Estimating root-zone soil moisture by assimilating remotely sensed biophysical states into modelling

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ABSTRACT

Thermal-infrared (TIR) satellite observations can be used as a powerful tool to estimate surface energy fluxes and vegetation water stress. There is a growing interest in assimilating remotely sensed TIR-based observations into Water and Energy Balance-Soil Vegetation Atmosphere Transfer (WEB-SVAT) models in order to improve their soil moisture estimations. Since the canopy thermal information of plants is linked to the soil water status of deeper layer through biophysical processes, employing a model that can realistically reproduce the surface-to-root-zone connection is critical for the efficacy of the model-observation integration. In the preliminary studies, limitations of the WEB-SVAT models in the parameterization of plant water uptake are identified and the potential benefits of integration with RS data are qualified. In the first step of this research, methods are explored to improve the soil water processes of a simple WEB-SVAT model (SWEB-SVAT) by adopting and incorporating an exponential root water uptake model with water stress compensation and establishing a more appropriate soil-biophysical linkage between root-zone moisture content, above-ground states and biophysical indices.

A new Multi-layer WEB-SVAT with Dynamic Root distribution (MWSDR) is developed by extending the existing model considering the impacts of plant root depth variations, growth stages and phenological cycle of the vegetation on plants transpiration. The sensitivity of surface energy fluxes to soil moisture reproduced by the new developed MWSDR is explored and compared with the original model and evaluated against the ground observations. Hydrometeorological and biogeophysical measurements collected from three experimental sites in Dookie, Victoria, Australia, Ponca, Oklahoma, USA, and Beltsville, MD, respectively, are used to validate the new model. Ground observations for three growing seasons (2002-2004) collected at the OPE study site are also used to verify the correlation between root-zone soil moisture and observed evapotranspiration (ET) and evaporative fraction (EF). The results of this thesis show the importance of having an adequate representation of vegetation-related transpiration process for an appropriate simulation of water transfer in a complicated system of soil, plants and atmosphere. Results demonstrate that the dynamic vegetation growth and root distribution scheme of MWSDR
significantly affects accurate representation of ET/EF versus the root-zone soil moisture and enhances the realism of biophysical and hydrological processes. On the other hand, MWSDR provides improved soil moisture, transpiration and evaporation predictions which highlights its proper model performance compared with the original SWEB-SVAT model.

In the next step, this thesis also examines how chosen model’s unique connection mechanism/strength between the surface variables and deeper soil layer information affects updating root-zone soil moisture using surface information through assimilation. The evaporative fraction (EF) derived from tower-based TIR measurements via the two-source energy balance model (TSEB) is assimilated into two different land surface models. Two models are used and compared to investigate the influence of coupling between surface variables and root-zone layer information on the efficacy of assimilating EF. Results show that improvement of root-zone soil moisture by assimilating TIR-based EF takes place only when the MWSDR model is used as the system’s model. It is attributed to the further details in the representation of vegetation dynamics and interactions between root depth and distribution with soil water content in the MWSDR model, which contributes to a more realistic coupling between surface energy fluxes and root-zone soil moisture resembling the observed correlation.
DECLARATION

This is to certify that

1. The thesis comprises only my original work towards the degree of Doctor of Philosophy.
2. Due acknowledgement has been made in the text to all other material used.
3. The thesis is fewer than 100,000 words in length, exclusive of tables, figures, bibliographies and appendices.

Mahboobeh Sadat Hashemian Rahaghi
PREFACE

This thesis is original and based on the studies I have conducted during my PhD candidature (year 2012-2016) at the University of Melbourne. The research outcomes of chapter 3 have been published in Advances in Water Resources journal, and chapters 4 and 5 are ready to be submitted for publications in journals.

I was the main investigator of these journal papers responsible for all the areas including concept formation, model development, model evaluation and analysing and discussing the results as well as majority of the manuscripts composition. My PhD principal supervisor Dr Dongryeol Ryu supervised my work and contributed to all the stages of the papers from concept formation to manuscript edits. My other supervisor Dr. Wade Crow provided valuable guidance during my research and contributed to the manuscripts and thesis reviewing. Dr. Bill Kustas and Dr. Fuqin Li also contributed to the manuscripts reviewing.
This thesis is the result of 4 years of intensive and exhausting work towards a worthwhile goal. It has been achieved with great support from many people during this adventure.

First and foremost, I would like to express my sincere gratitude to my PhD principal supervisor, Dr Dongryeol Ryu, for his constant guidance, encouragement and support throughout this journey. Without his support, this work would not be possible.

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I should also thank Rodger I. Young, Akuraju Venkata Radha and Robert Pipunic for their logistical support in operating and maintaining the Dookie site of the University of Melbourne as well as data collection and archiving.

Special appreciation is extended to the Australian Federal Government and The University of Melbourne for granting me the Endeavour International Postgraduate Research Scholarship (IPRS) and Australian Postgraduate Award (APA).

Finally, I would like to express my deepest gratitude to my parents, family and friends for their best wishes and especially to my partner, Mohammad, for his encouragement, companionship and support.
TABLE OF CONTENTS

ABSTRACT ........................................................................................................................................................... i

DECLARATION ........................................................................................................................................................ iii

PREFACE ............................................................................................................................................................... iv

ACKNOWLEDGMENTS ....................................................................................................................................... v

TABLE OF CONTENTS ..................................................................................................................................... vi

LIST OF TABLES .................................................................................................................................................. x

LIST OF FIGURES ............................................................................................................................................. xii

1. CHAPTER 1: INTRODUCTION .................................................................................................................. 1

2. CHAPTER 2: LITERATURE REVIEW AND RESEARCH QUESTIONS.............................................. 5

   2.1. Remote sensing retrievals of soil moisture ...................................................................................... 5

       2.1.1. Active and passive microwave remote sensing ................................................................. 5

       2.1.2. Thermal infrared remote sensing ..................................................................................... 7

   2.2. Using land surface models for soil moisture estimations ............................................................... 9

   2.3. Integrating models with observations via data assimilation ......................................................... 16

   2.4. Knowledge gaps and research questions .................................................................................. 22

3. CHAPTER 3: IMPROVING ROOT-ZONE SOIL MOISTURE ESTIMATIONS
   USING DYNAMIC ROOT GROWTH AND CROP PHENOLOGY .................................................. 28

   3.1. Introduction ........................................................................................................................................ 28
4.3.2. Evaluation of relationship between root-zone soil moisture and surface fluxes 78

4.4. Discussion and conclusions ................................................................................... 86

5. CHAPTER 5: IMPROVEMENT OF ROOT-ZONE SOIL MOISTURE BY ASSIMILATING EVAPORATIVE FRACTION INTO A SOIL VEGETATION ATMOSPHERE TRANSFER MODEL .................................................................................. 89

5.1. Introduction ............................................................................................................ 89

5.2. Materials and Methods ........................................................................................... 93

5.2.1. Land surface models ....................................................................................... 93

- Two-source energy balance model (TSEB) .......................................................... 94
- SWEB-SVAT model ............................................................................................. 95
- MWSDR model ..................................................................................................... 96

5.2.2. Site description ............................................................................................... 98

5.2.3. Data assimilation approach ............................................................................. 99

- EnKF Implementation ......................................................................................... 101
- EnKF Implementation using an empirical observation operator ....................... 103

5.3. Results and Discussions ....................................................................................... 108

5.3.1. Pre-analysis of models predictions ................................................................. 108

5.3.2. EF assimilation into SWEB-SVAT and MWSDR model ............................... 111

5.3.3. Implementation of data assimilation using an empirical observation operator 115
5.4. Discussion and Conclusions ................................................................................ 118

6. CHAPTER 6: SUMMARY AND CONCLUSIONS ..................................................... 121

   6.1. Overview.............................................................................................................. 121

   6.2. Conclusions.......................................................................................................... 122

   6.3. Challenges and recommendation for future work............................................. 126

REFERENCES ...................................................................................................................... 128
LIST OF TABLES

Table 3.1: Wheat growth stages and required growing degree day (GDD) ......................... 42
Table 3.2: Timing of various growth stages for Dookie data set in 2013 ......................... 44
Table 3.3: Timing of various growth stages for the Ponca data set ................................... 46
Table 3.4: Comparing timing of various growth stages with optical properties for the Ponca data set .................................................................................................................................. 47
Table 3.5: Coefficient of variation ($\sigma_C$) between measured and modelled soil moisture ($SM$) and latent heat flux ($LE$) at the Ponca site. Defined ranges in the column labels indicate the depth of soil layers in cm ................................................................................................................................ 48
Table 3.6: Linear correlation coefficient ($R$) between measured and modelled soil moisture ($SM$) and latent heat flux ($LE$) at the Ponca site. Defined ranges in the column labels indicate the depth of soil layers in cm ................................................................................................................................ 48
Table 3.7: Average relative error ($ARE$) between measured and modelled soil moisture ($SM$) and latent heat flux ($LE$) at the Ponca site. Defined ranges in the column labels indicate the depth of soil layers in cm ................................................................................................................................ 48
Table 3.8: Error statistics between measured and modelled daily total $ET$ (mm) at Ponca site,......................................................................................................................................................................................................................................................... 49
Table 3.9: Error statistics between measured and modelled soil moisture ($SM$) and latent heat flux ($LE$) using Dookie-2012 dataset, defined ranges in the column labels indicate the depth of soil layers .................................................................................................................................................. 51
Table 4.1: Normalised $\text{RMSE (NRMSE)}$ between measured and modelled surface and root-zone soil moisture ($SM$) and daily latent heat flux ($LE$)

Table 4.2: Linear correlation coefficients ($R$) between measured and modelled surface and root-zone soil moisture ($SM$) and daily latent heat flux ($LE$)

Table 4.3: Average relative error ($ARE$) between measured and modelled surface and root-zone soil moisture ($SM$) and daily latent heat flux ($LE$)

Table 4.4: Error statistics for modelled daily total ET (mm) between corn reproduction and full physiological maturity growth stages

Table 5.1: Cross-correlation of perturbations for soil moisture state variables of MWSDR model

Table 5.2: Error statistics of ET and EF predictions of three models comparing with observations

Table 5.3: Error statistics of root-zone soil moisture predictions before and after EF assimilation into MWSDR and SWEB-SVAT models

Table 5.4: Error statistics of root-zone soil moisture predictions of EF assimilation into SWEB-SVAT model using linear and exponential functions based on observed correlation

Table 5.5: Error statistics of root-zone soil moisture predictions of EF assimilation into MWSDR model using linear and exponential functions based on observed correlation
LIST OF FIGURES

Figure 2.1: Illustration of the different resistance in land surface models: (a) Penman, (b) Penman-Monteith (big-leaf/one-layer model), (c) Two-layer model and (d) Multi-layer model ................................................................................................................................. 10

Figure 3.1: A summary of 3 different cases comparing with SWEB-SVAT and MWSDR models ......................................................................................................................................................... 38

Figure 3.2: Simulated fraction of root length density of wheat in different layers of the root-zone ($F$), layer1: 10-30 cm, layer 2: 30-60 cm, layer 3: 60-90 cm, layer 4: 90-120 cm ..... 42

Figure 3.3: Comparing various model performances at Dookie study site in 2013 (a) and Ponca site (b) ........................................................................................................................ 50

Figure 3.4: Comparing various model performances in terms of surface (a) and root-zone (b) soil moisture using Dookie-2012 dataset ......................................................................................................................... 51

Figure 3.5: Cumulative modelled transpiration (a), observed evapotranspiration time series (b), modelled transpiration of SWEB-SVAT (c) and MWSDR (d) at Ponca site ....... 53

Figure 3.6: Cumulative modelled soil evaporation (a), surface soil moisture (b), modelled transpiration and soil evaporation of SWEB-SVAT (c) and MWSDR (d) at Dookie study site in 2013 ........................................................................................................................................................................... 54

Figure 3.7: Simulated water extraction by root (a), modelled soil moisture (b) at different stages, circles show the amount of variable at each layer (4-30, 30-60, 60-90, 90-120 cm), Dookie site-2013 ........................................................................................................................................................................... 56
Figure 3.8: Observed and simulated soil moisture by two models at different depths (0-30, 30-60, 60-90 cm) at Ponca site .................................................................57

Figure 4.1: Modelled soil evaporation (left), canopy transpiration time series (middle) and ratio of evaporation to transpiration (right) at OPE\textsuperscript{3} site............................................................73

Figure 4.2: Comparing model performances, surface (0-10cm) and root-zone soil moisture (0-100 cm) ..................................................................................................................75

Figure 4.3: Comparing model performances, root-zone soil moisture (0-100 cm) and daily LE predictions for MWSDR and WEB-SVAT models versus observations .................77

Figure 4.4: Scatter plots of root-zone soil moisture versus daily evapotranspiration (mm/d) for model predictions and observations during three growing seasons .................80

Figure 4.5: Scatter plots of root-zone soil moisture versus daily evaporative fraction for model predictions and observation during three growing seasons .........................80

Figure 4.6: Scatter plots of root-zone soil moisture versus daily observed evapotranspiration in three growing seasons, marked based on growth stages and net radiation (a, b, c), merging all data eliminating energy-limited conditions and low NDVI class (d), the purple curves show the exponential fitting to 2002 mid-season data ........81

Figure 4.7: Scatter plots of root-zone soil moisture versus daily observed evaporative fraction in three growing seasons, marked based on time in growth period and NDVI ......83

Figure 4.8: Scatter plots of observed root-zone soil moisture versus observed daily evaporative fraction marked based on NDVI (a) and growth stages (b), scatter plots of MWSDR modeled values marked based on growth stages (c) ........................................85
Figure 4.9: Scatter plots of soil moisture at different depth (a to d), weighted observe root-zone soil moisture (e) versus daily observed evaporative fraction, and weighted MWSDR modeled root-zone soil moisture (f) versus daily modeled evaporative fraction, marked based on growth stages ................................................................................................................................. 85

Figure 5.1: NDVI time series and the temporal partitioning of growth stages ............... 104

Figure 5.2: Scatter plot of observed root-zone soil moisture versus EF at 2pm (a) marked based on growth stages, (b) during the active growth period along with fitted linear and exponential functions ................................................................................................................................. 105

Figure 5.3: Scatter plots of observed weighted root-zone soil moisture versus EF at 2pm (a) marked based on growth stages, (b) during the active growth period along with fitted linear and exponential functions ................................................................................................................................. 107

Figure 5.4: (a) Daily EF and (b) daily ET estimations of MWSDR, WEB-SVAT and TSEB models comparing with observations ................................................................................................................................. 108

Figure 5.5: Comparing daily ET estimations of TSEB with (a) SWEB-SVAT and (b) MWSDR models ................................................................................................................................................................. 110

Figure 5.6: Soil moisture estimations of MWSDR and WEB-SVAT model comparing with observations ................................................................................................................................................................. 110

Figure 5.7: Scatter plots of root-zone soil moisture versus EF at 2pm marked based on growth stages for (a) MWSDR model, (b) SWEB-SVAT model and (c) observations ......... 111

Figure 5.8: Daily time series of modelled root-zone soil moisture, observations and results obtained from EF assimilation during the whole growing season into (a) SWEB-SVAT and (b) MWSDR models at 2pm, dotted vertical lines indicate EF observation times .......... 112
Figure 5.9: Kalman gain (low-pass filtered) time series of SWEB-SVAT- and MWSDR-based DA ................................................................. 113

Figure 5.10: Daily time series of SWEB-SVAT root-zone soil moisture results, observations and results obtained from EF assimilation based on h from observed (a) linear, (b) exponential relationships at 2pm, dotted vertical lines indicate EF observation times 115

Figure 5.11: Daily time series of MWSDR root-zone soil moisture results, observations and results obtained from EF assimilation based on h from observed (a) linear, (b) exponential relationships at 2pm, dotted vertical lines indicate EF observation times .......................... 117
1. CHAPTER 1: INTRODUCTION

Soil-moisture information is a key requirement in weather forecasting and environmental monitoring. Accurate representation of surface and root-zone soil moisture is required for the prediction of natural disasters, such as flooding and droughts and agricultural applications such as adequate crop and forage production. Given the inherent difficulty of making ground-based soil moisture measurements over a large scale area, various techniques have been developed to estimate soil moisture over a large region.

Remote sensing can be used as an ideal tool for global soil moisture mapping with high temporal frequency. Substantial efforts have been dedicated to the development of remote sensing techniques to retrieve the surface and/or root-zone soil moisture content. These efforts can be broadly categorized into microwave-based (e.g. Owe et al. 2001, Njoku et al. 2003) and thermal-infrared-based (e.g. Jackson et al. 1981, Anderson et al. 2007a, Anderson et al. 2007b) methods depending on the frequencies of the signal utilized for retrieval. For a long period of time microwave has been regarded as the most promising method to estimate large scale soil moisture but there are clear limitations in microwave soil moisture estimation. While the microwave retrieval techniques can produce surface moisture content even under cloudy conditions based on a firm physical model (i.e., soil dielectric model), resulting soil moisture estimate is limited by relatively low resolution and shallow penetration (approximately 5 cm) of the soil. In addition, the accuracy of microwave retrievals of soil moisture significantly decreases under moderate-to-dense vegetation due to interference effect (Verhoest et al. 1998, Hoeben & Troch 2000).

In comparison, even though the thermal infrared data cannot be obtained by satellite instruments under cloudy conditions, the surface thermal signature can provide very useful information about the moisture conditions at the top to the root-zone of soil at a better resolution. This method is not a stand-alone method instead it is rather combined with modelling. This method relies on the evapotranspiration (ET) estimations of remote sensing-based surface energy balance models. Evaporative fraction (EF) and the ratio of actual to potential evapotranspiration (PET) of vegetated surface are known to be proportional to the soil available water for vegetation. However, it should be mentioned
that the ability of thermal infrared data to provide soil moisture information may be limited to time/space locations where surface energy fluxes are water-limited.

Soil moisture content over large regions can also be estimated using land surface models. Although these models can produce continuous predictions of soil moisture, they have some limitations. For example, accuracy of the output soil moisture is sensitive to the availability/quality of the input forcing data and model parameters as well as the model structural errors. Global forcing data network is quite limited and the satellite forcing field has quite course resolution; thereupon, same as microwave data this method does not give high enough resolution.

Integrating additional information, such as the remotely sensed data into the modelling via data assimilation (DA) can improve the accuracy of the model-derived soil moisture. Data assimilation is a mathematical approach that enables updating model outputs using various available information (e.g. ground-based or remotely sensed observations). One of the advantages of this integrated model-observation approach is that it can produce continuous soil moisture estimates with minimized uncertainties in the periods between discrete observations.

Assimilation of microwave-derived surface soil moisture into land surface models have shown some improvements in the estimations of root-zone soil moisture (e.g. Reichle & Koster 2005, Reichle et al. 2002, Draper & Reichle 2015). However, there are some controlling factors determining the degree to which the root-zone can be accurately constrained via the assimilation of surface soil moisture estimates. The assimilation of surface soil moisture retrievals is ineffective at correcting root-zone soil moisture model predictions in case of limited vertical coupling between surface and root-zone layers (Kumar et al. 2009). In addition to the field soil texture which may limit the vertical redistribution of soil moisture anomalies (Li et al. 2010), the parametrization of model utilised in data assimilation system may effect on the vertical coupling of the root- and surface-zones.

Assimilation of products of thermal infrared (TIR) observations such as energy fluxes and soil moisture proxies (Crow et al. 2008, Li et al. 2010, Pipunic et al. 2008, Hain et al. 2012) or directly assimilation of thermal data (Crow et al. 2008) into the model in order to
estimate more accurate root-zone moisture have also been attempted. Although these studies demonstrated some improvements, it appears that they used simple/empirical linkage between surface thermal signals and root-zone soil moisture lacking a firm theoretical basis.

Prognostic water and energy balance (WEB)-soil vegetation atmosphere transfer (SVAT) models which enable the integration of TIR data or TIR-derived variables (e.g. predicted soil moisture or evapotranspiration) via data assimilation play an important role in data assimilation technique. There is strong biophysical process linking these surface variables to root-zone soil moisture and utilizing of this biophysical link requires biophysical model reproducing this process correctly. The connection between surface variables and root-zone states of the model is a substantial issue to produce superior profile soil moisture estimations by propagating surface information into deeper layers of soil. If the surface variable and root-zone states are correctly coupled in the model, knowledge of a change in surface variable would be more informative about root-zone change; whereas, over- or under-represented coupling strength may produce more errors. Over-simplifying the root biophysical processes and poor parametrization of evapotranspiration in the model may hamper the realistic representation of this connection and the ability of data assimilation to constrain root-zone soil moisture. Adapting dynamic plant biophysical components including dynamic rooting depth and distribution and remote sensing (RS)-based canopy resistance to existing model schemes may enable the models to have more realistic connection. This innovation may lead to not only better estimation of root-zone soil moisture, but also better linkage of root-zone moisture content to surface variables which will improve data assimilation efficiency.

Within the context described above, in this thesis the efficacy of using different model schemes in a data assimilation system to improve root-zone soil moisture predictions is explored. The primary aim of this thesis is to test whether the more realistic representation of connectivity between surface variables and root-zone states can improve model predictions via data assimilation techniques. By selecting a simple model with soil-vegetation-atmosphere-transfer (SVAT) scheme, various modifications for improving the model structure are explored by both integrating existing sub-models and utilising remote sensing indices. The original model is modified to have more layers in order to provide a
realistic dynamic root distribution. The impacts of plant root depth variations, growing stages and phenological cycle of plant on transpiration are considered in developing stages. Hydrometeorological and biogeophysical measurements collected from three experimental sites, one in Dookie, Victoria, Australia, another in Ponca, Oklahoma, USA and the other in Beltsville, Maryland, USA, are used to validate the new model. These data sets provide very distinct opportunity for assessing the new model by presenting a wide range of moisture status and field conditions. After the setting up of the model, the relationship between surface variables and root-zone soil moisture captured by new model is compared with predictions obtained from the original model and evaluated against the ground observations. Later, products of surface thermal-infrared data will be assimilated to both models to quantify how the connection between the surface variables and root-zone soil moisture of the model affects the efficiency and veracity of transferring the surface information into the root-zone through assimilation.

This research will adopt a broad range of modelling techniques (hydrological modelling and stochastic filtering) and observation datasets (in situ measurements of hydrological and meteorological data, surface spectral data). The significance of this research is in providing more accurate surface and sub-surface variables by improving the soil water processes of the model and in improving the efficacy of data assimilation technique using more realistic representation of soil water processes.

