having 42 vs 19 points of rainfall measurement for the same rainfall event during SGP'97, on July 10.

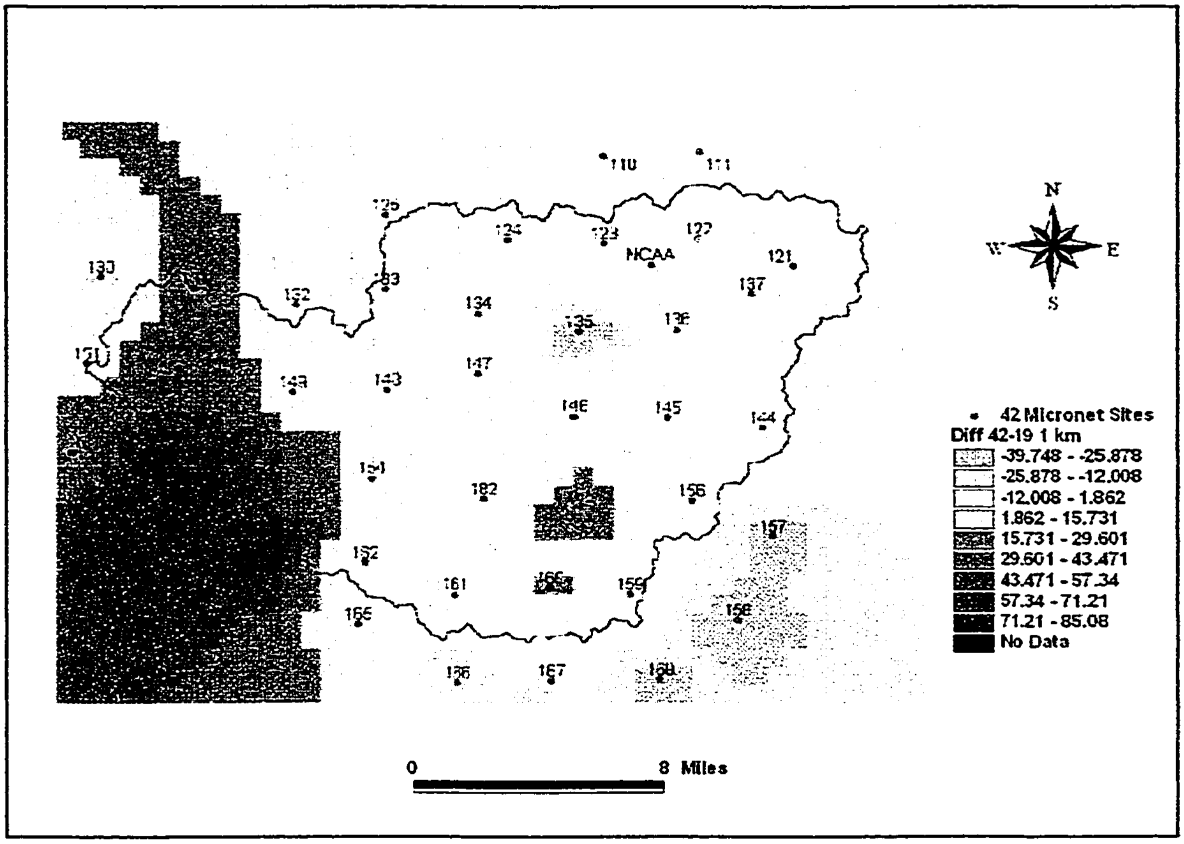


Figure 4.11a. Map showing Estar surface soil moisture (percent volumetric) observations during SGP'97, on July 11. An example of assimilation input data at the 1 km scale.