The thesis is structured around three main modules of work that constitute the Chapters 3-5, each of which contains its own introduction, methods, results and conclusions. Additionally, Chapter 2 provides a literature review of various methods for soil moisture estimations and the existing knowledge gaps and the research questions, which will be addressed in this research. Finally, chapter 6 summarises the thesis and outlines the conclusions that have been drawn during this research.
2. CHAPTER 2: LITERATURE REVIEW AND RESEARCH QUESTIONS

This chapter presents a detailed background regarding various methods of soil moisture estimation and the main advantages and limitations are discussed. It will also describe the previous studies in this area. Remote sensing methods and land surface models will be reviewed as two main methods of soil moisture estimation over a large scale area. Integrating models with remote sensing observations will also be explained as an advanced emerging method. Finally, based on the problems and limitations associated with the application of each method, the aim of this thesis is stated by demonstrating the knowledge gaps extracted from the literature review which support the research questions represented at the end of this chapter.

2.1. Remote sensing retrievals of soil moisture

A number of methods have been developed to estimate soil moisture using various satellite observations. Two most popular soil moisture sensing techniques are microwave and thermal remote sensing (RS) methods. Microwave remote sensing soil moisture estimation is based on a physical model, which exploits dielectric properties of wet soil. The microwave signal emitted (passive sensing) or reflected (active sensing) by the soil can be used to retrieve soil moisture content using the strong contrast between dielectric constants of dry and wet soil (Engman & Chauhan 1995). In contrast, thermal remote sensing methods infer root-zone soil moisture indirectly based on different thermal responses of the vegetation to sufficiency or limitation in available soil water (Jackson et al. 1981).

2.1.1. Active and passive microwave remote sensing

Operational microwave sensors of onboard satellite platforms have wavelengths in the range of a few centimetres to a few decimetres (L, C, X bands with 21, 4.3, 2.8 cm wavelength equivalent to the frequency of 1.4, 6.9, and 10.7 GHz). Microwave retrievals of soil moisture are limited to few centimetres of the soil profile (near-surface) due to the
limited penetration of these wavelengths into the soil (Njoku & Entekhabi 1996). Since soil moisture condition at deeper layer of soil behaves differently from the surface layer, soil moisture of shallow depth is not sufficient to obtain moisture information of deeper layers; while information about soil water storage conditions over the depth of approximately 1 meter or more is necessary for many agricultural and ecological applications.

Another limitation of microwave methods is that the accuracy of microwave signals significantly decreases under dense vegetation, such as in agricultural lands, where soil moisture information is of significant value (Jackson et al. 1982, Choudhury B.J. 1988, Schmugge et al. 1980, Verhoest et al. 1998, Hoeben & Troch 2000). Whilst effects of vegetation cover and land surface roughness are relatively mild for passive (radiometer) microwave measurement in comparison with active (radar) microwave sensing, space-borne passive microwave data suffers from low spatial resolution (a footprint scale of 40-60 km from currently available L-band satellite radiometers). A significant advantage of microwave retrieval techniques is that microwave signal can penetrate through most cloud covers and as a result these techniques can produce soil moisture under non-precipitating cloudy condition (Schmugge 1985).

Over the past decades there have been numerous microwave remote sensing studies using active and passive observations developing and evaluating some methods to retrieve soil moisture from microwave observations (e.g. Owe et al. 2001, Njoku et al. 2003, Bindlish et al. 2006). Some successful attempts have been made at soil moisture retrieval from Special Sensor Microwave/Imager (SSM/I) data (Jackson 1997, Lakshmi et al. 1997, Basist et al. 1998) and the Scanning Multifrequency Microwave Radiometer (SMMR) data (Owe et al. 1992, Choudhury B.J. 1988). One of the passive microwave satellites which has been most extensively validated to retrieve soil moisture is the Advanced Microwave Scanning Radiometer for the Earth Observing System (AMSR-E) operating from July 2002 to 2011 (Njoku et al. 2003, Bolten et al. 2010, Jackson et al. 2003). Land Parameter Retrieval Model (LPRM) developed by the VU University Amsterdam (VUA) and NASA is one of the most widely distributed soil moisture product of AMSR-E (Owe et al. 2008, De Jeu et al. 2009). Some previous validation studies (e.g. Rüdiger et al. 2009) revealed that LPRM products of AMSR-E may be used as a high quality soil moisture retrievals representing the high possible skill of microwave techniques. In 2012, the Advanced Microwave Scanning
Radiometer (AMSR-2) on the GCOM-W (Global Change Observation Mission-Water) was added to the network which inherits most of AMSR-E’s characteristics. Other prominent missions currently operational are the Soil Moisture and Ocean Salinity (SMOS) mission launched in 2009 and NASA’s Soil Moisture Active Passive (SMAP) mission launched in 2015.

2.1.2. Thermal infrared remote sensing

Remote sensing measurements of thermal infrared (TIR) wavelength (3 to 14 micrometers) which are typically applied to estimate the land surface temperature (LST), can be used as an alternative source of information to estimate soil moisture. Methods to retrieve soil moisture from TIR images are based on dependency of soil moisture condition to evolution of land surface temperature (e.g. Jones et al. 1998, Scott et al. 2003, Anderson et al. 2007a), as dry soil or stressed vegetation may result in higher LST than wet soil or well-watered vegetation. In a bare soil, due to changes in evaporative cooling effect, thermal signature from the surface is changing depending on the soil wetness. Plants typically control their stomata based on soil moisture content; if the soil is dry their close their stomata and leaf temperature goes up. In a vegetated area, when the canopy is under water stress, it cannot effectively transpire water (due to closed stomata and the failure of root water uptake), which results in high surface temperature.

Although vegetated surface temperature has been widely used to determine crop water stress (e.g. Jackson et al. 1981, Moran et al. 1994), use of crop water stress for the estimation of subsurface soil moisture is relatively new. The inverse approach that is using the effects of soil moisture content on the surface evaporative fluxes to calculate water stress has been used in many land surface models (LSM). It is assumed that evapotranspiration (ET) which is a composite of soil evaporation and canopy transpiration is largely controlled by soil moisture in the surface layer and the root-zone layer respectively; in general, dry soil profile leads to low ET and high surface temperature while wet soil profile increases ET and decreases surface temperature. Defining a semi-empirical linear or nonlinear relationship between soil moisture and water stress index (a function of surface evaporative fluxes) is a common method in agro-hydrological studies (e.g. Chen &
Dudhia 2001, Campbell & Norman 1998); this water stress index is used for reducing potential evapotranspiration (PET) to find the actual evapotranspiration (AET) (Allen et al. 2006).

On the contrary, it has been argued that difference between AET and PET can also be used as a sign of soil water stress (Scott et al. 2003). In this respect, some of the past studies attempted to relate TIR-based evapotranspiration (ET) data computed using diagnostic surface energy balance models, to the surface and root-zone soil moisture content (e.g. Anderson et al. 2007a, Anderson et al. 2011, Hain et al. 2009, Hain et al. 2011). Various soil moisture stress functions such as evaporative fraction \( EF = LE/(LE + H) \) and ratio of actual to potential evapotranspiration \( f_{PET} = AET/PET \) have been defined to relate ET products to available soil water of vegetated surface. Scott et al. (2003) utilized evaporative fraction calculated by the surface energy balance algorithm for land (SEBAL) model to estimate volumetric soil moisture using an exponential relationship. Hain et al. (2011) employed \( f_{PET} \) as a proxy for the root-zone soil moisture utilising a linear relationship between \( f_{PET} \) and available water fraction \( f_{AW} = (\theta - \theta_w)/(\theta_f - \theta_w) \) in which \( \theta \) is current moisture content, \( \theta_w \) and \( \theta_f \) are soil water contents at the wilting point and field capacity.

It should be noted that the water used by plants for transpiration originates from the whole profile of the soil which is in contact with the plants root, and the depth of root depends on the plant type and growth stage. Thus, remote sensing retrievals of evapotranspiration can be used only for estimations of soil moisture in the rooted depth of soil. In general, over dry surface or sparsely vegetated areas, surface stress detected from the TIR-based method is used to estimate surface moisture while detection of vegetation stress over moderate to dense vegetated areas leads to root-zone soil moisture estimation (Hain et al. 2012).

In addition to providing useful information about both surface and root-zone soil moisture by TIR-based methods, which is advantageous comparing with microwave methods, the spatial resolutions of thermal remote sensing sensors (from 60 m to 5 km) are generally much higher than passive microwave sensors (>40 km). However, application of thermal infrared images is limited because thermal radiation of land surface is interfered, if not completely blocked, by clouds.
Apart from estimating available water using evapotranspiration derived from TIR-based diagnostic surface energy balance models, there is another innovative method which assimilates TIR-based measurements (or estimations from the first approach) into prognostic land surface models for better estimation of soil moisture content. The main difference between these two methods is on how they treat surface temperature (Crow et al. 2005). Surface temperature along with air temperature, solar radiation, vegetation indices, wind speed and some other variables are all necessary information for a physically based RS algorithm to calculate energy fluxes and then link them to soil moisture. However, prognostic land surface models have their own different parameterisation, estimating surface and root-zone soil moisture without using surface temperature as the input data. TIR-based independently estimated surface temperature, energy fluxes and soil moisture proxies can be used as additional data to update the soil moisture predictions of land surface models via data assimilation system (e.g. Crow & Wood 2003, Pipunic et al. 2008, Crow et al. 2008, Hain et al. 2012). This method will be completely discussed in the next sections (2.2. and 2.3.).

2.2. Using land surface models for soil moisture estimations

A land surface model (LSM) is defined as a computational model describing ecological, hydrological and surface processes using atmospheric models (Bonan 1996). LSMS relate the biophysical interactions of land and atmosphere such as fluxes, momentum, long wave emission and albedo. The main task of LSMS is to simulate the partitioning of net radiation into the component fluxes including soil heat flux (G), latent heat flux (LE) related to transpiration and evaporation, and sensible heat flux (H) (Overgaard et al. 2006).

The evolution of land surface models during their long history, in terms of considering the land surface as an electrical circuit analogue, can be categorised in four stages as shown in Figure 2.1. It is assumed that the driven force for exchange of a quantity (e.g. temperature or vapour pressure) between two points (e.g. the land surface and the atmosphere) is the difference in potential of the quantity, and the exchange rate is controlled by the existing resistances. Penman (1948) estimated evaporation inspired from the electrical analogue assuming the atmosphere as the only source of resistance for evaporation of water from the
wet surface to the atmosphere (Figure 2.1a). This model has some fundamental drawbacks: only during and after the rainfall, the land surface behaves as a wet surface as assumed in the model; after drying out of the upper soil layer, water cannot be evaporated from the surface and the only way for transferring water to the atmosphere would be transpiration of vegetation controlled by their stomatal aperture. Monteith (1965) augmented the Penman method by considering an additional evapotranspiration control which was vegetation-dependent resistance estimated based on vegetation type, soil moisture content and weather condition (Figure 2.1b). Since this method considers the land surface as a homogeneous plane unresponsive to the difference of soil evaporation and vegetation transpiration, researchers defined this Penman-Monteith Model as “one-layer”, or “big-leaf” model. This model has been proven to work well under densely vegetated canopies (Monteith & Unsworth 1990). However, under sparse vegetation land cover, when soil surface and vegetation fluxes interact with each other, one-layer models will fail to accurately estimate the land-surface fluxes.

![Figure 2.1: Illustration of the different resistance in land surface models: (a) Penman, (b) Penman-Monteith (big-leaf/one-layer model), (c) Two-layer model and (d) Multi-layer model](image)

In order to overcome this failure two-layer models have been developed in which the soil surface is covered by a vegetation layer so that heat and water can be transferred to the atmosphere through this canopy layer, whereby the interaction of fluxes is conceivable (Figure 2.1c). In this structure, vegetation transpiration is controlled by stomata resistance similar to the “big-leaf” model and soil evaporation is controlled by substrate surface resistance. Thus water transfer is controlled by three aerodynamic resistances including leaf surface to canopy, soil surface to canopy and canopy to a reference height above the
vegetation layer. In the next generation two-layer approach was extended by adding more vegetation layers (Figure 2.1d). Such multi-layered model considers vertical structure of canopy fluxes for example from a forest with multiple vegetation types. Partial calculated fluxes of each layer are integrated to calculate the total flux over the whole canopy depth.

Based on the other method for classification of land surface models, the broad category of soil-vegetation-atmosphere transfer (SVAT) scheme encloses all the approaches partitioning the surface net radiation between sensible and latent heating (Crow et al. 2005). There are some structural differences between these methods in their treatment of RS-based surface temperature, which divides the SVAT approaches into two main classes: remote sensing (RS)-SVAT and water and energy balance (WEB)-SVAT.

In the RS-SVAT category, observations of surface radiometric temperature are used as an input for estimating flux components of the net radiation. The RS-SVAT models are grid-based methods and their resolution corresponds to the resolution of remotely sensed TIR imagery, which ranges from several meters to several kilometres based on the specifications of satellite instruments. However, they cannot provide continuous estimations of surface fluxes, instead, all the resulting energy fluxes are instantaneous because they are related to that time which satellite observations are available. The Two-Source Energy Balance (TSEB) model (Norman et al. 1995) and SEBAL model (Bastiaanssen et al. 1998) are some examples of RS-SVAT models.

Most of RS-SVAT approaches assume that net radiation \( (R_N) \) is available from observations of downward solar radiation, and then ground heat flux \( (G) \) is calculated as a simple function of net radiation, leaf area index (LAI), and time of day. Sensible heat \( (H) \) is estimated as:

\[
H = \rho C_p \frac{T_{\text{aero}} - T_a}{R_A}
\]  

(22-1)

where, \( \rho \) is the density of the air, \( C_p \) the specific heat of air at constant pressure, and \( R_A \) the aerodynamic resistance. \( T_a \) is the air temperature, and \( T_{\text{aero}} \) the aerodynamic temperature at the mean canopy air-stream. The latent heat \( (LE) \) can be calculated as a residual of the surface energy balance:
In fact, monitoring of daytime differences between estimates of $T_{aero}$ and observations of $T_a$ can be used to diagnose the water stress. According to past studies (e.g. Kustas & Norman 1996) the $T_{aero}$ value has a complex dependency to surface radiometric temperature ($T_{rad}$), vegetation characteristics and viewing angle. However, if there are typical uncertainties about 2–4 K in $T_{rad}$ observations, the accuracy of $T_{aero} - T_a$ estimation will be hampered (Kustas & Norman 1997). In response to this problem, the two-layer techniques such as TSEB model were developed to make use of $T_{rad}$ observations for computing soil and vegetation temperatures and heat fluxes. Two-layer models partition the surface radiometric temperature, $T_{rad}$, into the soil ($T_S$) and canopy ($T_C$) temperatures using the local vegetation cover fraction visible at the view angle of thermal sensor ($f(\theta)$) (Anderson et al. 2007a):

$$T_{rad}(\theta) \approx f(\theta)T_C + [1 - f(\theta)]T_S \quad (2-3)$$

Two-source models solve the soil and the canopy energy budgets separately, and compute the components of net radiation, sensible and latent heat fluxes as:

$$R_N = R_{N_S} + R_{N_C} \quad (2-4a)$$

$$H = H_S + H_C + G \quad (2-4b)$$

$$LE = LE_S + LE_C \quad (2-4c)$$

Other researches applied several modifications to the original TSEB model formulation. Deriving net radiation of soil and canopy using a more physically based algorithm (Campbell & Norman 1998), addressing the effects of row crops on wind decay and radiation divergence using clumped factor (described in Kustas & Norman 1999), adjusting gradual change in the Priestley–Taylor parameter used in the calculation of canopy transpiration under water stress condition and revising the soil resistance equations by changing of coefficients (described in Kustas & Norman 1997) are the most important amendments of this model during its evolutionary period.
The Atmosphere-Land Exchange Inverse (ALEXI) model is based on the TSEB model, which uses the morning surface temperature rise and removes the need of air temperature measurement (Anderson et al. 2007a). This model is insensitive to uncertainties of satellite-based TIR measurements due to its use of the difference between two observations at 1.5 and 5.5 hours after sunrise. The bias between TIR and the physical surface temperature is assumed to be cancelled off by taking this difference.

Considering the effects of detected soil water stress on the soil moisture estimation, Anderson et al. (2007a) found a strong relationship between the ratio of actual to potential evapotranspiration fluxes ($f_{PET}$) and the fraction of available water ($f_{AW}$) in the soil column using the obtained fluxes of ALEXI. Based on this finding, Hain et al. (2009) proposed unique relationships between $f_{PET}$ and $f_{AW}$. This study showed that $f_{AW}$ resulting from ALEXI, can be served as a proxy for the root-zone soil moisture in the vegetated areas. An important point in this study was that ALEXI $f_{PET}$ represents a merged soil moisture estimate, which is related to both surface and root-zone because it provides an estimate of water availability for both evaporation and transpiration. In fact, this method estimates the water availability of surface layer of non-vegetated soil for evaporation and water availability of root-zone layers over the vegetated areas for transpiration (Yilmaz et al. 2012).

The Surface Energy Balance Algorithm for Land (SEBAL) is an iterative RS-SVAT model computing the energy exchanges at the earth’s surface (Scott et al. 2003). Evaporative fraction calculated from Eq. (2-5) is an important indicator to express energy partitioning and it also has been used as a simple and direct indicator of root-zone soil moisture conditions in some studies related to this model (e.g. Bastiaanssen 2000, Scott et al. 2003)

$$EF = \frac{LE}{R_N - G}$$

Eq. (2-5)

The value of evaporative fraction is essentially between zero and unity and its behaviour is temporally stable. This index can be used as an appropriate indicator of water stress for vegetated areas acting as an alternative for $f_{PET}$ avoiding the complex definitions of potential evapotranspiration (Bastiaanssen 2000).
In the second category of SVAT model, coupled water and energy balance (WEB) equations are used for assessing the temporal variations of soil moisture and surface states. The main difference between this approach and RS-SVAT models is that surface temperature does not act as a forcing variable; rather it is a predicted value. WEB-SVAT models do not need TIR-based observations to extract soil moisture content; instead, they use observations such as precipitation and radiation and remotely sensed vegetation indices such as LAI. These models are more complicated and use more parameters not only for partitioning the surface energy budget but also as a multi-objective model, for predicting the surface states such as soil moisture.

WEB-SVAT approaches obtain energy flux predictions by parameterizing components of the surface energy balance \((R_n, H, LH, \text{and } G)\) as a function of surface aerodynamic temperature \((T_{aero})\), static parameters including soil and vegetation properties \((\Gamma)\), forcing variables such as precipitation and incoming radiation \((W)\), and current soil thermal \((Y)\) and hydrologic states \((\Theta)\) and numerically solving the balance equation (2-6) (Crow et al. 2005).

\[
R_n(T_{aero}, \Gamma, W) = H(T_{aero}, \Gamma, W) + LE(T_{aero}, \Gamma, W, \Theta) + G(T_{aero}, \Gamma, W, Y, \Theta) \tag{2-6}
\]

The model combines the flux predictions with rainfall observations and vertical subsurface modelling in order to predict the soil moisture content continually (Crow et al. 2008).

\[
\frac{d\Theta}{dt} = f(LE, \Theta, Y, \Gamma, W) \tag{2-7}
\]

Although WEB-SVAT models have a common conceptual basis, the parameterization of Eqs. (2-6) and (2-7) is very different for various models, which may result in predictions with large contrasts (Crow et al. 2005). Common Land Model (CLM) (Dai et al. 2003) and Noah (Hogue et al. 2005) are additional examples of WEB-SVAT models. They have been developed as a complex model with a multi-layer structure in order to suit a wide range of applications. One of the limitations of these global models is that they are not designed to address detailed biophysical process; simplified biophysics of model (for example in parameterisation of root biophysical processes) produce errors which hamper the ability of model to provide correct transpiration or soil moisture estimations. Integrating these models with other models simulating vegetation dynamics can make their biophysical structure
stronger; however, they will be more complex and some unexpected outcomes may be encountered.

A relatively simple WEB-SVAT model has been developed for some studies to make it more efficient to be integrated with remotely sensed observation systems (e.g. Crow & Reichle 2008, Crow et al. 2008, Li et al. 2010). In order to make a distinction between the name of this specific WEB-SVAT model and more generic WEB-SVAT, the former model is called SWEB-SVAT hereafter.

This simple WEB-SVAT model uses a two-layer vegetation-soil equations based on a force-shale concept for the soil water balance with a very similar resistances structure and radiation parameterization to the TSEB model (Crow et al. 2008). Two soil layers including surface-zone and root-zone are considered so that the surface layer is the top layer of the root-zone layer. Surface and root-zone soil moisture variations are calculated by the water balance equation represented as:

\[
\frac{d\theta_{sz}}{dt} = \frac{C_1}{d_{sz}} \left[ P_g - LE_S(\rho \lambda)^{-1} \right] - \frac{C_2}{f_d} (\theta_{sz} - \theta_{eq}) \tag{2-8a}
\]

\[
\frac{d\theta_{rz}}{dt} = \frac{1}{d_{rz}} \left[ P_g - LE_C(\rho \lambda)^{-1} \right] - LE_S(\rho \lambda)^{-1} - Q \tag{2-8b}
\]

where \( \theta_{sz} \) and \( \theta_{rz} \) are surface- and root-zone soil moisture contents, \( d_{sz} \) and \( d_{rz} \) surface- and root-zone depth, \( P_g \) throughfall, \( LE_S \) and \( LE_C \) soil and canopy latent heat flux, \( \rho \) density of air, \( \lambda \) latent heat of vaporisation, \( f_d \) the frequency of diurnal variations (24 hours), \( \theta_{eq} \) equilibrium surface volumetric moisture content, and \( Q \) the drainage from the bottom of the root-zone. \( C_1 \) and \( C_2 \) are force and restore coefficients for soil moisture, which are related to the soil characteristics.

As it mentioned earlier in this section, the estimates from WEB-SVAT models contain some uncertainty due to model deficiency in representing the surface and subsurface processes. The energy balance portion of SWEB-SVAT model calculates the soil and canopy temperature using an iterative process based on surface meteorological forces (e.g. solar radiation, wind speed, air temperature) and modelled soil moisture states. A key component of water and energy balancing part of Web-SVAT models which controls the surface temperature is canopy transpiration in which root layer soil moisture available for...
plant water uptake plays an important role. Using the lumped root-zone soil moisture as an input to calculate the total transpiration (which is the case for most of land surface models) means that the amount of water transpired by the plant is assumed to be uniformly distributed in the whole profile of the soil – regardless of the root vertical distribution. However, assigning proper proportion of root to different layers of root-zone leads to extract more water from the layers with high root distribution and helps to redistribute water correctly between the layers. One more example regarding the limitations of WEB-SVAT models is that although canopy resistance utilised for transpiration calculation is influenced by the vegetation characteristics, it is mainly calculated based on the water content in the whole root layer and soil texture-based resistance extremes. However, neglecting the effects of vegetation activities and plant phenological cycle may hamper the transpiration estimation and soil moisture prediction as a result.