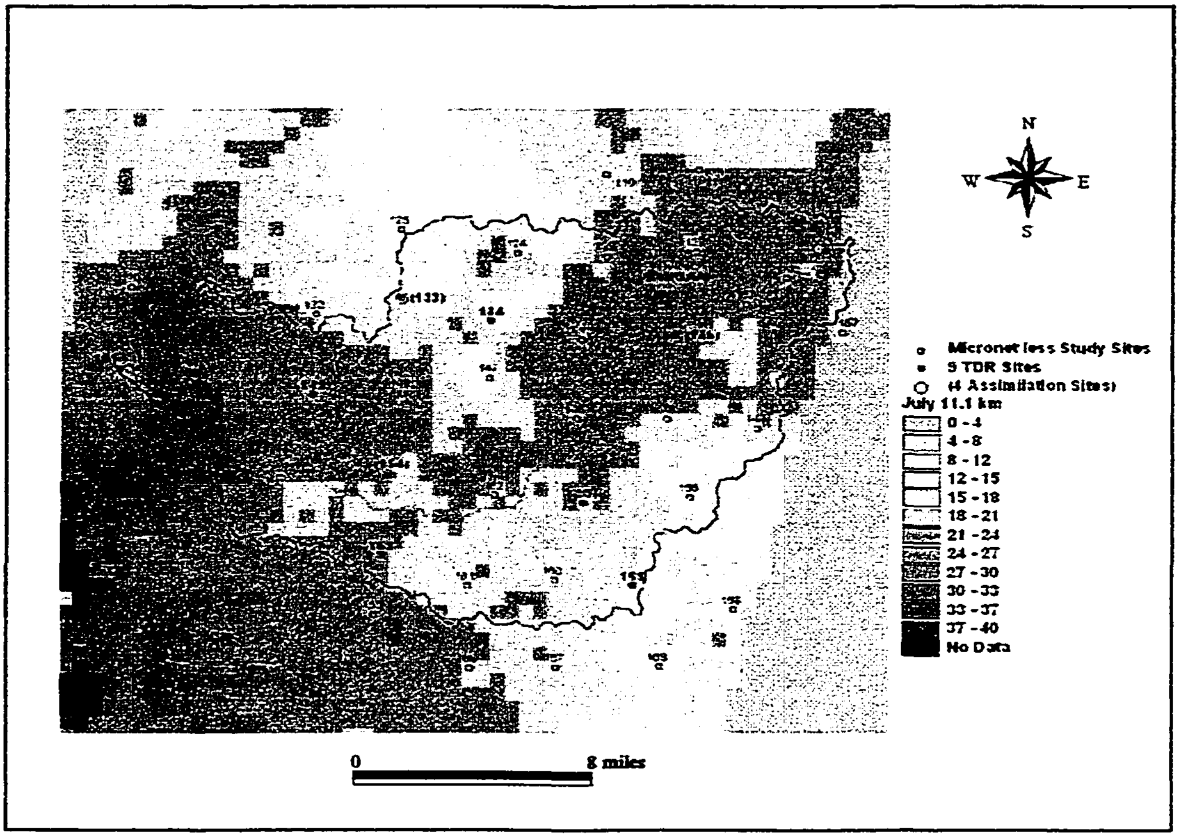


Figure 4.11b. Map showing Estar surface soil moisture observations (percent volumetric) during SGP'97, on July 13. An example of assimilation input data and 1/3 bar 2-day drainage data at the 1 km scale.

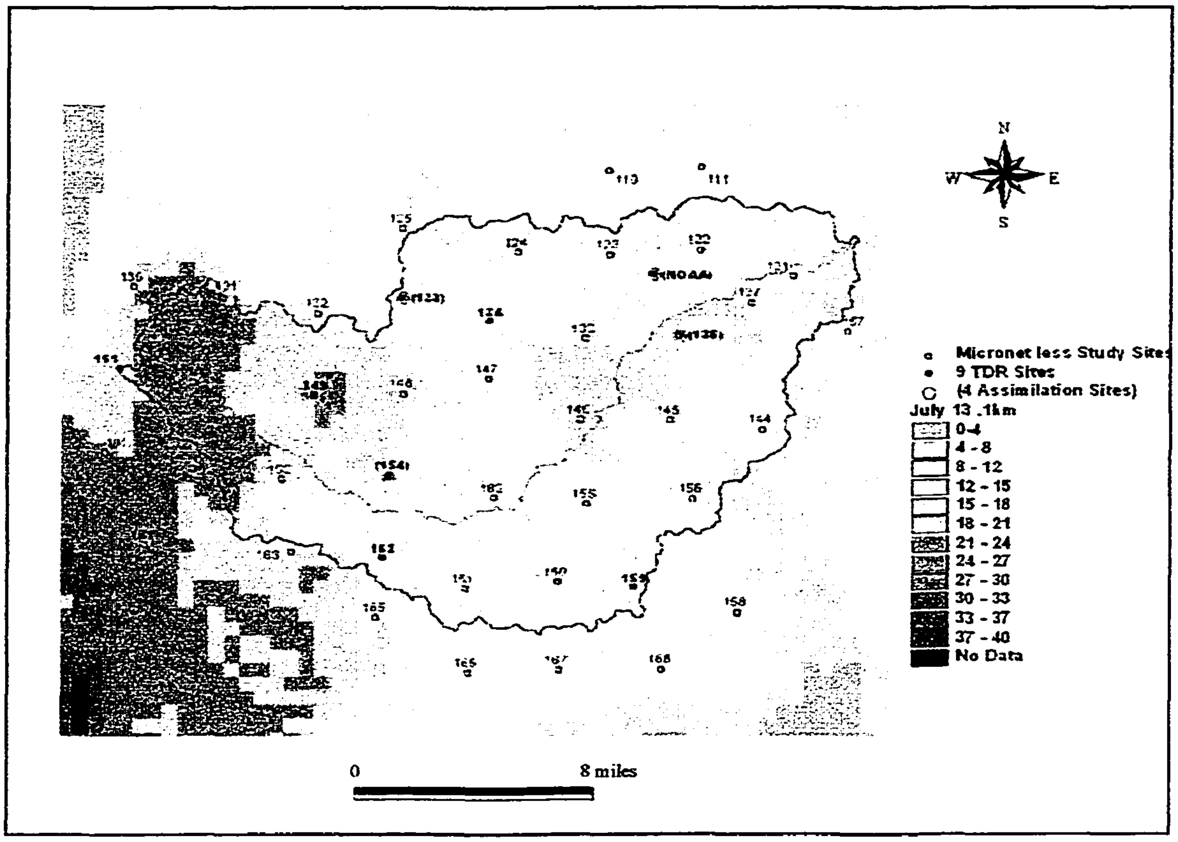
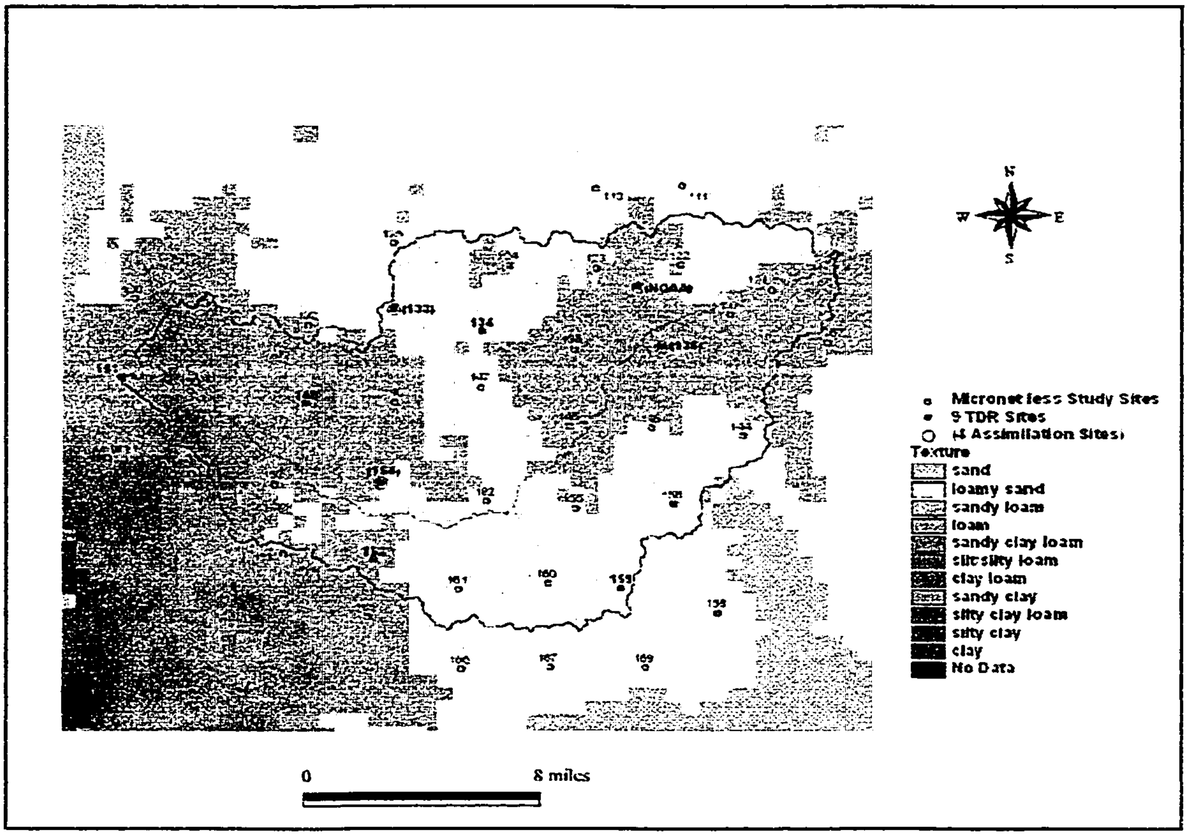