As noted before remote sensing observations can be integrated in the WEB-SVAT models to update the soil moisture predictions. There is longer history of assimilating microwave soil moisture into the land surface models (e.g. Entekhabi et al. 1994, Walker & Houser 2001), but recently there are several research works trying to assimilate thermal infrared products to improve root-zone moisture content estimations (e.g. Crow et al. 2008, Li et al. 2010, Hain et al. 2012).

### 2.3. Integrating models with observations via data assimilation

The first demonstration of using observed surface temperature assimilation in hydrological models was given in Lakshmi (2000). This paper shows that surface temperature can be used to correct the soil moisture due to incorrect precipitation in a two-layer model. Surface temperature (as well as vegetation index) has also been used to downscale passive microwave radiometer (AMSR-E) derived soil moisture using MODIS data (Fang et al. 2013). Downscaling algorithm is based on a regression relationship between daily temperature changes and daily average soil moisture and presented to produce an enhanced spatial resolution soil moisture product. The meteorological and oceanographic science communities adopted and developed a more sophisticated data
assimilation (DA) methods earlier (1970s) in order to produce accurate daily maps of weather (Li et al. 2009) but it has become a popular method in hydrological science in 2000s.

DA is a mathematical technique that makes the model outputs updatable using various available sources of information. DA is also called model-data synthesis or data-model fusion in different disciplines. This approach incorporates the observational data (e.g. ground-based or remotely sensed observations) with a land dynamic model covering theoretical understanding of the whole system. Although this method conceptually seems very popular, it is very hard to implement. The two main components of a DA system are a forward land dynamic model describing variations of the land states over time and an observation model relating land states estimations to observations. In addition to observed and predicted values, uncertainties associated with the observation, techniques and processing are also important to determine the final outcomes of this technique. Thus, estimation of uncertainties for observations and model parameters is an inevitable part of DA approach and comes into account as a distinctive characteristic.

Land DA is considered as a tool for optimal estimation of land surface state variables using a land surface model, remote sensing products and any other available a priori information. Remote sensing provides the opportunity to extract global soil content map of surface and/or root-zone. Both microwave and thermal-based soil moisture estimation techniques each possess their own unique set of advantages and limitations (Ahmad et al. 2011). One of the limitations of remote sensing methods is that the predictions are made for instantaneous times at which remote observations are available and it cannot produce the continuous predictions of soil moisture. On the other hand, continuous predictions of soil moisture content over large regions can be estimated using land surface models forced by atmospheric data. The existing uncertainties in model structure, model parameters and forcing data lead the model to have a large amount of errors if just running the model is considered without any constraints (Liang & Qin 2008). Satellite retrievals also contain errors due to imperfect measurement instruments and retrieval models. In the other words, both land surface models and remote sensing observations are not perfect and contain uncertainties. These uncertainties or errors are considered in the DA system and DA tries to incorporate them to improve the estimation accuracy of system’s state variables. Data
assimilation methods can act as an effective way to combine complementary information from model and remotely sensed observations of surface and provide preferable estimations with reduced error (Reichle et al. 2010). One of the advantages of this integrated model-observation approach is that it can produce continuous soil moisture estimates still achieving the accuracy of occasional ancillary observations whenever they are available.

Kalman filter (KF) presented by Kalman (1960), is the most common real-time updating scheme (Liu & Gupta 2007) which determines corrections based on the model and observations errors assuming that the error covariance matrices for the model forecast and the observation vector are known when new measurements are available (Evensen 1994). This method assumes linearity of the system for propagating the errors while some hydrological processes are moderately non-linear, which is the main limitation of this method. Variations of the Kalman filter including the Extended Kalman Filter (EKF) and the Ensemble Kalman Filter (EnKF) have been developed in order to deal with this limitation.

The EKF utilises local linear approximation to propagate the model error covariance matrix. Although application of this algorithm showed some successful results, it may provide instabilities or divergences due to the linear approximation of non-linear processes (Clark et al. 2008).

The ensemble Kalman filter (EnKF) is one of the most widely used assimilation techniques in the field of land surface data assimilation (e.g. Zhou et al. 2006, Hain et al. 2012). Zhou et al. (2006) showed that the EnKF can be applied as an efficient algorithm for assimilating remotely sensed retrievals into land surface models. This method provides more modern variation of Kalman Filter (KF) in which there is no need to linearize the model. This filter was introduced by Evensen (1994) as an alternative of the EKF when working with strong non-linear systems. Using a Monte Carlo approach, a large number of model runs in the same time period is used to calculate mean and covariance of the model which are taken as model uncertainty and the best estimation of the model state respectively. Usually a mean-zero Gaussian noise is used to perturb state variables, parameters and/or forcing data and generating the ensemble (Ryu et al. 2009). Synthetic soil moisture assimilation study has been used to compare the results of these two techniques and it has been concluded that
EnKF is more advantageous because of better quality of the forecasts statistic errors and lower calculation times (Reichle et al. 2002). Propagating the error/covariance information by a Monte Carlo ensemble, makes the EnKF able to represent almost any type of model errors (Crow & van den Berg 2010).

Both the EKF and the EnKF work sequentially based on two distinct steps: forecast step which estimates model variables and update step which corrects the estimations whenever an observation is available. The EKF system calculates a single estimate of the state vector and its uncertainty at each forecasting step and propagates them to the following time step. Whenever an observation is available, a correction based on observation errors and state uncertainty is made, and a new vector state is determined with a reduced uncertainty. On the other hand, the EnKF, propagates an ensemble of states vectors while the mean value is considered as the state vector estimate. It also calculates the state vector uncertainty based on the distribution of the ensemble in each time step. When a new observation is available, the whole ensemble of state vectors is updated, based on a weighting procedure involving both the state errors and the observation errors. The reduction of the state vector uncertainty is reflected in the reduction of the ensemble spread.

Many examples of the previous attempts of using data assimilation technique have been reported in the literature. Assimilation of microwave-derived surface soil moisture (Reichle & Koster 2005), direct assimilation of surface radiometric temperatures (LST derived from thermal remote sensing observations) (Crow & Kustas 2005), assimilation of energy flux estimates derived from surface radiometric retrievals (Pipunic et al. 2008), assimilating a root-zone soil moisture proxy based on surface energy flux estimates obtained from thermal remote sensing (Crow et al. 2008) and simultaneous assimilation of mutually independent soil moisture information obtained from microwave and thermal remote sensing sources (Li et al. 2010) are some examples of these attempts.

Previous attempts for assimilation of microwave-derived surface soil moisture into land surface models (e.g. Reichle & Koster 2005, Li et al. 2010), have reported lack of full satisfaction in improving root-zone soil moisture. It is shown that there are some controlling factors determining the degree to which the root-zone can be accurately constrained via the assimilation of surface soil moisture estimates. For example Li et al.
(2010) showed that soil textures allowing for the vigorous vertical redistribution of soil moisture anomalies (e.g. sandy soils) profit more from the assimilation of microwave soil moisture than soils in which such movement is actively retarded (e.g. clay and loamy soils). The processes of water and energy transfer from root-zone to the atmosphere are the basis of the soil-vegetation-atmosphere-transfer (SVAT) scheme of dynamic models which are utilised in data assimilation system. The model parametrization may also effect on the vertical coupling of the root- and surface-zones. The assimilation of surface soil moisture retrievals is ineffective at correcting root-zone soil moisture model predictions in case of limited vertical coupling. Therefore, other researches tried to assimilate products of TIR observations such as energy fluxes and soil moisture proxies into models (e.g. Crow et al. 2008, Pipunic et al. 2008, Li et al. 2010, Hain et al. 2012) to estimate more accurate root-zone moisture content, and some others tried to assimilate thermal data directly into the model (Crow et al. 2008).

Direct assimilation of surface radiometric temperature (LST) into land surface models is criticized because of existing absolute biases in the calculation of LST from satellite-based TIR observations (Bosilovich et al. 2007). Also, land surface temperature assimilation requires implementing comparison of satellite-based and model-based LST which is difficult and complicated due to lack of considering the view angle effects in most of LSMs (Holmes et al. 2012). In this respect, Crow et al. (2008) compared the results of assimilating TIR-based soil moisture proxy (using two source model (TSM)) with direct assimilation of LST measurements. They found that assimilation of soil moisture proxy based on surface energy flux estimations is superior, considering that relationship between root-zone soil moisture and LST is highly nonlinear and dependent on the accuracy of micrometeorological variables. The root-zone moisture estimation can be improved by assimilation of surface variables provided that the error in surface variables is linked to the error in root-zone soil moisture content. In other words, if there is no sensitivity between the surface states and the root-zone soil moisture, it is not expected to result in the correlation between the errors. Uncorrelated errors of surface variables and the root-zone soil moisture would not lead to a systematic improvement of the root-zone soil moisture by the data assimilation technique.
Although Pipunic et al. (2008) reported a successful assimilation of evapotranspiration (ET) observations derived from TIR images into a land surface model, Anderson et al. (2011) showed that TIR-based ratio of actual ET to potential ET \( f_{PET} = \frac{AET}{PET} \) is more correlated with soil moisture deficiencies in comparison with ET estimations. Using this finding Hain et al. (2012) preferred to use RS-based soil moisture proxy (ET predictions of ALEXI model normalized by potential ET) in assimilation technique rather than using RS-based ET.

In a data assimilation system, information about the predicted states can be inferred from the observed variables through the relationships expressed in the model’s governing equations. Surface information is propagated to the deeper soil layers through the model physics. Consequently, the connection between surface variables and root-zone soil moisture has an important role in determining the reliability and efficacy of data assimilation technique. Each WEB-SVAT model owns a different parametrization of soil moisture dynamics based on its particular scheme of soil and vegetation properties to calculate water and energy balance components (Crow et al. 2005). These differences in model schemes lead to variation in vertical coupling strength between the surface and subsurface variables. Also, the way that data assimilation technique propagates observed surface information into the deeper soil layers varies depending on the unique vertical connection strength of the chosen model. If the surface variable and root-zone states are correctly coupled in the model, knowledge of a change in surface variable would be more informative about root-zone change compared with those with the coupling strength over- or under-represented.

Some notable shortcomings in the WEB-SVAT models in the estimations of soil moisture, energy fluxes and their relationship with vegetation and soil have been reported in previous studies (e.g. Niu et al. 2011, Gayler et al. 2013). An important improvement of WEB-SVAT models in terms of surface and root-zone coupling can be achieved by modifying the existing simple representations of subsurface processes with the more realistic ones. For example, since root growth and root water uptake is often simplified in WEB-SVAT models (Overgaard et al. 2006), adopting more advanced vegetation dynamics from crop models, which consider the interaction of root depth and distribution with soil water content, may enhance the overground-underground connection of WEB-SVAT scheme.
As it mentioned before, studies examining the assimilation of thermal remote sensing observations to the SWEB-SVAT model have reported improvement in root-zone soil moisture estimations (e.g. Gao et al. 2015, Li et al. 2010). However it seems that simplification in the representation of dynamic surface-to-subsurface coupling – which is mediated by root biophysical processes and the transpiration parameterization – may result in unanticipated errors deteriorating the performance of data assimilation (Kumar et al. 2009). In this various model schemes are evaluated to show how the use of different model parametrisation affects the performance and results of data assimilation technique. The influence of different coupling strength on the accuracy and validity of data assimilation method in transferring surface information into the root-zone is evaluated.

### 2.4. Knowledge gaps and research questions

In this section the research objective which is estimating root-zone moisture content using integrated system of modelling and surface observations is discussed. Current important knowledge gaps and the defined research questions addressed in this thesis are also presented.

Although TIR-based approaches provide valuable information about root-zone soil moisture content, they contain some important knowledge gaps that make them imperfect. Here, some of the distinguished gaps are demonstrated by consolidating problems introduced in the previous sections. These knowledge gaps show how the limitations of different methods lead to attempting to improve the structure of the WEB-SVAT models by adopting dynamic vegetation components and then assimilating TIR-based data into the improved model in order to find the best estimation of root-zone soil moisture in this research.

- **Impact of the coupling between root-zone soil moisture and surface variables**

  The connection between surface variables and root-zone states of the model plays an important role in data assimilation techniques designed to produce superior profile soil moisture estimations by propagating surface information into deeper layers of soil. Evaluating the results of previous attempts in assimilating surface variables into the model
in order to improve root-zone soil moisture demonstrated that the over-simplifying the model biophysics may produce errors which hamper the ability of data assimilation to constrain root-zone soil moisture.

Previous attempts to assimilate land surface observations typically assumed a simple relationship between RS-based products and soil moisture. For example assuming a linear relationship between soil moisture and \( f_{PET} \) (Hain et al. 2011) can only provide a reasonable estimate of soil moisture when the soil is dry (moisture content below field capacity). In this case assimilation of soil moisture proxy may cause errors when the assumed correlation between the proxy and the actual soil moisture becomes no longer valid under wet soil condition. Apart from soil wetness range, the vegetation cover can also have an important effect on the relationship between soil moisture and surface fluxes. The assumption of a simple and high sensitivity of evapotranspiration to the soil moisture in WEB-SVAT models results in the spuriously high correlation between them.

Although using a model with strong vertical connection correlates root-zone increments strongly with surface innovations, it cannot guarantee higher efficiency for the data assimilation system because proximity to the real world coupling strength is also important. For example, if the model overestimates the sensitivity between surface and sub-surface states, it will always force the system to update the root-zone state but it does not mean that this update will always provide an improvement. Making a larger change in result cannot guarantee its closeness to the truth; on the contrary it may add more errors and inconsistency. As a result, a more accurate representing of the true coupling between surface fluxes and profile soil moisture can be more beneficial even if it shows a weaker surface variables-root-zone coupling.

Although the overestimation of connection between surface variables (such as energy fluxes) and soil moisture content is very common in land surface modelling, this relationship is highly conditional on the vegetation biomass and plant phenology. The model parametrization is very important in considering these aspects influencing the correlation between root-zone soil moisture and above ground variables such as energy fluxes. More realistic characterization of surface and subsurface processes of WEB-SVAT
models by adopting dynamic vegetation, may improve the surface-root-zone linkage resulting in improved efficacy of data assimilation.

- **Impact of root depth and distribution**

  One of the most important limitations of TIR-based RS-SVAT models is that the soil depth corresponding to the estimated water content is not clearly defined. Some of the approaches partition the soil profile just to the surface and root-zone layers (e.g. Anderson et al. 2007a), and some others trying to define the depth of each layer more precisely as predefined constant values considering the arbitrary rooting depth of particular species (e.g. Scott et al. 2003, Hain et al. 2009). Although WEB-SVAT models utilise soil layering, the plant root depth variations are not considered in the parametrization of the model. As it described before, TIR-based methods are based on the plant root photosynthesis activity in which plant transpire the water from the soil layers to the atmosphere. Root depth variation plays an important role in estimating soil water loss by transpiration because it determines the soil depth from which the roots can extract water. Plants cannot extract water beyond this depth and water available for transpiration depends on water content within this depth. The importance of dynamic nature of the plant root system is not limited to growth stage-based varying rooting depth; rather it includes root density and distribution. Considering uniform distribution and constant density – which is the case in most of WEB-SVAT models – assumes that the amount of water transpired by the plant is uniformly distributed in the whole profile of the soil while in reality plant behaves differently due to non-homogeneous nature of root. As a result, dynamic rooting depth and root distribution should be considered as a part of the model to estimate the soil water content more accurately.

  On the other hand, more realistic link between root water uptake to crop growth and water availability in each rooted layer of soil in the model, makes the dependency between profile soil moisture and evapotranspiration more accurate. Adopting the additional physics such as dynamic and non-uniform root growth and distribution in WEB-SVAT models seems to be required in order to appropriately capture the relationship between surface fluxes and profile soil moisture.
- **Impact of growing stages and phenological cycle of plant**

Most of conventional WEB-SVAT models assume that ET is proportional to spectrally observable biomass. As a result, existing ET partitioning schemes are based on some vegetation indices such as LAI. Considering the LAI-based canopy net radiation as a driving force for transpiration, the quantity of water uptake is somehow related to the biomass. It means crops have been simulated to extract more water when the leaf area is larger. However, it seems that this assumption may become invalid when vegetation goes through the mature stage because although LAI is a larger value at this stage, the plant starts decreasing the transpiration (Allen et al. 2006). Vegetation type and characteristics of various species as well as growth stages and phenological cycle of the plant have an influence on transpiration activity and these effects may change the estimation of root-zone soil moisture (Reich et al. 2003). Incorporating biophysical and seasonal plant behaviour to the models make it possible to improve the vegetation parameterization in evapotranspiration (ET) estimation and consequently root-zone soil moisture estimation of the model.

Since canopy resistance has been used to parametrized canopy transpiration in most of land surface models with a strong impact on transpiration estimation, it can be parameterized so that it reflects the strength of transpiration at different stages of plant growth. Although canopy resistance is also influenced by the vegetation characteristics, it is mainly calculated based on the water content in the whole root layer and resistance extremes. Resistance extremes are estimated based on soil texture, and the effect of plant activities is neglected in them. Use of constant canopy resistance extremes makes the final canopy resistance independent of growth stages in which plant has different transpiration power. Whereas, calculating plant transpiration considering plant biophysical fluctuations in the model may improve the estimation of root-zone soil moisture.

On the other hand, change in the estimations of transpiration and soil moisture may alter the relationship between surface fluxes and soil moisture content and makes it highly conditional on the plant phenology. Consequently, additional novel physics in WEB-SVAT models such as dynamic canopy resistance seems to be helpful to adequately and
realistically capture the relationship between surface flux and profile soil moisture across a range of crop growth stages.

Based on above knowledge gaps, the research is divided into two main parts, each addressing one main research question. To address these two main questions some sub-questions that target different aspects of the problem are defined. The first part focuses on answering the following question:

- What are the sources of sub-optimal/incorrect coupling between surface variables and root-zone states in the model?

To answer this question, several aspects of model scheme that can affect the estimations of surface variables (such as energy fluxes) and surface and root-zone soil moisture are explored. Specifically, four specific sub-questions are addressed:

- How can the representation of root growth (including dynamic rooting depth and distribution) be improved?
- How can a realistic dynamic growth component (including plant growth stages and phenological cycle) be made in the model?
- What are the effects of having each/all of these dynamic vegetation components on the model estimations?
- What are the effects of these model structure changes on the coupling between surface variables and root-zone states estimations?

The second part of this research builds on the first part and focuses on the following research question:

- If we reproduce more realistic coupling between root-zone soil moisture and surface variables, will that really improve soil moisture updates through data assimilation techniques?

To answer this question, modified model scheme (via the integrating dynamic vegetation components in previous stage) resulting in changes in the correlation between surface variables and root-zone soil moisture, is explored in a data assimilation system. Within this stage, two sub-questions are answered:
- How does the realistic connection between surface variables and root-zone soil moisture in dynamic model affect data assimilation results?
- What is the impact of using an empirical coupling between surface variables and root-zone soil moisture based on field observations on data assimilation results?
3. CHAPTER 3: IMPROVING ROOT-ZONE SOIL MOISTURE ESTIMATIONS USING DYNAMIC ROOT GROWTH AND CROP PHENOLOGY

3.1. Introduction

Soil moisture is a key requirement in environmental monitoring and hydrological prediction. Within the past several decades, various modelling techniques have been developed to simulate soil water movement coupled with biophysical and surface energy processes (Dai et al. 2003, Nijssen et al. 2001, Hogue et al. 2005). Soil-vegetation-atmosphere transfer (SVAT) schemes represent one of the most advanced modelling approaches, which can be applied to monitor water and energy exchanges (Noilhan & Planton 1989). The broad category of SVAT schemes include a wide variety of approaches that partition surface net radiation into sensible and latent heat fluxes (Crow et al. 2005). There are some structural differences between these methods in their treatment of surface temperature, which divides the SVAT approaches into two main categories: RS (Remote Sensing) and WEB (Water and Energy Balance) -SVAT (Crow et al. 2005). In the RS-SVAT category, thermal-infrared (TIR) satellite observations are used as an input to diagnostic models for estimating instantaneous surface energy flux components of net radiation. Since RS-SVAT models do not contain prognostic equations for soil temperature or soil moisture states, they can only generate estimates for non-continuous instances in which remotely-sensed surface temperature retrievals are available. The Two-Source Energy Balance (TSEB) model (Norman et al. 1995) and the Surface Energy Balance (SEBAL) model (Bastiaanssen et al. 1998) are examples of RS-SVAT models.

In the second category, prognostic water and energy balance (WEB) models are forced by meteorological input to assess the temporal variations of soil moisture and surface states. The main difference of this approach from the RS-SVAT models is that surface radiometric temperature is solved for via an internal surface energy balance which is coupled with a prognostic water balance calculation. As a result, WEB-SVAT models do not require remotely-sensed surface temperature observations and can be run continuously using meteorological observations. This enables the integration of TIR data or some of the
products of RS-SVAT methods (e.g. predicted soil moisture or evapotranspiration) via data assimilation to improve the soil moisture estimations. Typically, WEB-SVAT models are more complicated than RS-SVAT schemes and often contain a larger number of parameters not only for partitioning the surface energy budget but also as a multi-objective model for predicting surface water states and fluxes as well.

WEB-SVAT modelling approaches obtain energy flux predictions by parameterizing components of the surface energy balance, i.e. net radiation ($R_N$), sensible heat ($H$), latent heat ($LE$), and ground heat flux ($G$) as a function of surface aerodynamic temperature ($T_{aero}$), soil and vegetation properties, forcing variables such as precipitation and incoming solar radiation, thereby numerically solving the following energy balance equation:

$$R_N = H + LE + G.$$  (3-1)

The model combines the energy flux predictions with vertical subsurface soil water modelling in order to predict the soil moisture content continuously (Crow et al. 2008).

Although the WEB-SVAT models share a common conceptual basis, the parameterization of equations can vary for different models resulting in predictions with a large variation (Crow et al. 2005). The Common Land Model (CLM) (Dai et al. 2003) and Noah (Hogue et al. 2005) are some examples of WEB-SVAT models. They have been developed as complex models with multiple soil layers in order to suit a wide range of applications.

The estimates from WEB-SVAT models contain some uncertainty due to model parameters and forcing errors. In addition, model deficiency in representing the land surface processes makes the results more uncertain. Data assimilation methods can be used to reduce random soil moisture prediction errors by constraining the model with ground or remotely sensed observations of surface states. The connection between surface and root-zone states of the model plays an important role in data assimilation techniques designed to produce superior profile soil moisture estimations by propagating surface information into deeper layers of soil (Kumar et al. 2009). In this study we evaluate how a more realistic representation of the subsurface processes improves the surface-root-zone linkage and affects model performance in estimating surface and root-zone states. Subsequently, the improvements
can potentially lead to more appropriate results when surface observations are assimilated into the model.

The surface and root-zone coupling of WEB-SVAT models can be improved by adopting dynamic vegetation components. In general, WEB-SVAT methods parameterize plant transpiration using a stomatal resistance formulation that relates root-zone water availability to canopy conductance based on atmospheric demand. Root depth variation plays an important role in estimating soil water loss by transpiration because it determines the soil depth from which the roots can extract water. Plants cannot extract water beyond this depth and water available for transpiration depends on water content within this depth. The importance of dynamic nature of the plant root system is not limited to growth stage-based varying rooting depth; rather it includes root density and distribution. Considering uniform distribution and constant density – which is the case in most of WEB-SVAT models – assumes that the amount of water transpired by the plant is uniformly distributed in the whole profile of the soil while in reality plant behaves differently due to non-homogeneous nature of root. As a result, dynamic rooting depth and distribution should be considered as a part of the model to simulate the soil water movement more realistic (Gayler et al. 2013). On the other hand, soil textural properties, vegetation type and characteristics of various species as well as growth stages and phenological cycle of the plant have an influence on transpiration activity and these effects may change the estimation of root-zone soil moisture (Reich et al. 2003). Incorporating biophysical and seasonal plant behaviour using observable indices make it possible to improve the vegetation parameterization in evapotranspiration ($ET$) estimation and consequently root-zone soil moisture estimation of the model. Integrating WEB-SVAT models with other models simulating vegetation dynamics can make the aboveground-underground connection stronger; however, WEB-SVAT models will be more complex and some unexpected outcomes may be encountered.

Some crop models have plant growth and development linked dynamically to soil properties and moisture state driven by meteorological forcing. In these models, rooting depth and density is dynamically simulated as a function of various parameters such as soil moisture and temperature, crop and soil characteristics, climate and management variables such as irrigation and fertilizer application (Brun et al. 2006). Although representation of
vegetation components is typically more sophisticated in these models, their hydrological parameterisation for soil moisture and energy balance estimation is less complex than that in WEB-SVAT models. However, incorporating a relatively simple root growth model to a WEB-SVAT model can integrate the advantages of the crop models – considering the interaction of root depth and distribution with soil water content – with WEB-SVAT models.

A relatively simple WEB-SVAT model has been developed for some studies to make it more efficient to be integrated with remotely sensed observation systems and its state variables more compatible with observations (e.g. Crow et al. 2008, Crow & Reichle 2008, Li et al. 2010). In order to make a distinction between the name of this specific WEB-SVAT model and more generic WEB-SVAT, the former model is called SWEB-SVAT hereafter.

The SWEB-SVAT model uses a two-layer soil-vegetation equations based on a force-restore model proposed by Noilhan & Planton (1989) and adapted by Montaldo et al. (2001) for the soil water balance with a very similar aerodynamic resistance structure and radiation parameterization to the parallel version of two source energy balance (TSEB) (Norman et al. 1995). This model adopts the sophisticated scheme of TSEB model which provides separate estimation of transpiration and evaporation. Apart from the relative simplicity that enables easy modification of the soil water movement scheme and the vegetation parameterization, using the SWEB-SVAT model has other advantages. Independent observations of surface temperature and soil moisture can be assimilated into the model to update the model predictions. In addition, not only the remotely sensed ET from various one-source algorithms, but also the separate estimate of transpiration derived from TSEB or other two-source models can be integrated in to the model. Structural similarity between SWEB-SVAT and TSEB makes it more robust in the choice of observations that can be assimilated into the model.

The SWEB-SVAT model has been used to propose the concept that root-zone soil moisture can be improved by assimilating thermal remote sensing observations into the model (e.g. Crow et al. 2008, Li et al. 2010). Although these attempts demonstrated some improvements, it appears that the over-simplifying the root biophysical processes or the
transpiration parametrization of the model may produce errors which hamper the ability of data assimilation to constrain root-zone soil moisture (Kumar et al. 2009). As is for many land surface models, adding more layers with assigning proportion of root distribution to each layer helps to simulate water percolation between the layers and extracting water from each layer based on the root contribution (Gayler et al. 2014, Li et al. 2001).

In this paper the SWEB-SVAT model is extended to incorporate an exponential root water uptake model with water stress compensation proposed by Li et al. (2001). The model is modified to have more layers in order to provide a realistic dynamic root distribution. The impacts of plant root depth variations, growing stages and phenological cycle of plant on transpiration are considered in developing stages and the new developed model is validated using different data sets.

3.2. Materials and Methods

3.2.1. SWEB-SVAT model

The SWEB-SVAT adopts two soil layers, surface- and root-zone layers where the surface layer is a part of the root-zone layer. Surface and root-zone soil moisture variations are calculated by the water balance equation represented as:

\[
\frac{d\theta_{sz}}{dt} = \frac{C_1}{d_{sz}} \left[ P_g - LE_S (\rho \lambda)^{-1} \right] - \frac{C_2}{f_d} (\theta_{sz} - \theta_{eq}) \tag{3-2a}
\]

\[
\frac{d\theta_{rz}}{dt} = \frac{1}{d_{rz}} \left[ P_g - LE_C (\rho \lambda)^{-1} \right] - LE_S (\rho \lambda)^{-1} - Q \tag{3-2b}
\]

where \(\theta_{sz}\) and \(\theta_{rz}\) are surface- and root-zone soil moisture contents, \(d_{sz}\) and \(d_{rz}\) surface- and root-zone depth, \(P_g\) throughfall, \(LE_S\) and \(LE_C\) soil and canopy latent heat flux, \(\rho\) density of air, \(\lambda\) latent heat of vaporisation, \(f_d\) the frequency of diurnal variations (24 hours), \(\theta_{eq}\) equilibrium surface volumetric moisture content, and \(Q\) the drainage from the bottom of the root-zone. \(C_1\) and \(C_2\) are force and restore coefficients for soil moisture, which are related to the soil characteristics.
All the calculations of net radiations and heat fluxes are modelled same as the TSEB model (Norman et al. 1995) in order to partition the energy fluxes between soil and vegetation via separate energy balance equations as:

\[ R_{N,C} = H_C + LE_C \]  
\[ R_{N,S} = H_S + LE_S + G \]

Total surface fluxes are calculated by summing canopy and surface components as follows:

\[ R_N = R_{N,C} + R_{N,S} \]  
\[ H = H_C + H_S \]  
\[ LE = LE_C + LE_S \]

Canopy \((R_{N,C})\) and soil \((R_{N,S})\) components of net radiation are calculated based on the radiative transfer model of (Campbell & Norman 1998) using observations of downward solar radiation \((S_\downarrow)\) or \(R_S\) and calculated long wave radiation \((L_\downarrow)\).

\[ R_{N,C} = (1 - \tau_{longwave})(L_\downarrow + \varepsilon_S \sigma T_S^4 - 2 \varepsilon_C \sigma T_C^4) + (1 - \tau_{solar})(1 - a_lC)S_\downarrow \]  
\[ R_{N,S} = \tau_{longwave}L_\downarrow + (1 - \tau_{longwave})\varepsilon_C \sigma T_C^4 - \varepsilon_S \sigma T_S^4 + \tau_{longwave}(1 - a_lS)S_\downarrow \]

where \(\varepsilon, a_l\) and \(T\) are emissivity, albedo and temperature of soil \((S)\) and canopy \((C)\), respectively, \(\sigma\) the Stephan-Boltzman constant, and \(\tau\) is the canopy transmissivity for short wave \((solar)\) and long wave \((longwave)\) radiations.

Sensible heat fluxes from the vegetation and soil surface are calculated as:

\[ H_C = \rho C_p \frac{T_C - T_A}{R_A} \]  
\[ H_S = \rho C_p \frac{T_S - T_A}{R_A + R_{A,S}} \]

where, \(C_p\) is the specific heat of air at constant pressure. \(R_A\) is the above-canopy aerodynamic resistance and \(R_{A,S}\) the within-canopy soil aerodynamic resistance. \(R_A\) and \(R_{A,S}\) are parameterized based on surface roughness lengths, wind speed, and stability.
considerations presented for the parallel version of the TSEB in Norman et al. (1995). Li et al. (2005) showed that both parallel and series resistance parameterisation provided similar estimations of the latent and sensible heat fluxes. However, the parallel version of TSEB model is more sensitive to variation of model parameters, such as the clumping factor and fractional vegetation cover. On the other hand, it was shown that within a narrow range in vegetation cover fraction, the parallel network achieved a balance in the radiative temperature and convective heat fluxes between the soil and canopy component while the series version is unable to maintain the balance.

In contrast to TSEB, $LE_S$ and $LE_C$ are calculated based on the Eqs. (3-7).

$$LE_S = \rho C_p \gamma^{-1} [e_s(T_S) - e_a]/(R_{AS} + R_A + R_S) \quad (3-7a)$$

$$LE_C = \rho C_p \gamma^{-1} [e_s(T_C) - e_a]/(R_C + R_A) \quad (3-7b)$$

where, $\gamma$ is the slope of the saturation vapour pressure versus temperature curve, $e_s$ and $e_a$ are saturation and near-surface water vapour pressure, $R_S$ and $R_C$ are soil and canopy resistances which are a function of surface and root-zone soil moisture, respectively. The canopy resistance $R_C$ is estimated by:

$$R_C = \begin{cases} 
R_{C,max} & \theta_{rz} < \theta_w \\
(R_{C,min} - R_{C,max}) \frac{\theta_{rz} - \theta_w}{\theta^* - \theta_w} + R_{C,max} & \theta_w < \theta_{rz} < \theta^* \\
R_{C,min} & \theta_{rz} > \theta^*
\end{cases} \quad (3-8)$$

where $\theta^*$ and $\theta_w$ are the volumetric soil moisture levels at canopy stress and wilting point, respectively, resistance extremes $R_{C,max}$ and $R_{C,min}$ are specified based on typical literature values and consideration of soil texture (Li et al. 2010).

As a first step in computational stream of SWEB-SVAT model, initial values of $\theta_{sz}$ and $\theta_{rz}$ are used to calculate the soil and canopy resistances. Once these variables are given, all the fluxes in Eqs. (3-3) can be expressed in terms of canopy and soil temperature ($T_C$ and $T_S$). Newton-Raphsan method is used to derive solutions of Eqs. (3-3) for $T_C$ and $T_S$ simultaneously. The final output from the energy balance part of the model is the soil evaporation ($LE_S$) and canopy transpiration ($LE_C$), which are required to update soil moisture states in time via Eqs. (3-2).
3.2.2. Exponential root water uptake model with water stress compensation

Feddes et al. (1978) described the amount of water uptake as:

\[ S(h) = \alpha(h)S_{\text{max}}. \]  

(3-9)

In this equation \( \alpha \) represents the available soil water (dimensionless) as a function of soil water pressure head \( (h) \) and \( S \) is the sink term. The sink term is the rate of water extraction per unit depth of soil (Prasad 1988). \( S_{\text{max}} \) is the maximum water uptake, which is equivalent to the potential transpiration rate divided by the rooting depth. In Eq. (3-9), potential transpiration is assumed to be distributed homogeneously across the whole root-zone and consequently it will decrease uniformly as the water availability reduces. However, the root density and subsequent water uptake are typically reduced with depth. In order to model this profile distribution more realistically, an exponential relationship based on potential transpiration rate, root density and water availability was formed by Li et al. (1999) as represented in Eqs. (3-10). In this formulation the soil profile has been divided to \( n \) layers and \( i \) represents the layer number as:

\[ S_{\text{exp},i} = \frac{\alpha_i F_i P_t}{\Delta Z_i} \]  

(3-10a)

\[ F_i = \frac{\ln \left[ \frac{1 + \exp(-bZ_i)}{1 + \exp(-bZ_{i+1})} \right] + 0.5[\exp(-bZ_i) - \exp(-bZ_{i+1})]}{\ln \left[ \frac{2}{1 + \exp(-bZ_r)} \right] + 0.5[1 - \exp(-bZ_r)]} \]  

(3-10b)

where \( P_t \) is potential transpiration, \( \Delta Z_i \) layer thickness and \( F_i \) is the fraction of root length density in layer \( i \) described by the represented equation, \( Z_i \) is soil depth of layer \( i \), \( Z_r \) is root depth, and \( b \) is an empirical extinction coefficient of root distribution. Generally, soil properties and crop characteristics affect the selection of \( b \). Considering the effect of crop specifications, a smaller value of \( b \) (e.g. 0.02) is selected for crops with uniform distribution of root over the entire root depth such as wheat comparing with plants with large root mass in the first layer of soil such as soybean. Also, existence of hard subsoil, which restrict the root development in the deeper layers, can increase \( b \) (Li et al. 2000). However, the
calculation of $b$ based on the root density in the first 10 cm of soil ($F_{10}$) can compensate these effects to some extent:

$$b = \frac{24.66 F_{10}^{1.59}}{Z_r}$$ (3-11)

Since plant roots tend to uptake more water from the surface layer when the soil profile is wet (Nanymah & Black 1977), and the effect of water shortage in one part of the soil on water uptake can be compensated from the other parts that are not under stress (Lai & Katul 2000), Li et al. (2001) proposed the use of a weighted stress function defined based on root density and water availability:

$$S_{max,i} = \frac{P_i \beta_i}{\Delta Z_i}$$ (3-12a)

$$\beta_i = \frac{\alpha_i F_i^\lambda}{\sum_{i=1}^{n} \alpha_i F_i^\lambda}$$ (3-12b)

$$S_i = \frac{\alpha_i^2 F_i^\lambda P_t}{\Delta Z_i \sum_{i=1}^{n} \alpha_i F_i^\lambda}$$ (3-12c)

The unit-less parameter $\lambda$ in the model controls the water uptake distribution within the soil profile; with increased $\lambda$, more water is extracted from the upper layers, and consequently the fraction of water uptake from the lower layers decreases. Under non-stressed condition when $\lambda$ is equal to 0.01, it is very similar to the model of Feddes et al. (1978), distributing potential transpiration uniformly throughout the soil profile. In the case $\lambda = 0.25$, it produces a linear relationship between soil depth and water uptake which is very similar to the model represented by Hoogland et al. (1981). When $\lambda = 1$, it will be identical to the exponential model of Li et al. (1999). Ehlers et al. (1991) suggested $\lambda = 0.5$ based on the relative behaviour of special crops such as wheat and other cereals. Given that root growth is affected by soil physical and chemical conditions, considering an effective $\lambda$ corresponding to the behaviour of vegetation and soil properties is very important. For example, soil with a layer of hard subsoil can be simulated by setting $\lambda = 2$, which causes more water uptake from the upper layers of soil (Li et al. 2001). Ideally, $\lambda$ should be evaluated and assessed from field observations.
In summary, according to Feddes et al. (1978), actual transpiration can be calculated by multiplying potential transpiration of the whole profile of the soil by water stress; in the next model (Li et al. 1999), potential transpiration is divided layer-by-layer based on the root distribution ($P_t \times F_l$) prior to multiplying by water stress of each layer to calculate actual transpiration of that layer. In the third model (Li et al. 2001), potential transpiration is partitioned between the layers by $\beta_l$ which is a weighted stress function of soil water availability and root distribution of the layer. In the final model, more water is extracted from shallow layers before the water stress stage. Once the water stress is induced in the shallow layer, the peak water uptake occurs in the deeper layer. It means that most of water uptake comes from the deeper layers while surface layers do not have large effect on transpiration. The latter model incorporated into Soil Water Atmosphere Plant (SWAP) model (Van Dam et al. 1997) to estimate soil water content in a semi-arid area showed significantly improved deeper layer soil moisture estimation, especially in the late periods of crops growing season when the vegetation was under stress. They suggested that this model can be used for diverse cereal crops (Li et al. 2001).

### 3.2.3. Multi-layer WEB-SVAT with Dynamic Root distribution (MWSDR)

In this study a new model is adapted to improve the current scheme of SWEB-SVAT model by incorporating a sophisticated root distribution model that considers the dynamic nature of plant growth. The original SWEB-SVAT model is modified to include 5 layers to implement the vertical profile of root distribution. The impact of new parameterization of plants specifications on model performance, in terms of: i) estimating canopy resistances based on plant phenology and ii) adding more layers and assigning proportion of root distribution to each layer, are investigated before incorporating them to the original SWEB-SVAT model. As illustrated in Figure 3.1, three different cases are defined to evaluate the impact of incorporating various vegetation components to the model.

- **Case 1: RS-based dynamic canopy resistance**

  Since resistance extremes ($R_{C,min}$ and $R_{C,max}$) have a strong impact on transpiration estimation, they can be parameterized so that they reflect the strength of transpiration at
different stages of plant growth. Some researches showed that canopy resistance has a clear relationship with photosynthetic activities and other physiological characteristics of the canopy (Reich et al. 2003). Also, it has been shown that there is an approximately linear correlation between remote sensing (RS) based indices such as Normalised Difference Vegetation Index (NDVI) and Enhanced Vegetation Index (EVI) with both plant photosynthesis and canopy conductance (Huete et al. 2002). Variation of RS-based indices over time therefore, reflects the canopy resistance variations due to various vegetation type and phenological cycle during the growth period.

Use of constant $R_{c,min}$ and $R_{c,max}$ makes the final canopy resistance independent of growth stages in which plant has different transpiration power. In order to estimate the total canopy resistance based on plant phenology, minimum canopy resistance may be estimated as a function of a remote sensing index such as NDVI as a scaling factor. This new canopy
resistance extreme will be scaled based on water stress function and applied to calculate canopy transpiration.

Estimating canopy resistance extremes as a function of RS-based indices has been used in several different ways. For example, Van Dijk (2010) suggested use of PCI (photosynthetic capacity index) to calculate maximum canopy conductance \( G_{s,max} \) which is the reciprocal of minimum canopy resistance as:

\[
G_{s,max} = k \times PCI
\]

(3-13)

defining \( k \) as a constant value. By inverting Eq. (3-13), \( R_{c,min} \) is calculated as:

\[
R_{c,min} = \frac{1}{G_{s,max}} = \frac{1}{k \times PCI} = \frac{k_2}{PCI}
\]

(3-14)

Other remotely sensed vegetation indices such as NDVI can be used to apply vegetation-dependent values in Eq. (3-14). In this case, in order to verify only the impact of dynamic canopy resistance, a new canopy resistance calculated as a function of NDVI is used for transpiration calculation and the results will be compared with the original SWEB-SVAT model.

**Case 2: Multiple soil layers**

The original SWEB-SVAT uses a force-restore equation for soil moisture calculation of thin surface layer. Soil moisture variation of the root layer, which includes the surface layer, is controlled by transpiration, evaporation from surface layer and drainage out the bottom of the layer according to Eqs. (3-2). In order to have more separate layers, one surface layer and four root-zone layers are defined using a simple conceptual model of soil moisture. Surface and root-zone soil water content for every time step are calculated for this multi-layer model based on the following equations subtracting soil evaporation \( LE_S \) from the surface layer and fraction of canopy water uptake associated to each layer \( LE_{C,n} \) from the subsurface layers.

\[
\frac{d\theta_{sz}}{dt} = \frac{1}{d_{sz}} [P_g - LE_S(\rho \lambda)^{-1} - q_{1\rightarrow 2}] \tag{3-15a}
\]
\[
\frac{d\theta_{rz,n}}{dt} = \frac{1}{d_n} \left[ q_{n-1\rightarrow n} - LE_{C,n}(\rho \lambda)^{-1} - q_{n\rightarrow n+1} \right] \quad (3-15b)
\]

where \( q_{n\rightarrow n+1} \) shows the water flux from layer \( n \) to layer \( n+1 \) (redistribution) assuming Darcy equation:

\[
q_{n\rightarrow n+1} = K_{\theta,n} \left[ \frac{\psi_{m,n} - \psi_{m,n+1}}{0.5(d_n + d_{n+1})} \right] + K_{\theta,n} \quad (3-16)
\]

\( K_{\theta} \) is hydraulic conductivity, \( \psi_m \) matric potential and \( d_n \) depth of soil layer.

The energy balance portion of SWEB-SVAT model calculates the soil and canopy temperature using an iterative process based on surface meteorological forces (e.g. solar radiation, wind speed, air temperature) and modelled soil moisture states. A key component of this balancing controlling the surface temperature is canopy transpiration in which root layer soil moisture available for plant water uptake plays an important role. Using the lumped root-zone soil moisture as an input to calculate the total transpiration means that the amount of water transpired by the plant is assumed to be uniformly distributed in the whole profile of the soil – regardless of the root vertical distribution. Having multiple soil layers is inevitable when adding a root growth component to the model. Therefore, in order to verify only the impact of adding multiple separate layers, the calculated total transpiration is divided between the layers based on the depth and the results will be compared with the original SWEB-SVAT model. The specific part of transpiration which is provided from the \( n^{th} \) layer is presented by \( LE_{C,n} \) in Eq. (3-15b).

- **Case 3: Dynamic root depth and distribution**

As demonstrated in section 2.2., root density distribution and moisture condition of different soil layers are the key factors in water uptake estimation. The root water uptake distribution can be parametrized by incorporating exponential root density distribution proposed by Li et al. (2001) at multiple soil layers. In the new-defined multi-layer soil profile (Case 2) it is also possible to constrain the root to uptake water from each layer based on the wetness of that specified depth. In this case \( LE_{C,i} \) is calculated for each layer based on the water content and root density. Similar to the exponential model, transpiration contribution of each layer can be calculated as:
The final total transpiration ($LE_C$) will be the sum of partial transpiration calculated for each layer ($LE_{C,i}$).

$$LE_C = \sum_{i=1}^{n} LE_{C,i}$$  \hspace{1cm} (3-18)

Root depth ($Z_r$) and empirical extinction coefficient of root distribution ($b$), are required to calculate the fraction of root length density in layer $i$ ($F_i$) as was described by Eq. (3-10b). Since root depth changes by time, there is a need to have a dynamic rooting depth in the model. The variable $b$ can be calculated if there is information about the fraction of root length density in the top 10% of the root-zone ($F_{10}$) using Eq. (3-11). Typical rooting depth ($Z_r$) and $F_{10}$ as a function of growth stages were reported in several researches. For example Li et al. (2001) estimated this information based on wheat growth stages from collected ground data by Campbell et al. (1977). There are various ways to find the approximate date of individual plant growth stages. Miller (1999) and Wise et al. (2011) describe the identification of growth stages of wheat based on the shape and size of the over-ground biomass. In the case that in situ crop growth observations are not available, region- and crop-specific timing tables of growth stages or simple models simulating those timing tables can be employed (McMaster et al. 1992). However such tables are not able to determine the growth stages in all the conditions because air temperature can dramatically affect the time required for plant to reach different growth stages (Ritchie & NeSmith 1991). Miller et al. (2001) suggested using growing degree days (GDD) based on actual daily average air temperature as a simple and precise way to predict the time of certain plant stage. Here it is assumed that plants require a specific amount of heat to transition between developmental stages. Miller et al. (2001) and Bowden et al. (2008) collected field observations to show the growing degree days required to reach various plant stages for several crops. With air temperature observations and such tables, the timing of various growth stages in the selected data set can be predicted.