Figure 4.11c. Map showing soil texture derived from ESTAR 2-day drainage data during SGP'97, on July 13 at 1 km scale.



5. SUMMARY, CONCLUSIONS AND RECOMMENDATIONS

The interactive use of selective experimentation and computational modeling is an efficient way to devise and evaluate new approaches for solving many issues in hydrologic research. A prime example for application of this concept is research involving soil moisture dynamics. Soil moisture links the hydrologic cycle and the energy budget of land surfaces by governing the partitioning of surface radiative energy between latent and sensible heat fluxes. Accurate measurement of soil moisture is essential to many areas of environmental, agricultural, and water resource management. Validated data sets of *in situ* soil moisture data are considered a priority to successfully evaluate new hydrologic theories, models, and remote sensing techniques. According to a recent agenda for land surface hydrology research and a call for the second international hydrological decade, the use of remotely sensed surface soil moisture data assimilation into hydrologic models has received considerable attention (Entekhabi et al., 1999). By combining a one-dimensional coupled heat and moisture diffusion model for porous media and radiative transfer model, Entekhabi et al. (1994) theoretically demonstrated the feasibility of estimating the soil moisture and temperature profiles by solving the "inverse" problem using simulated time-varying remote sensing measurements as upper boundary conditions. Walker et al. (2001) reported in a recent study that only a few studies have assimilated near-surface soil moisture data into a hydrologic model with the objective to improve predictions of evapotranspiration or runoff, or to estimate profile soil moisture for a one-dimensional soil column using synthetic data, and a very short update interval..

The goal of this research was to evaluate the use of limited soil data information, surface soil moisture data assimilation, and soil water modeling in estimating root zone soil water content and soil hydraulic properties at several locations within the Little Washita River Watershed (LWRW) in south central Oklahoma. The results of the work are based on the interactive use of good quality experimental field work, computational modeling, and the technique of direct insertion data assimilation. This type of research approach is unique in that, to date, such a study has not been presented in the literature. The sections below summarize the results for each chapter in this thesis, followed by an overall summary.

Experimental TDR Field Calibration

In Chapter 2, four calibration methods were evaluated for determining volumetric profile soil water content from time domain reflectometry (TDR) data at nine locations within the Little Washita River Watershed (LWRW). Comparisons were made between soil water content as determined by the factory calibration, two methods of site-specific calibration, and a general calibration technique. Values of soil water content determined by each calibration method were compared to the actual soil-core water content data taken at the time of calibration, as well as to an independent collection of soil-core samples. Method 1 is the factory calibration which uses average values for model coefficients that were derived from extensive laboratory work and theoretical analysis. Method 2 fits a site-specific linear regression of TDR time delay on measured soil-core water content. Regression analysis for nine field sites gave coefficients of determination (r^2) between 0.74

and 0.87. Root mean square errors (RMSE) ranging from 0.031 to 0.042 $m^3\ m^{-3}$ were obtained with Method 2, compared to a range of 0.032 to 0.078 $m^3\ m^{-3}$ using the factory calibration. An alternative approach using the factory calibration equation and site-specific values for the ratio of TDR time delay in dry soil, to that in air, was adopted as Method 3 that resulted in a RMSE range of 0.032 to 0.057 $m^3\ m^{-3}$. In Method 4, a general equation was developed from a linear regression performed on the data from all sites. The general calibration equation was then applied to TDR time delay data for each site. The results from Method 4 had a range in RMSE of 0.035 to 0.051 $m^3\ m^{-3}$. All field calibration methods show that it is necessary to include very low water content data in determining absolute water content. When compared to the factory calibration, all three field calibration methods improved the measurement of soil water content, with Method 2 providing the most accurate results, being within 3 to 4% of measured values.