As shown in Table 3.1, different growth stages of wheat used in the new model have been adapted from Bowden et al. (2008).
Table 3.1: Wheat growth stages and required growing degree day (GDD)

<table>
<thead>
<tr>
<th>Growth Stages</th>
<th>Planting</th>
<th>Emergence</th>
<th>Three Leaf</th>
<th>Five Leaf</th>
<th>Shot Blade</th>
<th>Dough</th>
<th>Maturity</th>
<th>Harvesting</th>
</tr>
</thead>
<tbody>
<tr>
<td>GDD</td>
<td>-</td>
<td>100</td>
<td>300</td>
<td>605</td>
<td>1300</td>
<td>1475</td>
<td>2175</td>
<td>2475</td>
</tr>
</tbody>
</table>

Since the information about rooting depth and $F_{10}$ is available only within specified growth stages, linear interpolation is used to estimate root growth and density variation between two different stages. These assumptions make it possible to calculate $F_i$ as a continuous dynamic value based on the biophysical states of the plant. $F_i$ calculated for each layer in Ponca site are presented in Figure 3.2 versus time. It should be noted that Day 1 in the figure is 63 days after planting when there is some root biomass in the second layer. The fraction of root length density in the upper layer decreases with time. This decrease is balanced by an increase in deeper soil layers, which is consistent with our expectation concerning root growth behaviour.

In order to verify the impact of dynamic root depth and distribution alone (separate from the impact of adding multiple soil layers), the results of Case 3 will be compared with the results of Case 2.

![Figure 3.2: Simulated fraction of root length density of wheat in different layers of the root-zone ($F$), layer1: 10-30 cm, layer 2: 30-60 cm, layer 3: 60-90 cm, layer 4: 90-120 cm](image)

The new MWSDR model will include all the above changes described in Case 1 to 3. This new model enables the simulation of water percolation between the soil layers and extracting water from each layer based on the root contribution and plant phenology during the growth period.
3.2.4. Test sites and datasets

To test the utility of new model for soil moisture and energy fluxes prediction, this study uses hydrometeorological, biophysical and spectral data gathered from two different sites: the Dookie experimental site in Victoria, Australia and the Ponca site in Oklahoma, USA.

- Dookie site

One of the data sets used in this study has been collected from instruments installed at the Dookie campus of the University of Melbourne. This study site is a rainfed field rotationally cultivated with wheat and canola. A Spectro-Eddy-Covariance (SEC) system installed at the tower station provided data required for latent, sensible and soil heat fluxes measurements and all the necessary meteorological data including wind speed, air temperature, relative humidity and rainfall. The monitoring began on 19 August 2012 and continued until the end of 2014. Soil moisture was measured by two sets of sensors including 36 profile soil moisture systems which measured continuous soil moisture at depths of 0-4 cm, 0-30 cm, 30-60 cm, 60-90 cm, 90-120 cm. Surface reflectance system of the tower including multispectral radiometers and thermal radiometer, measured surface reflectance at six spectral bands and TIR temperature every 5 minutes. VIS/NIR radiometer data was used to provide biophysical indices including NDVI, NDWI (Normalized Difference Water Index), PRI (Photochemical Reflectance Index) and CWSI (Crop Water Stress Index). The reflectance measurement system also contained sky and ground facing sensors which could measure the incoming and outgoing radiations.

Field data collected from the wheat study site is used in this study to run the models on a 30-minutes time step. The actual time periods of interest are 24 May 2013 to 17 December 2013 which is concurrent with seeding and harvesting time, respectively, and from 19 August to 7 December 2012 which reflects a starting date around 90 days after sowing.

The timing of various stages of plant growth was determined based on GDD values calculated from observed mean daily air temperature. Available photos from the site were used to verify the timing of different stages of crop growth. These photos were also used to compare the visual characteristics of the plant with the information provided in Miller
(1999) and Wise et al. (2011) about the shape and size of the over-ground biomass at each stage. Estimated dates of growth stages, assumed root depth and $F_{10}$ corresponding to each stage – from Li et al. (2001) – for 2013 dataset are reported in Table 3.2.

This timing was also used to simulate LAI from minimum of 0.1 m at crop emergence to a maximum of 6 m at the dough stage. A piecewise linear model was used to interpolate LAI between these two end points. The same piece-wise linear interpolation was used for canopy height ($h_c$), based on a final crop height of 0.91 m. Maximum LAI and canopy height are provided from available information from the field. The original 30-minute tower-based NDVI measurements collected between 11am and 2pm (local time) were averaged to produce daily time series of NDVI and a 16-day moving window averaging was applied to produce the final daily NDVI values; the results were employed in the MWSDR model simulation.

Table 3.2: Timing of various growth stages for Dookie data set in 2013

<table>
<thead>
<tr>
<th></th>
<th>Planting</th>
<th>Emergence</th>
<th>Three Leaf</th>
<th>Five Leaf</th>
<th>Shot Blade</th>
<th>Dough</th>
<th>Maturity</th>
<th>Harvest</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>GDD</strong></td>
<td></td>
<td>-</td>
<td>100</td>
<td>300</td>
<td>605</td>
<td>1300</td>
<td>1475</td>
<td>2175</td>
</tr>
<tr>
<td><strong>Days after Planting</strong></td>
<td></td>
<td>-</td>
<td>9</td>
<td>29</td>
<td>60</td>
<td>123</td>
<td>136</td>
<td>181</td>
</tr>
<tr>
<td><strong>Calendar</strong></td>
<td>24 May</td>
<td>1 Jun</td>
<td>21 Jun</td>
<td>22 Jul</td>
<td>23 Sep</td>
<td>6 Oct</td>
<td>20 Nov</td>
<td>17 Dec</td>
</tr>
<tr>
<td><strong>Root Depth</strong></td>
<td>0.15</td>
<td>0.60</td>
<td>0.90</td>
<td>1.20</td>
<td>1.20</td>
<td>1.20</td>
<td>1.20</td>
<td>1.20</td>
</tr>
<tr>
<td><strong>$F_{10}$</strong></td>
<td>-</td>
<td>1</td>
<td>0.40</td>
<td>0.40</td>
<td>0.32</td>
<td>0.28</td>
<td>0.21</td>
<td>0.21</td>
</tr>
</tbody>
</table>

Using a preliminary evaluation of soil texture in the lab, soil texture was classified as sandy loam and appropriate values for all the parameters were selected referring to the look up table of various soil types presented in Rawls et al. (1982). However, considering the compact soil structure with higher bulk density at the deeper layers, smaller saturated hydraulic conductivity values were assumed for three lower layers of multi-layer model.

The depth of surface and root-zone layers of both models is assumed to be equal to 10 cm and 120 cm, respectively. Soil moisture probes at the surface were installed vertically in the depth ranges of 0-4 cm and 0-30 cm. In order to reduce the influence of thickness difference of the first layer between model and observations, a weighted average of 0-10 cm soil moisture is used to evaluate the predicted 0-10 cm surface soil moisture. The weighting coefficients were determined based on the overlapping fractions between the
layers (unit weight for 0-4 cm and 1/3 weight for 0-30 cm observed soil moisture). The average of soil moisture measurements available at 0-30, 30-60, 60-90, and 90-120 cm is used as representative of root-zone soil moisture observation.

- **Ponca site**

The AmeriFlux network ([http://ameriflux.lbl.gov](http://ameriflux.lbl.gov)) provides continuous measurements of water and energy exchanges under various time scales at experimental sites located in North America, Central America, and South America. Level 2 data from the “Ponca” wheat cropland AmeriFlux site, located 16 km north of Ponca City, Oklahoma, was selected for this study. This site is planted with winter wheat in mid-fall and harvested in early summer each year (Hanan et al. 2002). The selected half-hourly data has been collected from early November 1998 to mid-June 1999. At the site, daily soil moisture measurements are available for the soil depths: 0-15, 15-30, 30-60, 60-90 and 0-90 cm. Water and heat fluxes were measured at 4.5 m above the surface using the eddy-covariance sensors. All other meteorological data required as input which included incoming solar radiation, air temperature and pressure, relative humidity, wind speed and rainfall were collected at nominally 5 m above the ground. Soil type is silty clay loam in the upper 0.6 m of soil underlain by a thick heavy clay horizon and lower horizons are carbonated due to limestone bedrock (Hanan et al. 2002). Maximum canopy height was assumed as 0.91 m according to the provided information in the website.

The depth of surface layer for both models is assumed to be equal to 10 cm. Likewise, the 0-15 cm soil moisture measurement at the site is used as the surface soil moisture observation. Different depth specifications between the model and ground measurements can result in slightly-different soil moisture temporal dynamics; however; here we assume that the apparent soil depth difference was insignificant. Since there are no observations beyond 90 cm soil depth, the root-zone depth of SWEB-SVAT model is assumed to be 90 cm and available measured soil moisture in the 0-90 cm interval is considered as representative of root-zone soil moisture. The MWSDR model is defined based on four separate root-zone layers to the depth of 120 cm; however, the weighted averaged modelled soil moisture at 0-90 cm depth is compared with the results of SWEB-SVAT and observations.
Since soil moisture during the first two months of the plant growth is not available for this period, Ponca site simulations started from 1 January which is between three-leaf and five-leaf wheat growth stages. Several ground-based LAI values are available in Ponca site which are used in the model assuming a piecewise linear model providing LAI between two subsequent observations. Field measurement of Green LAI, defined in Haboudane et al. (2004), is used in place of NDVI because the MODIS NDVI is not available during the Ponca analysis period. To ensure the suitability of Green LAI, the Green LAI values collected later in 2000-2001 were compared with the MODIS NDVI and it resulted in linear correlation coefficient of 0.75. A total of 10 Green LAI measurements during the 1998-1999 cropping season were linearly interpolated and rescaled to NDVI to be used for MWSDR.

The time of various stages of plant growth was determined based on GDD values calculated from observed air temperature as shown in Table 3.3 along with assumed root depth and \( F_{10} \) corresponding to each stage.

<table>
<thead>
<tr>
<th>Growth Stages</th>
<th>Planting</th>
<th>Emergence</th>
<th>Three Leaf</th>
<th>Five Leaf</th>
<th>Shot Blade</th>
<th>Dough</th>
<th>Maturity</th>
<th>Harvest</th>
</tr>
</thead>
<tbody>
<tr>
<td>GDD</td>
<td>-</td>
<td>100</td>
<td>300</td>
<td>605</td>
<td>1300</td>
<td>1475</td>
<td>2175</td>
<td>2475</td>
</tr>
<tr>
<td>Days after Planting</td>
<td>-</td>
<td>12</td>
<td>28</td>
<td>101</td>
<td>170</td>
<td>181</td>
<td>216</td>
<td>229</td>
</tr>
<tr>
<td>Calendar</td>
<td>early Nov</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>late May</td>
<td>mid Jun</td>
</tr>
<tr>
<td>Root Depth</td>
<td>-</td>
<td>0.15</td>
<td>0.60</td>
<td>0.90</td>
<td>1.20</td>
<td>1.20</td>
<td>-</td>
<td>1.20</td>
</tr>
<tr>
<td>( F_{10} )</td>
<td>-</td>
<td>1</td>
<td>0.40</td>
<td>0.40</td>
<td>0.32</td>
<td>0.28</td>
<td>-</td>
<td>0.21</td>
</tr>
</tbody>
</table>

The leaf visual properties of the Ponca site are presented and compared with the estimated stages in Table 3.4Table 3.4: Comparing timing of various growth stages with optical properties for the Ponca data set. All the dates are compatible with the provided plant properties. For example, as reported from the field, after 206 days when the leaves are brownish-yellow, head and stems are green, the estimated stage is close to maturity and harvesting had not yet taken place. According to GDD based stages, 206 days after planting is close to complete maturity which is in agreement with the field observations. Also the Ponca field calendar indicated that maturity is reached in late May and harvesting time is mid-June, which (again) is compatible with estimated dates of growth stages.
Table 3.4: Comparing timing of various growth stages with optical properties for the Ponca data set

<table>
<thead>
<tr>
<th>Date</th>
<th>Fay of Year</th>
<th>Species or plant element</th>
<th>Days after planting</th>
<th>Stage</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mar 25, 1999</td>
<td>84</td>
<td>Green leaves</td>
<td>145</td>
<td>Between five leaf and shot blade</td>
</tr>
<tr>
<td>Apr 20, 1999</td>
<td>110</td>
<td>Top most green leaves</td>
<td>170</td>
<td>Five leaf</td>
</tr>
<tr>
<td>May 8, 1999</td>
<td>128</td>
<td>Green and brownish-yellow leaves &amp; grain head</td>
<td>188</td>
<td>Close to dough</td>
</tr>
<tr>
<td>May 18, 1999</td>
<td>138</td>
<td>Green and brownish-yellow leaves &amp; grain head</td>
<td>198</td>
<td>Between dough and maturity</td>
</tr>
<tr>
<td>May 26, 1999</td>
<td>146</td>
<td>Green stems, brownish-yellow leaves &amp; grain head</td>
<td>206</td>
<td>Close to maturity, no harvesting yet</td>
</tr>
</tbody>
</table>

3.3. Results

3.3.1. Impacts of adding vegetation components

In order to evaluate the impact of each proposed change to the model, the three cases detailed above are compared with the baseline using the Ponca dataset. Soil moisture and latent heat estimates at 2 pm for each case are compared with the original SWEB-SVAT and new MWSDR models – including all of vegetation-based changes. The discrepancy between measured and simulated values is used to calculate a coefficient of variation ($C_v$) which is defined as the ratio of the root mean square error ($RMSE$) to the mean of observations ($\mu_O$),

$$C_v = \frac{RMSE}{\mu_O}$$  \hspace{1cm} (3-19)

as represented in Table 3.5. The value of $C_v$ is normalized to account for variations in the extent and magnitude of the variables, which makes it easier to compare datasets with different mean values. Pearson’s linear correlation coefficient ($R$) showing the mismatch in temporal pattern of observations ($O$) and predictions ($M$) time series, presented in Table 3.6. $R$ defined as the covariance of the variables ($cov(M,O)$) divided by the product of their standard deviations ($\sigma$),

$$R = \frac{cov(M,O)}{\sigma_M \cdot \sigma_O}$$  \hspace{1cm} (3-20)
Averaged Relative Error (ARE) is reported in Table 3.7 to show discrepancies in the measured and simulates means. ARE is defined as the ratio of bias ($\mu_M - \mu_O$) to the mean of observations ($\mu_O$).

$$ARE = \frac{\mu_M - \mu_O}{\mu_O}$$

(3-21)

to be independent from the extent and magnitude of the variables.

Since there are no separate root layers for the SWEB-SVAT model and Case 1, the relevant cells to these statistics are empty in the tables.

Table 3.5: Coefficient of variation ($C_v$) between measured and modelled soil moisture ($SM$) and latent heat flux ($LE$) at the Ponca site. Defined ranges in the column labels indicate the depth of soil layers in cm.

<table>
<thead>
<tr>
<th></th>
<th>SM (0-10)</th>
<th>SM (0-30)</th>
<th>SM (30-60)</th>
<th>SM (60-90)</th>
<th>SM (0-90)</th>
<th>LE</th>
</tr>
</thead>
<tbody>
<tr>
<td>SWEB-SVAT</td>
<td>0.255</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>0.191</td>
<td>0.739</td>
</tr>
<tr>
<td>Case 1</td>
<td>0.256</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>0.192</td>
<td>0.697</td>
</tr>
<tr>
<td>Case 2</td>
<td>0.241</td>
<td>0.273</td>
<td>0.249</td>
<td>0.169</td>
<td>0.194</td>
<td>0.728</td>
</tr>
<tr>
<td>Case 3</td>
<td>0.205</td>
<td>0.167</td>
<td>0.182</td>
<td>0.068</td>
<td>0.120</td>
<td>0.664</td>
</tr>
<tr>
<td>MWSDR</td>
<td>0.207</td>
<td>0.124</td>
<td>0.132</td>
<td>0.056</td>
<td>0.080</td>
<td>0.489</td>
</tr>
</tbody>
</table>

Table 3.6: Linear correlation coefficient ($R$) between measured and modelled soil moisture ($SM$) and latent heat flux ($LE$) at the Ponca site. Defined ranges in the column labels indicate the depth of soil layers in cm.

<table>
<thead>
<tr>
<th></th>
<th>SM (0-10)</th>
<th>SM (0-30)</th>
<th>SM (30-60)</th>
<th>SM (60-90)</th>
<th>SM (0-90)</th>
<th>LE</th>
</tr>
</thead>
<tbody>
<tr>
<td>SWEB-SVAT</td>
<td>0.579</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>0.521</td>
<td>0.619</td>
</tr>
<tr>
<td>Case 1</td>
<td>0.615</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>0.525</td>
<td>0.619</td>
</tr>
<tr>
<td>Case 2</td>
<td>0.741</td>
<td>0.559</td>
<td>0.158</td>
<td>0.441</td>
<td>0.461</td>
<td>0.609</td>
</tr>
<tr>
<td>Case 3</td>
<td>0.819</td>
<td>0.530</td>
<td>0.200</td>
<td>0.272</td>
<td>0.338</td>
<td>0.634</td>
</tr>
<tr>
<td>MWSDR</td>
<td>0.755</td>
<td>0.809</td>
<td>0.681</td>
<td>0.540</td>
<td>0.747</td>
<td>0.835</td>
</tr>
</tbody>
</table>

Table 3.7: Average relative error (ARE) between measured and modelled soil moisture ($SM$) and latent heat flux ($LE$) at the Ponca site. Defined ranges in the column labels indicate the depth of soil layers in cm.

<table>
<thead>
<tr>
<th></th>
<th>SM (0-10)</th>
<th>SM (0-30)</th>
<th>SM (30-60)</th>
<th>SM (60-90)</th>
<th>SM (0-90)</th>
<th>LE</th>
</tr>
</thead>
<tbody>
<tr>
<td>SWEB-SVAT</td>
<td>0.097</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>0.105</td>
<td>0.275</td>
</tr>
<tr>
<td>Case 1</td>
<td>0.106</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>0.118</td>
<td>0.170</td>
</tr>
<tr>
<td>Case 2</td>
<td>0.074</td>
<td>0.113</td>
<td>0.168</td>
<td>-0.156</td>
<td>0.106</td>
<td>0.227</td>
</tr>
<tr>
<td>Case 3</td>
<td>0.077</td>
<td>0.015</td>
<td>0.120</td>
<td>0.049</td>
<td>0.061</td>
<td>0.208</td>
</tr>
<tr>
<td>MWSDR</td>
<td>0.051</td>
<td>-0.011</td>
<td>0.090</td>
<td>0.039</td>
<td>0.039</td>
<td>0.189</td>
</tr>
</tbody>
</table>

The error statistics for Case 1 and the SWEB-SVAT model in Table 3.5 to Table 3.7 show that a NDVI-based canopy resistance does not lead to a noticeable improvement in estimating canopy transpiration of the model nor a significant change in estimated soil moisture. Also, comparing the statistics of Case 2 with SWEB-SVAT shows that soil moisture estimates of surface layer and total root-zone do not improve significantly after
adding four separate root layers, neglecting dynamic rooting depth and density. This implies that an introduction of multiple soil layers alone assuming uniform root distribution does not affect the final simulation of soil moisture. In addition, for both cases, latent heat flux statistics are relatively unchanged. Therefore, the only clear advantage of Case 2 is the improved vertical resolution of the soil moisture showing moisture profile.

In contrast, more profound changes are seen when introducing vertical heterogeneity in the root biomass distribution and root-water uptake (i.e. moving from Case 2 to Case 3 and the full MWSDR case). Lower $C_v$ and $ARE$ for most of the variables shows that Case 3 simulates the water content better than Case 2 even though the correlation coefficient represents low relation for some of the layers. Latent heat flux shows a slight improvement after adding the exponential root density to the model in Case 3. However, comparing the full MWSDR model statistics with the SWEB-SVAT model illustrates the following clear improvements in soil moisture and energy flux estimates:

- an approximately 10% decrease of $C_v$, 20% increase of correlation and 6% less bias for root-zone soil moisture estimates, and
- a greater than 20% decrease of $C_v$, more than 20% increase of correlation and less than 10% decrease of bias in latent heat flux estimates.

This implies that MWSDR model – including all of the above mentioned changes – performs better than the SWEB-SVAT model.

Table 3.8 represents the values of above statistics for daily total $ET$ (mm). Mean absolute error ($MAE$) and root mean square error ($RMSE$) of daily $ET$ are also presented. $RMSE$ is reduced from 1.213 mm for SWEB-SVAT model to 0.773 mm for MWSDR model. Whereas the magnitude of the reduction in bias ($MAE$) is not as large as $RMSE$, it shows some improvement.

Table 3.8: Error statistics between measured and modelled daily total $ET$ (mm) at Ponca site,

<table>
<thead>
<tr>
<th></th>
<th>$C_v$</th>
<th>$R$</th>
<th>$ARE$</th>
<th>$RMSE$</th>
<th>$MAE$</th>
</tr>
</thead>
<tbody>
<tr>
<td>SWEB-SVAT</td>
<td>0.652</td>
<td>0.686</td>
<td>0.261</td>
<td>1.213</td>
<td>0.486</td>
</tr>
<tr>
<td>Case 1</td>
<td>0.604</td>
<td>0.696</td>
<td>0.156</td>
<td>1.124</td>
<td>0.290</td>
</tr>
<tr>
<td>Case 2</td>
<td>0.639</td>
<td>0.679</td>
<td>0.213</td>
<td>1.190</td>
<td>0.397</td>
</tr>
<tr>
<td>Case 3</td>
<td>0.587</td>
<td>0.687</td>
<td>0.196</td>
<td>1.093</td>
<td>0.365</td>
</tr>
<tr>
<td>MWSDR</td>
<td>0.415</td>
<td>0.884</td>
<td>0.193</td>
<td>0.773</td>
<td>0.359</td>
</tr>
</tbody>
</table>
Simulated root-zone soil water content using various models based on Ponca and Dookie-2013 datasets are compared qualitatively with observations in Figure 3.3. The results of Case 2 model performance are represented in addition to SWEB-SVAT and MWSDR soil moisture estimations. The visual comparison of time series shows a relatively significant improvement in the deep layer soil moisture prediction at both sites due to the use of a non-uniform root distribution (MWSDR) whereas simply adding more layers (Case 2) to the model has little impact relative to the original model.

As it can be seen in Figure 3.3a, there is a very large increase in root-zone water content at the Dookie site around day 20 in 2013. This sudden increase of deeper layer soil water content from 15% to 35% in just a few days at this site is not physically plausible except perhaps as a result of a ground water intrusion to the upper layers. Consultation with the field managers revealed that such groundwater intrusions are common in this area. However, neither this model nor any other land surface model have a way to consider the problem of ground water intrusion a priori.

![Figure 3.3: Comparing various model performances at Dookie study site in 2013 (a) and Ponca site (b)](image)

It is difficult to prefer the results of one model over the others due to the big difference between observed and predicted root-zone soil moisture of Dookie-2013 dataset. However, the only good match in the trend of soil moisture changing is occurred at the last part of the period (around day 160) when the observations and the MWSDR model do not show moisture reduction, while other models still simulate soil moisture decreasing.
Better correspondence in the trend of change in moisture in the results of new model with the observed values of Ponca site confirms higher correlation found in the statistics of MWSDR model.

The error statistics of MWSDR and SWEB-SVAT results using the Dookie-2012 dataset are reported in Table 3.9. Comparing these statistics reveals a decrease of bias and random errors and an increase of correlation associated with the application of the MWSDR model.

<table>
<thead>
<tr>
<th></th>
<th>SM (0-10)</th>
<th>SM (0-120)</th>
<th>LE</th>
</tr>
</thead>
<tbody>
<tr>
<td>SWEB-SVAT</td>
<td>0.480</td>
<td>0.140</td>
<td>0.625</td>
</tr>
<tr>
<td>MWSDR</td>
<td>0.267</td>
<td>0.051</td>
<td>0.531</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th></th>
<th>R</th>
<th>ARE</th>
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<tbody>
<tr>
<td>SWEB-SVAT</td>
<td>0.867</td>
<td>0.332</td>
</tr>
<tr>
<td>MWSDR</td>
<td>0.934</td>
<td>0.141</td>
</tr>
</tbody>
</table>

Figure 3.4 represents predicted surface and root-zone soil moisture using various models based on the Dookie-2012 datasets in comparison with observations. The simulated soil water content using MWSDR model shows more compatibility with observed data during the last part of the season. SWEB-SVAT maintains its continuous water extraction from the soil profile due to water availability and other conducive conditions but MWSDR model decreases the canopy transpiration since the crops are close to maturity at this stage.
There is a high similarity between the results of Case 2 and SWEB_SVAT model confirming the aforementioned inefficiency of Case 2 in improving SWEB-SVAT model predictions. The application of multiple soil layer structure in Case 2 helps to improve surface soil moisture predictions as represented in Figure 3.4a; however, surface soil moisture simulated by MWSDR model shows more proximity to the observations.

### 3.3.2. Transpiration rate

Differences in estimated actual transpiration between the SWEB-SVAT model and the MWSDR model at Ponca site are illustrated in Figure 3.5c and Figure 3.5d respectively. Cumulative transpiration calculated from both models and cumulative potential transpiration are shown in Figure 3.5a. At the beginning of the period, when there is no water stress ($\alpha = 1$), root water update is equal to the maximum amount of transpiration or calculated potential transpiration. The transpiration rate decreases comparing to potential transpiration due to water stress around day 90. On the other hand, comparing the cumulative transpiration of two models shows that transpiration calculated by the MWSDR model is significantly higher than the estimations by the SWEB-SVAT model. The time series of calculated transpiration of the models presented in Figure 3.5c and Figure 3.5d also confirm this difference. Another important difference here is the distinct patterns of calculated transpiration during the period. The pattern provided by MWSDR model seems physically intuitive in that it predicts much more water uptake during the active growth stages and less extracted water at the start and the end of the period; whereas the estimated transpiration pattern by SWEB-SVAT model changes from low values at the beginning of the period to the higher values at the end. The temporal pattern produced by MWSDR more closely matches observed evapotranspiration in the field shown in Figure 3.5b. This implies that although simulated LAI – used for both models – declines after day 120, the SWEB-SVAT model structure is not able to change the transpiration rate efficiently. Cumulative transpiration calculated from the new model levels off in the last part of the analysis period because daily transpiration steeply decreases. Although there is no water stress near the end of the simulation time (Figure 3.3b), water uptake decreases when the crops are approaching to the harvest time. This behaviour is modelled by NDVI-based canopy resistance of the MWSDR model, considering less transpiration strength in the
maturity stage. The observed evapotranspiration time series (Figure 3.5b) confirms that total evapotranspiration decreases close to the end of the period to around 3 mm/d while SWEB-SVAT model overestimates transpiration at this time (around 5 mm/d).

The same trend can be recognised in the transpiration results achieved from Dookie site. However, because soil is dry at the final part of the period, this decline in the water uptake rate starts sooner.

### 3.3.3. Soil evaporation rate

Differences in estimated soil evaporation between the original model and the new model at Dookie site in 2013 are illustrated in Figure 3.6c and Figure 3.6d. Cumulative soil evaporation calculated from two models are represented in Figure 3.6a. At the beginning of the period, when there is no or small crop cover, evaporated water from the soil surface
calculated from both models are relatively equal. Soil evaporation rate estimated by MWSDR model, decreases comparing to SWEB-SVAT model around day 70.

![Graphs showing cumulative modelled soil evaporation, surface soil moisture, modelled transpiration and soil evaporation of SWEB-SVAT and MWSDR at Dookie study site in 2013.](image)

Figure 3.6: Cumulative modelled soil evaporation (a), surface soil moisture (b), modelled transpiration and soil evaporation of SWEB-SVAT (c) and MWSDR (d) at Dookie study site in 2013

Considering low wind speed and less solar radiation reaching the crop-covered soil surface, water availability at the surface layer is the most important factor influencing soil evaporation. The SWEB-SVAT model is able to parameterise the portion of solar radiation reaching the surface using LAI; also observed wind speed is used as an input to the model, but water content of the surface layer may be calculated much wetter than it is using a lumped root layer. The thick wet root layer of SWEB-SVAT model acts as a large water supply to replenish the evaporated water from the surface due to the force-restore algorithm. The larger amounts of estimated bare soil evaporation resulted from the SWEB-SVAT model may be an outcome of this model structure. However, MWSDR model assigns higher water uptake by the plant root from the upper root-zone layer. Consequently, the soil layer beneath the soil surface becomes more water-stressed and less able to
replenish the surface evaporated water. Figure 3.6b represents simulated surface soil water content using both models in comparison with observations. For the second part of the period SWEB-SVAT based surface soil moisture overestimates the observations and can therefore support the larger values of SWEB-SVAT based soil evaporation showed in Figure 3.6a.

As seen in Figure 3.6d, the results of new model seem more realistic; MWSDR soil evaporation becomes less than transpiration as the crop grows, significantly increasing fractional canopy cover during the mid-growth season; whereas at the start of the growing period, soil evaporation is more than plant transpiration which is consistent with low vegetation cover conditions. The transpiration rate decreases close to the harvesting time when the crop matures and in the senescence stage resulting in soil evaporation exceeding transpiration.

### 3.3.4. Water uptake distribution

Different patterns in water extracted by root from the soil profile as simulated by the MWSDR model are represented in Figure 3.7a at various growth stages at Dookie field in 2013. Figure 3.7b shows the modelled soil water contents at the same dates.

At the five-leaf stage, when there is no water stress, this modified model simulates extracting most of the water from the surface layer. Although root depth assumed to be 0.9 m at this stage, the amount of water uptake from the layers below 0.3 m depth is close to zero. At the shot blade stage, water stress of the surface layer developed and deeper layers are wetter than top layers as shown in Figure 3.7b. As this point, the plant starts extracting some water from deeper layers; however, the pattern of water extraction does not change and maximum water extracted by root, is still transpired from the surface layer. Low water availability in the surface layer and relatively greater root density in the deeper layers leads the model to extract more water from the second layer (30-60 cm depth) versus the surface layer at the dough time stage. During subsequent days to the maturity stage, after drying out the surface layer, the deeper layers provide more water required for transpiration than the shallower layers due to more available water in the deeper layers as shown in Figure 3.7b.
A visual comparison between measured soil water content and simulated values from different models at various growth stages of the plant is presented in Figure 3.8. Since comparing the soil moisture estimations of the MWSDR model with the SWEB-SVAT model is not possible at different soil depth, this figure compares MWSDR model with Case 2. Apart from the proximity of absolute soil moisture estimates of MWSDR model and observations – which is reflected in lower $RMSE$ values (Table 3.5) – the relative pattern of soil water variation in different soil layers, shows more similarity with the observations.

The pattern of water extraction of Case 2 is almost the same for all the stages because it is parameterised to extract the same amount of water from each layer due to its assumption of uniform root distribution. That always simulates deep layers wetter than surface layer.

MWSDR model provides higher water content for deep layers at the beginning of the period (Figure 3.8a) but the second soil layer becomes drier than others at maturity stage (Figure 3.8d). This pattern of soil moisture change in different layers is very similar to that of observed moisture content.

This pattern shows more water extraction from the second layer between dough time and maturity stage when there is more root density in the second layer and the first layer is less wet. This indicates that adding more vegetation component to the model results in a considerable improvement in water uptake estimations from different parts of the root-zone during the growing season.
3.4. Discussion and conclusions

Results of the experiments show that separate application of a NDVI-based canopy resistance (case 1) or adding four separate root layers (case 2) does not improve soil moisture and latent heat estimations significantly. Comparing error statistics of case 2 and 3 with SWEB-SVAT model indicates that having multiple root layers does not affect the final simulation of soil moisture unless the assumption of uniform root – and water uptake – distribution changes. Considering dynamic root density in Case 3 provides a relatively more reliable water content simulation comparing with models with uniform root distribution. Quantitative and graphical comparison of MWSDR model including all of the above mentioned modifications with SWEB-SVAT model represents a substantial improvement in model estimates of profile soil moisture and evapotranspiration. A lower coefficient of variation, higher correlation coefficient and less bias in comparing simulated
with measured variables all indicate that incorporating proper vegetation components into the SWEB-SVAT can improve the accuracy of its soil moisture and evapotranspiration predictions. A considerable reduction in RMSE of daily total ET also supports this result.

Verifying the transpiration rate shows the improved patterns of calculated transpiration using MWSDR model, representing more similarity with the trend of observed total evapotranspiration. This pattern shows more water uptake during the active growth stages and less extracted water both early in the simulation time (when the crop is emerging) and late in the season after the crop has reached maturity. Vegetation characteristics are incorporated into the original SWEB-SVAT transpiration part via LAI only, to divide net radiation between canopy and soil. Although canopy resistance is also influenced by the vegetation characteristics, it is mainly calculated based on the water content in the whole root layer and resistance extremes \( R_{C,min} \) and \( R_{C,max} \). SWEB-SVAT resistance extremes are based on soil texture, and the effect of plant activities is neglected in them. In this model, considering the LAI-based canopy net radiation as a driving force for transpiration, the quantity of water uptake is somehow related to the biomass. It means crops have been simulated to extract more water when the leaf area is larger. This model similar to other conventional land surface models assumes that ET is proportional to spectrally observable biomass. However, it seems that this assumption may become invalid when vegetation goes through the mature stage because although LAI is a larger value at this stage, the plant starts decreasing transpiration (Allen et al. 2006). The results of this study shows that calculating plant transpiration considering plant root location and plant biophysical fluctuations in the model improves the estimation of root-zone soil moisture.

MWSDR soil evaporation rate shows a good relation with the crop growth. It represents a substantial decrease when the plant covers the soil and a large increment at low vegetation condition. However, in most land surface models, utilizing a lumped root layer with uniform redistribution of soil water – due to the assumption of uniform plant root distribution – may hamper the simulation of soil water movement. Having a large reservoir of soil water underneath the surface layer may make the surface layer remain wetter than reality resulting in large bare soil evaporation. According to the results of Case 2, just adding more soil layers is not sufficient to improve the percolation of soil water between
the layers. However, assigning maximum proportion of root distribution to the upper root-zone layer leads to extract more water from the layer immediately below the surface, preventing that to supply water for the surface layer.

Verifying water uptake distribution and its dependency to the water stress and root contribution of each layer represents the ability of MWSDR model to provide more reliable pattern of soil water variation in different soil layers. Assuming an evenly distributed root makes the layer by layer water extraction pattern almost the same for all the stages. However, the process of water percolation in MWSDR model is very different among the sub layers dependent on the root location. The rooted surface layer of soil dries more quickly because plant roots are able to extract more water from this part, while the water content of other soil layers does not change by root activities. After drying out this layer, the plant will face limited available water for transpiration and it will try extracting more water from the second rooted layer. This pattern of soil moisture extraction leads to an improved soil water distribution simulated by MWSDR model as the pattern of soil water variation in different soil layers shows more similarity with the observations.

The improvements of new MWSDR model in terms of soil moisture and latent heat flux estimations, overall transpiration, evaporation rates and water uptake distribution are representative of better performance of this modified SWEB-SVAT model.

The results show the importance of an adequate representation of vegetation-related transpiration process for an appropriate simulation of water transfer in a complicated system of soil, plants and atmosphere. Incorporating a newly implemented sub-model to simulate root growth dynamics and considering the plant phenology, enhances the performance of SWEB-SVAT model.

In addition to the open-loop model performance, acknowledging that these two models differ significantly in complexity of subsurface soil moisture processes, propagation of surface state updates along the soil profile via data assimilation may vary strongly depending on the selection of model. More realistic characterization of surface and subsurface processes using dynamic vegetation, which results in more accurate estimations for both surface and root-zone states, may result in improved efficacy of data assimilation.
Further works to evaluate the efficacy of MWSDR’s improved root-zone water processes for land surface data assimilation is warranted.

In this work, the MWSDR model has been evaluated for field-scale soil moisture estimates using tower-based input data. In order to apply MWSDR at broader spatial scales, it needs to be implemented and verified at larger spatial support under diverse climatic and vegetation conditions. For example, when MWSDR is implemented at the spatial support scale of the Global Land Data Assimilation System (GLDAS), 0.25-degree, using regional and global meteorological input, extra uncertainties originating from input forcing error and sub-grid-scale heterogeneity can cause a significant degradation of the model performance. Moreover, MWSDR’s crop-specific root-growth and other general phenological characteristics mean that including non-uniform crop types within a grid cell would be undesirable as well as heterogeneity in soil textural properties affecting water content and root distribution. Adopting the concept of the Hydrologic Response Unit (HRU) as in the Soil and Water Assessment Tool (SWAT; (Neitsch et al. 2005)) is one potential strategy for implementing a spatially distributed version of MWSDR over larger spatial extent. However, more rigorous evaluation of MWSDR for various spatial, climatic and crop conditions is warranted.
4. CHAPTER 4: EFFECTS OF DYNAMIC VEGETATION COMPONENTS ON THE COUPLING BETWEEN ROOT-ZONE SOIL MOISTURE AND SURFACE FLUXES

4.1. Introduction

Soil moisture is a key land surface variable controlling the exchange of water and energy between the soil and the lower atmosphere. As a result, the application of hydrologic and atmospheric processes in agriculture, weather prediction and flood forecasting requires the accurate representation of surface and root-zone soil moisture (Koster et al. 2004, Oglesby 1991). In order to address the inherent difficulty of ground-based soil moisture measurements over large areas, substantial efforts have been made to develop models for estimating spatially distributed soil moisture (e.g. Dai et al. 2003, Nijssen et al. 2001, Ek et al. 2003). The water and energy balance-soil vegetation atmosphere transfer (WEB-SVAT) scheme represents one of the common land surface modelling approaches, which can be applied to the dynamic prediction of soil moisture as well as land surface water and energy fluxes (Noilhan & Planton 1989). The WEB-SVAT modelling approach is based on the application of prognostic equations to predict energy fluxes, soil moisture and thermal states based on the atmospheric forcing variables such as precipitation, temperature, wind speed, and incoming solar radiation.

As a way to improve the model-based root-zone soil moisture prediction, the assimilation of various remotely sensed (RS) data into land surface models has also been examined. The assimilation of microwave-derived surface soil moisture into WEB-SVAT models, for example, has improved estimates of root-zone soil moisture (e.g. Reichle & Koster 2005, Reichle et al. 2002, Draper & Reichle 2015). However, there are a number of factors determining the degree to which the root-zone can be accurately constrained via the assimilation of surface soil moisture estimates. For example, the assimilation of surface soil moisture retrievals is ineffective at correcting root-zone soil moisture model predictions in case of either limited vertical coupling between surface and root-zone layers (Kumar et al. 2003).
2009) and the presence of certain soil textures which limit the vertical redistribution of soil moisture anomalies (Li et al. 2010).

Due to the linkage between canopy thermal information with the soil water status of deeper layers, the assimilation of thermal-infrared (TIR)-derived surface variables such as radiometric temperature, energy flux estimates and soil moisture proxies into WEB-SVAT models has also been examined (e.g. Crow & Kustas 2005, Pipunic et al. 2008, Jones et al. 1998, Reichle et al. 2010). However, the efficacy of assimilating TIR-derived surface states relies on the model’s realistic representation of soil water processes providing an appropriate linkage between root-zone moisture and the evapotranspiration.

When assimilating TIR-based energy fluxes (EF or ET) to update the root-zone soil moisture, the error covariance between the surface fluxes and root-zone states is largely determined by the model’s soil water physics. Consequently, the model’s representation of surface variables vs. root-zone soil moisture can affect the efficacy of the assimilation. The parameterization of the vegetation-soil water processes to calculate water and energy balance components varies across different WEB-SVAT models (Crow et al. 2005), which can lead to variations in coupling strength between the surface energy fluxes and subsurface moisture states (Calvet & Noilhan 2000, Kumar et al. 2009).

The importance of accurately representing the coupling between energy fluxes and soil water states is not limited to data assimilation; it is also important for a range of other applications such as irrigation scheduling, drought monitoring and land-atmosphere feedback studies. For example, surface fluxes have been used as simple and direct indicator of root-zone soil moisture conditions in general and as a tool for determining crop consumptive water use, crop water stress detection and irrigation activities (e.g. Bastiaanssen 2000, Moran 2003). The ratio of actual evapotranspiration (AET) to potential evapotranspiration (PET) known as crop water stress index has been shown to be closely correlated with soil moisture content (Jackson et al. 1981, Moran et al. 1994) which led to use it for important farm applications as irrigation scheduling and prediction of crop yield (e.g. Irmak et al. 2000, Pinter Jr et al. 2003). Bastiaanssen (2000) concluded from investigating different observed data sets that evaporative fraction is a promising temporally stable indicator to express energy partitioning and is directly related to the soil
moisture conditions. He suggested using evaporative fraction as an alternative for the ratio of AET/PET to indicate crop water stress, as it avoids the intricate definitions related to potential evapotranspiration. Considering the relationship between AET/PET and soil moisture, Anderson et al. (2011) utilised a new drought index (evaporative stress index (ESI)) quantifying anomalies in the ratio of actual to potential ET to overcome the limitations of precipitation-based standard meteorological drought indices. In all of these cases the relationship between soil moisture and surface energy fluxes is affected by the stage of crop growth or vegetative development (defining vegetation cover and root depth) and solar radiation (Bastiaanssen 2000) and it is critical to represent this coupling accurately to reliably invert surface flux estimates to track soil moisture availability.

The inherent limitations of WEB-SVAT models have important implications on the models’ capability to reproduce accurate relationship between root-zone soil moisture and surface energy fluxes (such as ET and EF). Some notable shortcomings in the WEB-SVAT models in the estimations of energy fluxes, soil moisture and their relationship with vegetation and soil have been reported in previous studies (e.g. Niu et al. 2011, Gayler et al. 2013). For example, parameterising plant transpiration using a stomatal resistance for a given atmospheric demand is a common approach in WEB-SVAT methods. Although growth stages and phenological cycle of the plant have an influence on the stomatal resistance and transpiration activity (Reich et al. 2003), they are neglected in most land surface models. Also, root depth and density variation also plays an important role in estimating soil water loss by transpiration; however, most WEB-SVAT models assume uniform root distribution and constant root density (with time), which leads to uniformly distributed root-water extraction from the soil profile.

An important improvement of WEB-SVAT models in terms of coupling between surface variables and root-zone soil moisture can be achieved by modifying the existing simple representations of subsurface processes with the more realistic ones. For example, since root growth and root water uptake is often simplified in the WEB-SVAT models (Overgaard et al. 2006), adopting more advanced vegetation dynamics from crop models, which consider the interaction of root depth and distribution with soil water content, may enhance the overground-underground connection of WEB-SVAT scheme (the connection of soil surface-vegetation-atmosphere exchange with subsurface and root-zone water
availability). Hashemian et al. (2015) extended a conventional simple WEB-SVAT model (SWEB-SVAT) (Crow et al. 2008, Li et al. 2010) to have more complexity in the representation of plant growth and root water uptake. The evaluations of new model (multi-layer WEB-SVAT with dynamic root distribution (MWSDR)) using in situ data demonstrated more accurate soil moisture and energy flux predictions. Here, we extend upon this earlier work by explicitly examining the impact of these changes on the coupling between root-zone soil moisture and energy flux predictions. This novel investigation is important for a variety of reasons such as application of this coupling in water resources management (e.g. determination of the consumptive use of water by crops in irrigated agriculture) and disaster prediction (e.g. using water stress indices for drought monitoring). It is also useful in order to assess how the assimilation of surface variables is able to improve the model estimations and if the applied dynamic vegetation components are likely to facilitate robust assimilation.

4.2. Materials and Methods

4.2.1. Land surface model

Two separate land surface models are used in this study. Both SWEB-SVAT and MWSDR modelling strategies are based on the partitioning of net radiation ($R_N$) into sensible heat ($H$), latent heat ($LE$), and ground heat ($G$) fluxes based on the TSEB model (Norman et al. 1995) which divides energy fluxes between soil (subscript $S$) and canopy (subscript $C$) components via separate energy balance equations as:

$$R_{N,C} = H_C + LE_C$$  \hspace{1cm} (4-1a)

$$R_{N,S} = H_S + LE_S + G$$  \hspace{1cm} (4-1b)

The physically-based radiation model of Campbell & Norman (1998) is used to calculate canopy ($R_{N,C}$) and soil ($R_{N,S}$) components of net radiation based on observed downward solar radiation and calculated long wave radiation.