The results of this work demonstrate that use of a simple linear relationship between soil water content and TDR time delay output provides an easy means for obtaining site-specific field calibrations. The results from nine field sites with different soil physical properties show that use of a site-specific linear regression approach reduces measurement error, as well as the range of error, when compared to soil moisture values obtained using the factory calibration. It was also found that in collecting soil moisture samples for the regression analysis, it is important that the data set include very low moisture samples in order to determine absolute water content. It should be emphasized that great care should be taken during the collection of soil samples in an effort to minimize sample error. For example, a small error in the measurement of bulk density can have considerable effects on calculating the volumetric water content. It can be concluded from this work that measured dielectric data should be calibrated to the water content of the actual soil involved for determining absolute water content, otherwise the measured soil water content should be considered in relative terms.

Use of Limited Soil Data Information

In Chapter 3, the use of limited soil data information (e.g., texture name only) was evaluated as input for the Root Zone Water Quality Model (RZWQM) in modeling profile soil water content. Calculated profile water contents for 0-60 cm were compared to actual measurements made periodically over the same period of time. Comparisons between RZWQM simulated and measured TDR soil water content values demonstrate the model's capability to provide acceptable estimates of average soil water content at five sites within the LWRW. Experiments were conducted on several different soil types and modeled for a one-month period. Variable levels of physical and hydraulic input data were applied in the model, as well as the use of field or laboratory measurements of soil hydraulic properties. Results show the smallest errors in predicted water content were achieved using either limited input data (texture name only) or hydraulic properties determined *in situ*, with root mean square errors (RMSE) ranging from 0.012 to 0.018 $m^3\ m^{-3}$. Hence, it is concluded that the model was adequate to its purpose, under the limited conditions of the verification made.

This study illustrates how soil type, different levels of input data, and differences in soil hydraulic parameter estimation or measurement influence the capability of the

RZWQM in simulating average profile soil water content under rangeland conditions. Generally, the model provided satisfactory results, especially considering that no soil hydraulic properties were calibrated or optimized, though measured (site-specific) hydraulic properties were used in some cases. In addition, the environmental and site conditions for the experimental study were quite different from those reported in previous RZWQM evaluation and calibration studies (Hanson et al., 1998; Ma et al., 1998; Wu et al., 1999). The experimental time-scale for this work was also considerably shorter than what is normally applied to the model, in order to coincide with other studies during the SGP97 Hydrology Experiment. It does not appear that the shorter time-scale had any appreciable effect on model results, though some studies have suggested that soil moisture predictability may be related to modeled time-scale (Schlosser and Milly, 2000).

Results presented here are consistent with previous studies that evaluated the capability of the RZWQM to predict soil water content, but also show that use of a limited input data set or soil hydraulic properties obtained in the field using relatively simple techniques provided the best estimates of average profile soil water content. These findings illustrate the potential application for modeling profile soil water content based on very limited soil data information and support the use of soil hydraulic properties obtained from remotely sensed surface soil moisture data as model input.

Surface Soil Moisture Data Assimilation

In Chapter 4, an extensive set of field data was used in combination with direct insertion of surface soil moisture data assimilation and soil water modeling to estimate root zone soil water content at a point in the field, something which is uncommon in the literature. The modeling approach was based on the use of limited soils data information since in practical terms, this is usually the case. Surface soil moisture sample data was obtained during SGP97 from June 18 - July 16, 1997 and used as a surrogate for microwave moisture data. Data assimilation of surface soil moisture improved model estimates to a depth of 15 cm at all sites and at three sites to a depth of 30 cm. Of particular significance with data assimilation, model estimates more closely matched the measured dynamic fluctuations of soil moisture in the top 30 cm in response to rainfall events. This may indicate that data assimilation of surface soil moisture tends to compensate for any errors that might be due to rainfall measurements or the partitioning of rainfall into runoff and infiltration. There was no significant improvement in soil water estimates below the 30 cm depth.