Sensible heat fluxes from vegetation and the soil surface are calculated as:
\[ H_C = \rho C_p \frac{T_C - T_A}{R_A} \]  \hspace{1cm} (4-2a)

\[ H_S = \rho C_p \frac{T_S - T_A}{R_A + R_{AS}} \]  \hspace{1cm} (4-2b)

where \( \rho \) is density of air, \( C_p \) the specific heat of air at constant pressure, \( T_A, T_S \) and \( T_C \) temperature of air, soil and canopy respectively. \( R_A \) is the above-canopy aerodynamic resistance and \( R_{AS} \) the within-canopy aerodynamic resistance. \( R_A \) and \( R_{AS} \) are parameterized based on surface roughness lengths, wind speed, and stability considerations for the parallel version of TSEB presented in Norman et al. (1995).

\( LE_S \) is calculated as:

\[ LE_S = \rho C_p \gamma^{-1} [e_S(T_S) - e_a] / (R_{AS} + R_A + R_S) \]  \hspace{1cm} (4-3)

where \( \gamma \) is the slope of the saturation vapour pressure versus temperature curve; \( e_S \) and \( e_a \) are saturation and near-surface water vapour pressure; and \( R_S \) is soil resistance which is an empirical function of surface soil moisture.

The SWEB-SVAT model parameterizes \( LE_C \) as:

\[ LE_C = \rho C_p \gamma^{-1} [e_S(T_C) - e_a] / (R_C + R_A) \]  \hspace{1cm} (4-4)

where \( R_C \) is canopy resistance which is a function of root-zone soil moisture (\( \theta_{rz} \)) estimated by:

\[ R_C = \begin{cases} 
R_{C,max} & \text{if } \theta_{rz} < \theta_w \\
 \frac{(R_{C,min} - R_{C,max})}{\theta^* - \theta_w} \frac{\theta_{rz} - \theta_w}{\theta^* - \theta_w} + R_{C,max} & \theta_w < \theta_{rz} < \theta^* \\
R_{C,min} & \text{if } \theta_{rz} > \theta^* 
\end{cases} \]  \hspace{1cm} (4-5)

where \( \theta^* \) and \( \theta_w \) are the volumetric soil moisture levels at field capacity and wilting point, respectively. Resistance extremes \( R_{C,max} \) and \( R_{C,min} \) are specified based on typical literature values and consideration of soil texture (Li et al. 2010). Although canopy resistance is also influenced by the vegetation characteristics, it is mainly calculated based on the water content in the whole root layer and resistance extremes (\( R_{C,min} \) and \( R_{C,max} \)).
SWEB-SVAT resistance extremes are based on soil texture, and the effect of plant activities is neglected in them.

The SWEB-SVAT model has a two-layer soil water balance scheme based on a force-restore model (Noilhan & Planton 1989, Norman et al. 1995). This model divides the soil column into surface- and root-zone layers where the root-zone layer surface includes the surface layer completely. The water balance equations for surface and root-zone soil moisture are parametrized as:

\[
\frac{d\theta_{sz}}{dt} = \frac{C_1}{d_{sz}}[P_g - LE_S(\rho\lambda)^{-1}] - \frac{C_2}{f_d}(\theta_{sz} - \theta_{eq}) \tag{4-6a}
\]

\[
\frac{d\theta_{rz}}{dt} = \frac{1}{d_{rz}}[P_g - LE_C(\rho\lambda)^{-1}] - LE_S(\rho\lambda)^{-1} - Q \tag{4-6b}
\]

where \(\theta_{sz}\) and \(\theta_{rz}\) are surface- and root-zone soil moisture contents, \(d_{sz}\) and \(d_{rz}\) surface- and root-zone depth, \(P_g\) throughfall, \(\lambda\) latent heat of vaporisation, \(f_d\) the frequency of diurnal variations (24 hours), \(\theta_{eq}\) equilibrium surface volumetric moisture content, and \(Q\) the drainage from the bottom of the root-zone. \(C_1\) and \(C_2\) are force and restore coefficients for soil moisture which are related to the soil characteristics.

Vegetation characteristics are incorporated into SWEB-SVAT transpiration estimates only via the leaf area index (LAI). In particular, LAI is utilised in the model to calculate canopy transmissivity for short wave (\(\tau_{solar}\)) and canopy albedo (\(al_c\)) which are used to divide net radiation between canopy and soil. This model considers the LAI-based canopy net radiation as a driving force for transpiration; therefore, the quantity of water uptake is somehow related to the biomass. It means crops have been simulated to extract more water when the leaf area is larger. Like other conventional land surface models, SWEB-SVAT assumes that plant transpiration increases monotonically as a function of spectrally observable biomass. However, this assumption may become invalid when vegetation goes through the mature stage because although LAI is a larger value at this stage, the plant starts decreasing transpiration (Allen et al. 2006).

In contrast, the MWSDR model adapts a sophisticated root distribution model that considers the dynamic nature of plant growth to improve the water and energy balance coupling of the SWEB-SVAT. Since having multiple soil layers is required when adding a
root growth component, the original SWEB-SVAT model is modified to include several layers (the number of layers depends on the soil type of the study site). The new MWSDR model also includes a new parameterization of canopy resistance based on plant phenology.

Surface and root-zone soil moisture contents of the MWSDR model are calculated for every time step based on the following equations. Soil evaporation ($LE_s$) is subtracted from the surface layer and fraction of canopy water uptake associated to each layer ($LE_{c,i}$) from the subsurface layers. In this formulation $i$ indexes a particular layer number:

$$\frac{d\theta_{sz}}{dt} = \frac{1}{d_{sz}} \left[ P_g - LE_s(\rho \lambda)^{-1} - q_{1\rightarrow 2} \right]$$

(4-7a)

$$\frac{d\theta_{rz,i}}{dt} = \frac{1}{d_i} \left[ q_{i-1\rightarrow i} - LE_{c,i}(\rho \lambda)^{-1} - q_{i\rightarrow i+1} \right]$$

(4-7b)

where $q_{i\rightarrow i+1}$ is the water flux from layer $i$ to layer $i+1$ (redistribution) following the Darcy equation:

$$q_{i\rightarrow i+1} = K_{\theta,i} \left[ \psi_{m,i} - \psi_{m,i+1} \right] \left[ 0.5(d_i + d_{i+1}) \right] + K_{\theta,i}$$

(4-8)

$K_{\theta}$ is the hydraulic conductivity, $\psi_m$ the matric potential, and $d_n$ depth of soil layer.

The MWSDR model is parametrized by incorporating an exponential root water uptake model with water stress compensation as proposed by (Li et al. 2001). In addition, this model constrains the root to extract water from each layer based on varying root distribution and soil wetness of that specified depth. The transpiration contribution of each layer ($LE_{c,i}$) is calculated for each soil layer based on the water content and root density as:

$$LE_{c,i} = \frac{\alpha^2 F_i}{\sum_{i=1}^{n} \alpha_i F_i} P_t$$

(4-9)

where $n$ represents the number of layers, $P_t$ is potential transpiration, $\alpha$ the available soil water (dimensionless) as a function of the volumetric soil moisture, and $F_i$ is the fraction of root length density in layer $i$ described by the Eq. (4-10):

$$F_i = \frac{ln \left[ \frac{1 + \exp(-bZ_i)}{1 + \exp(-bZ_{i+1})} \right] + 0.5[\exp(-bZ_i) - \exp(-bZ_{i+1})]}{ln \left[ \frac{2}{1 + \exp(-bZ_r)} \right] + 0.5[1 - \exp(-bZ_r)]}$$

(4-10)
Here, \( Z_i \) is soil depth of layer \( i \); \( Z_r \) is varying root depth; and \( b \) is an empirical extinction coefficient of root distribution. The coefficient \( b \) is calculated based on the root density in the first 10 cm of soil \( (F_{10}) \) as:

\[
b = \frac{24.66F_{10}^{1.59}}{Z_r}
\]  
(4-11)

Due to the time evolution of crop root depth and density, there is also a need to have a dynamic rooting depth in the model. Typical crop rooting depths \( (Z_r) \) and \( F_{10} \) (or \( b \)) as a function of growth stages are available within the literature (e.g. Li et al. 2001, Dwyer & Stewart 1986, Dwyer et al. 1988). Growing degree days (GDD) calculated based on actual daily average air temperature can be used as a simple and precise way to predict the time of certain plant stage (Miller et al. 2001). Simulating varying \( Z_r \) and \( b \) using this information can be used to provide dynamic estimates fraction of root density \( (F_i) \) used in the calculation of transpiration contribution from each soil layer \( (LE_{C,i}) \).

Total transpiration \( (LE_C) \) is the sum of partial transpiration calculated for each layer \( (LE_{C,i}) \):

\[
LE_C = \sum_{i=1}^{n} LE_{C,i}
\]  
(4-12)

Another dynamic vegetation component which is used in the parameterisation of MWSDR model involves the canopy resistance estimation. Use of constant minimum and maximum canopy resistances \( (R_{C,min} \text{ and } R_{C,max} \text{ in Eq. (4-5)}) \) makes the final canopy resistance \( (R_C) \) independent of growth stages in which plant has different transpiration power. In order to estimate the total canopy resistance based on plant phenology, the minimum canopy resistance of MWSDR model is estimated as a function of measured/estimated NDVI as a scaling factor:

\[
R_{C,min} = \frac{k}{NDVI}
\]  
(4-13)

with a constant \( k \) specified for the vegetation type.

In summary, two major modifications were implemented into the MWSDR model: the exponential and dynamical root growth, and the new canopy resistance parameterization as a function of NDVI. Hashemian et al. (2015) quantified sensitivity of the model results to
these modifications by implementing each modification separately and both of them in combination, respectively. The results show that separate application of a NDVI-based canopy resistance or adding multiple separate root layers does not improve model estimations significantly. Comparing error statistics of different cases indicates that having multiple root layers does not affect the final simulation of soil moisture unless the assumption of uniform root – and water uptake – distribution changes. However, the application of the MWSDR model, including all of the above mentioned modifications, represents a substantial improvement in model-based estimates of profile soil moisture and evapotranspiration.

4.2.2. Test site and datasets

This study uses hydro-meteorological, biophysical and spectral data gathered during three consecutive (2002–2004) growing seasons at the USDA Optimizing Production Inputs for Economic and Environmental Enhancements (OPE3) experimental site located in Beltsville, Maryland of the US. During the growing season, land cover at the site is rain-fed cultivated corn typically planted in May or June and harvested in October or November. Local soil texture at the site is several meters of sandy loam overlying an impermeable clay lens (Gish et al. 2005). Micro-meteorological data such as solar radiation, air temperature, vapour pressure, wind speed and precipitation data required by both SWEB-SVAT and MWSDR are obtained from instrumentation mounted on a 10-m tower above the corn canopy. Eddy covariance instruments are also mounted at the same height to measure LE and H. Incoming and outgoing shortwave and longwave radiation are measured at 4.5 m above ground level. Profile soil moisture measurements are taken by sensors at 10, 30, 50 and 80 cm depths (Gish et al. 2005). A vertically integrated top 1-m representation of root-zone soil moisture ($\theta_{rz}$) is obtained as a weighted average (based on soil layer depth) of soil moisture observations at various depths.

Regarding the growing season rainfall, soil moisture and latent heat observations, the 2002 growing season is remarkably dry, followed by a wetter-than-average 2003, and 2004 is a typical case with relatively normal level of precipitation (Crow et al. 2008).
A piecewise linear model is assumed for LAI temporal dynamics of each growing season based on the available extensive LAI observations in 2004 integrating with yearly planting information and limited LAI observations of other years. The LAI measurements close to maturity stage of the crop depict different maximum values for different years. The same piecewise linear interpolation model is assumed for canopy height ($h_c$), based on a minimum of 0.1 m and a maximum of 2 m crop height. Since NDVI is employed in the MWSDR model, the 16-day composite 250 m MODIS NDVI is used for the MWSDR simulation.

The depths of surface and root-zone layers for the SWEB-SVAT model are set to 10 cm and 100 cm respectively. Layer depths of MWSDR model are set to 10 cm for surface layer and 30 cm for the three root-zone layers in order to make them approximately match with the measurement depths at the field. Soil hydraulic parameters are assigned referring to the values for sandy loam from Noilhan & Planton (1989) and Cosby et al. (1984). In order to improve the performance of the SWEB-SVAT soil moisture predictions, the default value of 4.34 for $b$ – recommended for the generic sandy loam – is modified to a calibrated value of 2.8. However, the MWSDR model performs better with the default value of $b$ for the upper soil layers and the calibrated $b$ for the deepest layer.

### 4.2.3. Evaluation metrics

In order to verify the performance of the models, a set of error metrics are used to compare the model estimations with the observed ground data.

The discrepancy between measured and simulated values ($d$) is calculated as:

$$d = M - O$$

where $M$ and $O$ denote simulation and observation vectors, respectively. This study involves the use of normalised $RMSE$ ($NRMSE$), which is defined as the ratio of the root mean square error ($RMSE$) to the mean of the ground observations ($\mu_O$),

$$NRMSE = \frac{RMSE}{\mu_O}$$

where
\[ RMSE = \sqrt{\frac{\sum_{i=1}^{N} d_i^2}{N}} \]  

(4-16)

and \( N \) is the length of time series. The advantage of using this statistic in place of \( RMSE \) is its ability to show the extent of variability in relation to the mean of the variable. The value of \( NRMSE \) is independent of the extent and magnitude of the variables, which makes it easier to compare datasets with different mean values. The other metrics used for this evaluation is Pearson’s linear correlation coefficient \((R)\) defined as the covariance of the variables, \( cov(M,O) \), divided by the product of their standard deviations \((\sigma)\),

\[ R = \frac{cov(M,O)}{\sigma_M \cdot \sigma_O} \]  

(4-17)

The Averaged Relative Error \((ARE)\) is also used to quantify the mean bias between the measured and simulates values scaled by the mean of observations. Specifically, \( ARE \) is defined as the ratio of bias \((\mu_M - \mu_O)\) to the mean of observations \((\mu_O)\):

\[ ARE = \frac{\mu_M - \mu_O}{\mu_O} \]  

(4-18)

### 4.3. Results

#### 4.3.1. Evaluation of SWEB-SVAT and MWSDR models

In this section the performance of the models in terms of soil moisture and energy flux estimations is verified via comparison with the observed ground data using a set of error metrics. Surface (0-10 cm) and root-zone (0-100 cm) soil moisture and daily latent heat estimations of the MWSDR model using three-year OPE\(^3\) dataset are compared with those from the original SWEB-SVAT and results are summarized in the Table 4.1 to Table 4.3. Total daily latent heat flux is calculated only during the period of the day when solar radiation is larger than zero.

The ET predictions reported here are sum of the soil evaporation and the canopy transpiration during the growing season, which are presented separately in Figure 4.1 for
each year. Figure 4.2 compares the time series of model predictions with observed soil moisture at the OPE3 site.

Table 4.1: Normalised RMSE (NRMSE) between measured and modelled surface and root-zone soil moisture (SM) and daily latent heat flux (LE)

<table>
<thead>
<tr>
<th></th>
<th>OPE3-2002</th>
<th>OPE3-2003</th>
<th>OPE3-2004</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>SWEB-SVAT</td>
<td>MWSDR</td>
<td>SWEB-SVAT</td>
</tr>
<tr>
<td>NRMSE</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>SM (0-10 cm)</td>
<td>0.413</td>
<td>0.200</td>
<td>0.148</td>
</tr>
<tr>
<td>SM (0-100 cm)</td>
<td>0.264</td>
<td>0.116</td>
<td>0.121</td>
</tr>
<tr>
<td>LE (daily)</td>
<td>0.573</td>
<td>0.449</td>
<td>0.269</td>
</tr>
</tbody>
</table>

Table 4.2: Linear correlation coefficients (R) between measured and modelled surface and root-zone soil moisture (SM) and daily latent heat flux (LE)

<table>
<thead>
<tr>
<th></th>
<th>OPE3-2002</th>
<th>OPE3-2003</th>
<th>OPE3-2004</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>SWEB-SVAT</td>
<td>MWSDR</td>
<td>SWEB-SVAT</td>
</tr>
<tr>
<td>R</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>SM (0-10 cm)</td>
<td>0.617</td>
<td>0.901</td>
<td>0.752</td>
</tr>
<tr>
<td>SM (0-100 cm)</td>
<td>0.782</td>
<td>0.981</td>
<td>0.833</td>
</tr>
<tr>
<td>LE (daily)</td>
<td>0.441</td>
<td>0.707</td>
<td>0.823</td>
</tr>
</tbody>
</table>

Table 4.3: Average relative error (ARE) between measured and modelled surface and root-zone soil moisture (SM) and daily latent heat flux (LE)

<table>
<thead>
<tr>
<th></th>
<th>OPE3-2002</th>
<th>OPE3-2003</th>
<th>OPE3-2004</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>SWEB-SVAT</td>
<td>MWSDR</td>
<td>SWEB-SVAT</td>
</tr>
<tr>
<td>ARE</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>SM (0-10 cm)</td>
<td>0.191</td>
<td>0.010</td>
<td>-0.028</td>
</tr>
<tr>
<td>SM (0-100 cm)</td>
<td>0.175</td>
<td>-0.080</td>
<td>0.015</td>
</tr>
<tr>
<td>LE (daily)</td>
<td>-0.150</td>
<td>-0.153</td>
<td>-0.117</td>
</tr>
</tbody>
</table>

The results of models using the 2002 dataset show noticeable improvement in the performance of MWSDR compared with the original SWEB-SVAT model. Smaller normalised RMSE for both surface (approximately 20%) and root-zone (approximately 15%) soil moisture estimations of MWSDR model presents less deviation from the observation. Larger correlation coefficient for MWSDR also indicates improvement of the similarity between temporal pattern of the modelled and the observed surface (approximately 30%) and root-zone (approximately 20%) soil moisture time series. Lastly,
MWSDR’s ARE shows smaller bias in the soil moisture estimations especially for the surface layer (approximately 20%). Visual comparison of soil moisture time series confirms that the soil moisture predictions of deep layer for 2002 dataset are significantly improved in the MWSDR model (Figure 4.2b). Also, surface soil moisture predictions derived from MWSDR for 2002 datasets show significantly higher similarity with observations compared with the results from the SWEB-SVAT model (Figure 4.2a).

Latent heat estimation statistics of 2002 dataset also illustrate a significant improvement in the results of MWSDR model by showing roughly 12% decrease in NRMSE and a 25% increase in $R$ (Table 4.1 and Table 4.2). In order to analyse the factors contributed to the improved ET prediction, the soil evaporation and the canopy transpiration are compared

![Figure 4.1: Modelled soil evaporation (left), canopy transpiration time series (middle) and ratio of evaporation to transpiration (right) at OPE$^1$ site](image)

**Figure 4.1**: Modelled soil evaporation (left), canopy transpiration time series (middle) and ratio of evaporation to transpiration (right) at OPE$^1$ site
separately. Estimated soil evaporation trends of both models are generally similar in 2002 (Figure 4.1a), but the MWSDR estimates show lower values when the surface soil layer becomes very dry (around day 80 to day 130 in Figure 4.2a), whereas SWEB-SVAT model predicts higher level of moisture for the top layer of soil and soil evaporation is estimated higher at this stage. On the contrary, the estimated canopy transpiration of the models (Figure 4.1b) present distinct patterns for each model. MWSDR model predicts higher water uptake in the mid-growing season while the root-zone layer is almost dry (Figure 4.2b) whereas the canopy transpiration parameterization of SWEB-SVAT model does not allow the model to estimate high level of water extraction beyond field capacity (about 0.16 for this field). Overall, the ET performance statistics for MWSDR demonstrate superior performance to SWEB-SVAT in predicting ET. The ratio of evaporation to transpiration (Figure 4.1C) shows distinct fluctuations in the predictions of SWEB-SVAT model during the mid-season of 2002 while the results of MWSDR model represent steadier trend during this period. The contribution of small precipitation events seems to largely affect the SWEB-SVAT predictions of this ratio while the root-zone layer is almost dry. Also at the first part of the season when the soil is less-covered by vegetation, MWSDR estimated evaporation to transpiration ratio is larger than SWEB-SVAT estimations and distinctly above 1 which demonstrates more evaporation than transpiration during the early season.

With the exception of a slightly-higher error of MWSDR in root-zone soil moisture results, the predictions of both models are generally similar during the wet 2003 period. Comparison of LE predictions with observation shows that both models underestimate ET during the early portion of the 2003 growing season (from day 1 to day 30). Crow et al. (2008) reported extremely low radiometric temperature during this period suggesting the presence of standing water. None of the models are able to provide this extremely high level of latent heat flux arising from the overall wetness of the surface in this period. The MWSDR model yields ET mostly from the surface soil evaporation and less canopy transpiration at the early stage of the growing season (Figure 4.1f) due to the undeveloped crop cover. This results in a larger underestimation of ET by MWSDR during early portions of the 2003 growing season; however, the MWSDR model estimates ET more accurately during later part of the growing season (from day 80 to day 105). As shown in Figure 4.1f, the evaporation to transpiration ratio estimations from the two models are
generally comparable during the mid-season when ET is mostly from transpiration (ratio is less than 0.5) and the canopy is not under stress.

Figure 4.2: Comparing model performances, surface (0-10cm) and root-zone soil moisture (0-100 cm)

With the exception of a slightly-higher error of MWSDR in root-zone soil moisture results, the predictions of both models are generally similar during the wet 2003 period. Comparison of LE predictions with observation shows that both models underestimate ET
during the early portion of the 2003 growing season (from day 1 to day 30). Crow et al. (2008) reported extremely low radiometric temperature during this period suggesting the presence of standing water. None of the models are able to provide this extremely high level of latent heat flux arising from the overall wetness of the surface in this period. The MWSDR model yields ET mostly from the surface soil evaporation and less canopy transpiration at the early stage of the growing season (Figure 4.1f) due to the undeveloped crop cover. This results in a larger underestimation of ET by MWSDR during early portions of the 2003 growing season; however, the MWSDR model estimates ET more accurately during later part of the growing season (from day 80 to day 105). As shown in Figure 4.1f, the evaporation to transpiration ratio estimations from the two models are generally comparable during the mid-season when ET is mostly from transpiration (ratio is less than 0.5) and the canopy is not under stress.

The results of 2004 represent a moderate improvement in the correlation coefficient of the MWSDR model - especially for soil moisture (more than 10%). That implies relatively better results in terms of more similarity in timing and shape between predictions and the observed time series of LE and soil moisture. Since ARE and NRMSE also represent a slight improvement (less than 10%) in the root-zone soil moisture, the overall improvement in the profile soil moisture is noticeable (Figure 4.2f). However, nearly similar error values of ARE and RMSE for surface soil moisture does not represent a remarkable improvement in the soil moisture prediction of the surface layer (Figure 4.2e). As was the case in 2003, temporal patterns in simulated soil evaporation and canopy transpiration are similar however evaporation to transpiration ratio estimated from MWSDR model shows larger values at the early stage of the growing period.