Based on the results of this chapter, a value representing the soil water content at 1/3 bar, which is related to texture class, may be obtained from surface soil moisture 2-day field drainage data after a sufficient wetting of the profile. This value may then be used as hydraulic input data for the model to a depth of 30 cm. The results indicate that use of this value as an average for the profile is only applicable where soil texture is uniform with depth.

Also presented in this chapter is a conceptual approach for model applications at the watershed scale based on a minimum set of required data necessary to execute RZWQM in a spatially distributed format. The results of Chapter 3 and those in Chapter 4 indicate that the model should provide reasonable estimates of profile soil moisture using the necessary meteorological input, data assimilation of surface soil moisture, 1/3 bar θ_v, and soil texture name based on the large-scale data format presented in Chapter 4. Thus, application of the model in a spatially distributed format is anticipated using similar but more exact data sets to evaluate the use of surface soil moisture data assimilation for profile soil moisture estimation at the watershed scale. As mentioned earlier, application of this methodology will require a GIS-based distributed hydrologic model which incorporates data assimilation and spatially variable meteorological data and surface parameters into model formulations.

Overall Summary

The results of this thesis should be viewed as a basic step towards better understanding the relative merits of surface soil moisture data assimilation in soil water modeling to estimate root zone soil water content based on field and modeling experimental analyses. Results presented here should serve as a link between theoretical concepts and field research that is based on the complimentary analysis of each. In essence, theoretical concepts have been extended to real world applications through comprehensive and valid field experimentation. Thus, the results of this research support much of the theoretical and synthetic work found in the literature today. However, further work is necessary to make a complete assessment of the methodology presented in this thesis. One aspect of future research would be to extend the spatial scale of application using a GIS-based distributed hydrologic model, as discussed in Chapter 4. Though four field sites were chosen in this work to represent a cross-section of soil types in the LWRW, extending this investigation to an additional five sites or more should certainly provide interesting challenges for future research.

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APPENDIX A

Model Scenario Descriptions

Scenario Name	Description
RZS1	For each soil layer the model is supplied soil textural-class name only. Based on texture class, the model uses soil physical and hydraulic default values as input for particle size fraction, bulk density, porosity, and 1/3 bar soil water content (F13). Saturated hydraulic conductivity (Ks) is estimated by Method 2 described in Chapter 3.
RZS2	For each soil layer the model is supplied site-specific lab-measured particle size fraction and bulk density from which the model derives soil texture and assigns the corresponding F13 default values. Ks is estimated according to Method 1 described in Chapter 3.
RSZ3	Same as RZS2 with the exception that F13 is explicitly specified and was measured in the laboratory on soil cores.
RZS4	Same as RZS3 but F13 values were measured in situ based on 2-day drainage data taken at each site during infiltration experiments.
RZS5	The model is supplied soil texture name and field measured values of F13 and Ks. F13 values were the same as in RZS4 and Ks was taken as the average conductivity for the profile based on steady-state infiltration. Thus Ks was the same for each layer at a given site.
RZS7, 7a, 7b	Same as RZS1 with adjustments made to 1/3 bar θ_v (RZS7, 7b) or Ks (RZS7a) in an effort to match modeled θ_v to measured θ_v values.
RZS10	Same as RZS1 with 0-5 cm surface θ_v assimilation.
RZS11	Same as RZS10 using 1/3 bar θ_v obtained from surface θ_v 2-day drainage data as the profile average value.
RZS12	Same as RZS10 accounting for plant water uptake.

CURRICULUM VITAE

Gary Claude Heathman was born in Jasper, Texas on June 22, 1953. In December 1977 he earned his B.S. degree in Forestry and in May 1981 the M.S. degree in Soil Science from Texas A & M University in College Station, Texas. After finishing his M.S. degree he spent six months working on a collaborative project between Texas A & M and the French government at an international research center (I.N.R.A.) located in Avignon, France. He then took a research and teaching assistant position in the soil physics department at New Mexico State University in Las Cruces, NM.

From 1982 to 1993 he served as a soil scientist at the United States Department of Agriculture (USDA) Agricultural Research Service (ARS), National Agricultural Water Quality Laboratory in Durant, Oklahoma. Between 1993 and 2000 he was reassigned as supervisory soil scientist-in-charge at the USDA-ARS field office in Chickasha, Oklahoma. He is currently a soil scientist stationed at the USDA-ARS laboratory in El Reno, Oklahoma. He, his wife, and two children live in Norman, OK.