Figure 4.3 compares SWEB-SVAT and MWSDR predictions of root-zone (0-100 cm) soil moisture and daily latent heat with ground-based observations in the scattergrams. Plotted points represent lumped daily data from the 2002, 2003 and 2004 growing seasons. This figure suggests a superior performance for the MWSDR model with regards to both surface energy flux and root-zone soil moisture.
Results can also be parsed to examine within-season variability relative to the single year results shown in Table 4.1 to Table 4.3. Since most differences between the results of two models can be found in mid-season of the growing period (Figure 4.2) which is a critical stage in plant growth, Table 4.4 breaks down aggregated results for each growing season as a function of corn crop growth stages. Table 4.4 summarizes mean absolute error (MAE) and root mean square error (RMSE) of daily ET during the period between the reproduction phase (first corn silks appear and the pollination starts) and the full physiological maturity phase (corn kernels achieve their maximum dry weight). Timing of these stages are extracted based on the provided key-event information of the OPE\(^3\) site (Li et al. 2010).

According to Table 4.4, RMSE is reduced dramatically from 2 mm/d for SWEB-SVAT model to 0.6 mm/d for MWSDR model during this period of 2002. Although the reduction in RMSE of 2004 dataset is smaller than that in 2002, it still shows considerable improvement. Statistics of 2003 predictions do not illustrate a notable change.
Table 4.4: Error statistics for modelled daily total ET (mm) between corn reproduction and full physiological maturity growth stages

<table>
<thead>
<tr>
<th></th>
<th>RMSE</th>
<th>MAE</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>SWEB-SVAT</td>
<td>MWSDR</td>
</tr>
<tr>
<td>OPE3-2002</td>
<td>2.052</td>
<td>1.922</td>
</tr>
<tr>
<td>(Day 60-83)</td>
<td>0.637</td>
<td>0.542</td>
</tr>
<tr>
<td>SWEB-SVAT</td>
<td>0.531</td>
<td>0.399</td>
</tr>
<tr>
<td>MWSDR</td>
<td>0.523</td>
<td>0.381</td>
</tr>
<tr>
<td>OPE3-2004</td>
<td>0.717</td>
<td>0.556</td>
</tr>
<tr>
<td>(Day 64-121)</td>
<td>0.497</td>
<td>0.399</td>
</tr>
</tbody>
</table>

The time series of observed profile soil moisture show unusually dry levels during the 2002 growing season. In contrast, 2003 is wetter than normal especially during the early stage of the growing period, and 2004 is a relatively normal season. The results demonstrate that MWSDR model soil moisture and ET predictions are superior to the SWEB-SVAT model under high water stress whereas the models present similar error statistics when the overall soil wetness remains high during the growing period.

Presumably, the MWSDR model benefits from water stress compensating part of its root water uptake parameterization. In this model, the crop root system is capable of extracting more water from the wetter layers during the dry season; while the SWEB-SVAT model just relies on the overall wetness of the whole depth and reduces water extraction under water-stressed condition. On the other hand, estimating a dynamic canopy resistance based on the crop phenology and as a function of remotely sensed vegetation index, has a remarkable influence on the water extraction simulation of the MWSDR model. This part of the MWSDR scheme enables the model to extract water from wet layers of soil and maintain high level of canopy transpiration in spite of the overall dryness of the soil profile.

4.3.2. Evaluation of relationship between root-zone soil moisture and surface fluxes

In order to assess the coupling strength of the models for ET/EF and the root-zone soil moisture, the correlation of predicted surface fluxes with estimated root-zone soil moisture is evaluated and compared with the real correlation expressed in ground-based observations. The coupling strength is visualized by plotting ET/EF versus root-zone states time series to demonstrate their correlation. The scatter plots show the type and degree of
their correlation for a qualitative assessment. Figure 4.4 and Figure 4.5 present the scatter plots of root-zone soil moisture versus daily evapotranspiration and the evaporative fraction (EF) respectively. The predictions/observations of different years are marked in different colors. According to the figures, SWEB-SVAT outputs present a roughly linear correlation between ET/EF and soil moisture, which is not observed in the MWSDR outputs nor the observations. Particularly, the scatter plot of the SWEB-SVAT outputs in 2002 presents a substantial difference from the observed values.

The assumption of a simple and high sensitivity of evapotranspiration to the soil moisture in SWEB-SVAT model results in the spuriously high correlation between them. This strong coupling may come from parameterising the canopy resistance solely as a function of profile soil moisture and neglecting the effect of crop phenology on transpiration strength. However, the variation in evaporative demand and the contribution of small precipitation events largely affecting ET flux, add noise to this relationship and make the spread represented in the graph. Given that 2002 growing season is remarkably dry, profile soil moisture shows low water availability for canopy transpiration; constraining canopy transpiration based on this low root-zone soil moisture in SWEB-SVAT model provides low ET resulting the high correlation represented in Figure 4.4b. However despite the relatively dry total soil profile, various layers with roots may contain different (and enough) amount of water, enabling the crops to transpire regularly as it can be inferred from relatively high observed ET for low profile soil moisture in Figure 4.4c. Comparing observed soil moisture of various layers shows that the deepest layer (70-100 cm) is mostly the driest layer while it has the lowest effect on the plant transpiration due to the lowest plant root fraction in that layer. On the other hand, since canopy resistance of MWSDR model is defined as a function of NDVI which links the plant transpiration to plant phenology, it will force the model to extract more water from the root-zone even under stressed condition (soil moisture less than field capacity) compared with the SWEB-SVAT model in which canopy resistance is only a function of soil moisture. Consequently, more realistic links between canopy resistance and root water uptake to crop growth and water availability in each rooted layer of soil in MWSDR model, decrease the dependency between profile soil moisture and evapotranspiration which seems to make the correlations in the model more accurate (Figure 4.4a). The MWSDR ET do not decline in 2002 by
decreasing the soil wetness, instead it shows different patterns at different growth stages. The pattern of changes in MWSDR-based ET versus soil moisture is generally compatible with those of observed data.

Figure 4.4: Scatter plots of root-zone soil moisture versus daily evapotranspiration (mm/d) for model predictions and observations during three growing seasons

(a) (b) (c)

Figure 4.5: Scatter plots of root-zone soil moisture versus daily evaporative fraction for model predictions and observation during three growing seasons

(a) (b) (c)

The net result of high ET versus soil moisture correlation of the SWEB-SVAT model is a more pronounced correlation between EF and soil moisture under water-limited condition presented in Figure 4.5b. Observed EF shows a dependency to the profile soil moisture at the small part of the scatterplot with low soil moisture conditions while the other parts of the graph does not show any sensitivity (Figure 4.5c). The difference between the scatterplots of observations versus SWEB-SVAT results implies that although most land surface models (like SWEB-SVAT) assume excessive correlation under water limited condition, there are other environmental and biological factors influencing this relationship. Although some discrepancies remain, the MWSDR-based EF versus soil moisture plot does a better group capturing overall trends in the relationship between observed EF and soil moisture.
In order to verify the effects of seasonal cycle of net radiation \( (R_N) \) and plant phenology, the correlation between soil moisture and ET is evaluated with respect to \( R_N \) and NDVI changes. NDVI has been used to develop some methodologies for assessing crop phenology (e.g. Gao et al. 2015). Here, in order to link the crop phenology to NDVI, since maximum and minimum NDVI for various growing seasons differ, NDVI larger than its seasonal mean value is assumed as representative of the active growth period. NDVI smaller than this value indicates the initial growth stage after sowing or last stage close to maturity. Three broad growth stages are defined as: early, mid-term and last days in the growing season, categorising simply based on the days after planting and NDVI range. Figure 4.6 shows the observed ET versus soil moisture relationship marked/categorized by growth stages, NDVI and the net radiation.

Figure 4.6: Scatter plots of root-zone soil moisture versus daily observed evapotranspiration in three growing seasons, marked based on growth stages and net radiation (a, b, c), merging all data eliminating energy-limited conditions and low NDVI class (d), the purple curves show the exponential fitting to 2002 mid-season data

Categorising the scatterplots based on NDVI provides two distinct classes of high and low vegetation biomass. The low NDVI plots (< mean of NDVI range) can be divided to two other groups based on different growth stages i.e. early (red points in Figure 4.6) and late (green points in Figure 4.6) stages of the growing period while the plots with high NDVI
values (>mean of NDVI range) mark mid-growing season (blue points in Figure 4.6a, Figure 4.6b and Figure 4.6c). On the other hand, the scatterplots are categorised based on the mean of net radiation range to represent high (circles) and low (triangles) net radiation during the whole period. Grouping based on the net radiation shows that high level of ET is usually produced due to increasing of net radiation.

At early stage of the growing season during the crop germination and establishment stage, crop water extraction from the root-zone layer is small and ET occurs mainly as bare soil evaporation resulting in a relatively small total ET for the given soil wetness. The ET rate also decreases towards the end of the growing season when the crop reaches physiological maturity. At the same time, soil is mostly at the driest condition at the end of the cropping period, which makes this stage distinctive from the early wet stage (Figure 4.6a, Figure 4.6b and Figure 4.6c). Low NDVI clusters in 2002 and 2004 include the early and late portions of the growing period with low transpiration strength irrelevant to the profile soil moisture at these stages. 2003 dataset represents a linear relationship between soil moisture and ET in low NDVI class; however, this linearity is not associated with soil moisture. As it mentioned before, due to the presence of standing water at the beginning of the growing season plus high level of energy, ET shows very high unexpected values at this time. On the other hand, the soil is drier at the end of the period in which the net radiation is mostly low. As a result, these two groups of data construct a linear correlation in the scatterplot which is a good example showing lack of causality despite having a high correlation.

ET is driven mainly by the vegetation during the mid-season stage. At this stage when the plant is fully developed, and greatest fractional cover minimizing the influence of soil evaporation, the evapotranspiration rate increases significantly to the maximum level if there is no water and energy limitation. During the 2002 growing season, the observed ET/soil moisture relationship follows a relatively exponential trend at mid-season due to high water stress conditions. On the other hand, the 2002 and 2004 datasets present the highest range of ET at this stage in the presence of high net radiation and high soil moisture which reduces the sensitivity between ET and soil moisture significantly. Considering the $R_W$ range in the scatterplots, lower values of ET in this class seem to driven by the energy-limitations rather than the soil moisture limitations. Eliminating energy-limited conditions
and low NDVI class of data, exponential relationship between soil moisture and ET is more obvious as shown in Figure 4.6d.

Figure 4.7 presents the correlation between measured soil moisture content and observed evaporative fraction for each of the OPE3 growing seasons considering NDVI changes and plant growth stages. Similar to Figure 4.6 the scatterplots can be categorised in two groups of data by high and low NDVI. Again, the early and the late stages of the plant growth are distinctive. The 2002 dataset features very clear exponential correlation between soil moisture and EF at the active crop stage. However, there appears to be no sensitivity between soil moisture and EF during the middle of the 2003 and 2004 growing seasons. Since a linear relationship is recognised for the low NDVI cluster of 2003 (as a result of above-mentioned linear correlation between ET and soil moisture), it should be emphasised again that this trend seems completely stochastic due to the specific conditions of soil moisture. In summary, Figure 4.7 presents a good correlation between soil moisture and EF just for the peak growth period of 2002 while the other years do not show any apparent sensitivity.

![Figure 4.7: Scatter plots of root-zone soil moisture versus daily observed evaporative fraction in three growing seasons, marked based on time in growth period and NDVI](image)

Although the results from these three years look different, a consistent trend emerges if all the datasets are combined in one plot. Figure 4.8 shows observed daily EF versus root-zone soil moisture categorized based on NDVI as an indicator showing crop phenology. This simple parameterization is efficient in terms of transferability because NDVI data is readily available from remote sensing sources and can be widely applied to separate out the graph based on the crop phenology. However, if the actual growth stages are available from the field observation, this partitioning can be implemented by the field-based thresholds.
Separating the points in the scatterplot based on high and low values of NDVI in Figure 4.8a reveals an exponential trend showing high sensitivity of ET to soil moisture over the water stressed conditions at active growth period of all the years. On the other hand, separating initial stage and last stage from the low NDVI class results in a more explicit graph (Figure 4.8b). Figure 4.8c shows the results of MWSDR model which is relatively consistence with observed data.

Since the sensitivity of ET/EF to soil moisture emerges just at the active growing period when the soil is under stress, applying a linear model for the whole season in land surface processes would likely cause large estimation errors. It would also result in large updating errors when surface observations such as EF, ET, or other predictors linked to these variables are assimilated to update the root-zone soil moisture. For example, referring to Figure 4.4b and Figure 4.5b, parameterisation of ET as a fixed function of soil moisture, even under low vegetation cover, in the prognostic model would result in erroneous ET and soil moisture predictions or updates.

Figure 4.8 represents the relationship between soil moisture and EF which correlates high EF to high soil moisture content during the mid-season of the growing period while the soil is relatively dry. However, high EF does not indicate whether high moisture content exists in the surface layer or deeper layers of the soil profile. Apart from the wetness of different layers of soil, plant transpiration activity depends on the depth and density of the plant root. Plant water extraction scheme may vary based on the wetness of soil layers if there are enough roots in those layers (Li et al. 2001). In order to verify the effect of soil depth on this relationship, Figure 4.9 compares soil moisture at different depths against observed EF. Correlation between EF and soil moisture at active crop growth stage remains high at the upper layers (Figure 4.9a and Figure 4.9b) and reduces towards the deeper layers (Figure 4.9c and Figure 4.9d). Since the canopy transpiration is largely controlled by soil moisture in the rooted layers of soil and there is less density of crop root at the deeper layers of soil, finding difference in the correlation of various layers is expected. On the other hand, surface soil moisture (0-10 cm) represents high correlation with EF at initial stage whereas deeper layers (e.g. 70-100 cm) soil moisture show less correlation with EF under low vegetation condition when surface soil evaporation is dominant.
Correlation between EF and profile soil moisture may be influenced by considering the most effective layers of soil in transpiration activity and the contribution of each layer in estimated EF. However, an effective averaging of soil moisture in various layers such as weighted average based on root distribution in each layer, strengthens the sensitivity and improves predictability (Figure 4.9e and Figure 4.9f).
4.4. Discussion and conclusions

Evaluating the performance of the SWEB-SVAT and MWSDR models demonstrates that MWSDR model performs consistently throughout the three growing seasons while the performance of SWEB-SVAT changes between very low accuracy in 2002 and accurate results in 2003. The improved functional performance of the MWSDR is revealed both in the closeness of predicted surface and root-zone soil moisture to the observations and in the pattern and accuracy of evapotranspiration. The results illustrate the strong correlation between getting reliable estimates in surface and root-zone soil moisture and surface fluxes due to their interdependence. Comparing different subsurface schemes of two models demonstrates that a more detailed representation of the subsurface processes in parallel with considering the dynamic vegetation growth in MWSDR model leads to more accurate estimations of surface fluxes and soil moisture states.

The exponential or piecewise linear relationship between ET/EF and soil moisture is utilised in the ET parametrisation of most WEB-SVAT models (e.g. Scott et al. 2003, Anderson et al. 2007b, Hain et al. 2009) providing a high correlation between these variables similar to the one shown in Figure 4.4b and Figure 4.5b. However, although the overestimation of correlation between ET/EF and soil moisture content is common in land surface modelling, OPE\textsuperscript{3} observations show that this relationship is highly conditional on the vegetation biomass, plant phenology and net radiation. Also the overall wetness of soil at different stages of plant growth is very determinative for this correlation. Very close similarity between the results of MWSDR model and observations in Figure 4.4 (simulated and observed ET versus root-zone soil moisture) and Figure 4.5 (simulated and observed EF versus root-zone soil moisture) illustrates that this model parametrization is successful in capturing the aspects influencing the correlation between root-zone soil moisture state and above ground variables such as evaporative fluxes. In this field incorporating dynamic vegetation components such as dynamic root growth, non-uniform root distribution and NDVI-based canopy resistance in MWSDR model has improved the dependency of evapotranspiration to both crop phenology and water stress.

Verifying the correlation between surface fluxes and root-zone soil moisture under active growing season demonstrates high dependency only under water stress condition of this
period. This complies with earlier studies showing that retrieval of soil moisture from
diagnosed evaporative fluxes should be reasonable when there is water stress, but
sensitivity would be lost as soil moisture exceeds the stress point (Hain et al. 2009, Hain et
al. 2011). Also it is clarified that the linear/exponential correlation between
evapotranspiration and soil moisture performs well under moderate to dense vegetation but
the accuracy decreases under low vegetation conditions (Hain et al. 2009). Looking at the
other side of this relationship and pointing to its implications in data assimilation technique,
the existing correlations show that root-zone soil moisture can only be updated efficiently
when surface flux products of remote sensing methods or any other resources are supplied
at critical range of soil moisture and vegetation activity. Sensitivity at a short range of soil
moisture is a fundamental limitation for the applications of this relationship, however, it
may not matter in most cases because people do not care about soil wetness when there is
no water stress condition. There is much interest however in water use efficiency: how the
fraction of evaporation versus transpiration changes with cover and moisture conditions.
Since transpiration goes into biomass production and ultimately yield, while evaporation is
considered a loss to biomass production, more accurate estimation of these fluxes by the
MWSDR model which leads to more realistic relationship between evaporative fluxes and
soil moisture is the strength of this model.

Although using a model with strong vertical connection in a data assimilation system
correlates root-zone increments strongly with surface innovations, it cannot guarantee
higher efficiency for the data assimilation system. For example, if the model overestimates
the sensitivity between surface fluxes and sub-surface states by extending that to the whole
growth period, root-zone states will become sensitive to the surface updates even under low
vegetation condition. The sensitivity overestimation, will always force the system to update
the root-zone state but it does not mean that this update will always provide an
improvement. Making a larger change in result cannot guarantee its closeness to the truth;
on the contrary it may cause more errors in the final results when the errors in surface
fluxes are not correlated to errors in soil moisture of deep layers e.g. early or late in the
season. In this case having less correlation between surface flux and root-zone soil moisture
is more likely to produce appropriate results. As a result, even a reduction in model
coupling can be beneficial – if it results in a more accurate representing of the true coupling
between surface fluxes and profile soil moisture. In a more specific language, in an EnKF
implementation, the accurate specification of the Kalman gain requires that the model
accurately capture the coupling between observations (here EF and ET) and model states. If
this coupling is not adequately represented, the EnKF analysis will be degraded.

As a precursor to data assimilation application, it is interesting to look at how the changes
implemented in MWSDR model impact the modeled relationship between root-zone soil
moisture and surface fluxes (i.e., the observable variables that might be conceivably
assimilated into the model). Different coupling strength of SWEB-SVAT and MWSDR
models – resulting from different parameterisation of subsurface dynamics – can help to the
proper selection of a model as the system’s model component of a data assimilation system.
It can make a sense of what happens if one tries to assimilate the surface fluxes to each of
the SWEB-SVAT or MWSDR models. Considering the results of MWSDR model shows
that ET/EF is not constrained by soil moisture under non-stressed vegetated area in which
there will be no benefit in data assimilation; however, under stressed condition in the active
growing season there is a high dependency which may provide good results upon applying
the data assimilation method. It is inferred from the results that although MWSDR model
assume a high correlation between soil moisture and evapotranspiration under water limited
condition similar to most of the land surface models, it considers other environmental and
biological factors influencing this relationship. The additional physics in MWSDR (versus
the SWEB-SVAT) such as dynamic and non-uniform root growth and distribution and
dynamic NDVI-based canopy resistance appear to be required in order to appropriately
capture the relationship between surface fluxes and profile soil moisture.

As a summary although this research highlights the conditions which should be excluded
when using ET products as a way to estimate root-zone soil moisture, the more important
contribution is the need for additional novel physics in SWEB-SVAT model as a sample of
conventional land surface models to adequately capture the relationship between surface
flux and profile soil moisture across a range of crop growth stages.
5. CHAPTER 5: IMPROVEMENT OF ROOT-ZONE SOIL MOISTURE BY ASSIMILATING EVAPORATIVE FRACTION INTO A SOIL VEGETATION ATMOSPHERE TRANSFER MODEL

5.1. Introduction

Satellite remote sensing (RS) provides the opportunity to derive global maps of surface and/or root-zone soil moisture. This technique can be broadly categorized into microwave-based (e.g., Owe et al. 2001, Njoku et al. 2003) and thermal-infrared-based (e.g., Jackson et al. 1981, Anderson et al. 2007a, Anderson et al. 2007b) methods depending on the frequencies of the signal utilized for retrieval. Although microwave and thermal-based soil moisture estimation techniques each possess their own unique set of advantages (Ahmad et al. 2011), all RS-based soil moisture observations are prone to errors and available only sporadically. On the other hand, continuous predictions of soil moisture content can be estimated using land surface models forced by meteorological inputs. However, uncertainties in model structure, model parameters and forcing data induce error in model forecast (Liang & Qin 2008). Data assimilation (DA) techniques try to combine model predictions and observations based on their mutual uncertainties to improve the estimation accuracy of system’s state variables. One of the advantages of this integrated model-observation approach is that it can produce continuous soil moisture estimates with minimized uncertainties in the periods between discrete observations. Data assimilation can also simultaneously ingest information from multiple sources to update model outputs. This approach incorporates the observational data with a land dynamic model that encapsulates theoretical understanding of the whole system (Liang & Qin 2008). Thus, the two main components of a DA system are a forward land dynamic model describing variations of the land states over time and an observation operator relating land states estimates to observations.

The assimilation of microwave-derived surface soil moisture into land surface models has been examined in a number of past studies (e.g., Reichle & Koster 2005, Reichle et al. 2002). However, an emerging technique to improve the root-zone soil moisture is to
assimilate surface thermal infrared data or other products of the TIR data, such as energy fluxes estimated from TIR-based diagnostic models, to update root-zone soil moisture.

Generally, past studies have used two major schemes for the assimilation of remotely sensed TIR data into models to improve soil moisture estimations. One approach is to directly assimilate thermal infrared (TIR) observations of surface radiometric temperature (Crow et al. 2008) and the other approach assimilates products of TIR observations such as energy fluxes and soil moisture proxies (e.g., Crow et al. 2008, Pipunic et al. 2008, Li et al. 2010, Hain et al. 2012). Direct assimilation of surface radiometric temperature (LST) into land surface models (LSM) faces challenges associated with potentially large relative biases between the model-derived LST and the satellite-based TIR observations (Bosilovich et al. 2007). The view angle effect impacting TIR-based LST retrievals, but unaccounted for in most of LSMs, is another complicating factor (Holmes et al. 2012). In this respect, Crow et al. (2008) compared the results of assimilating TIR-based soil moisture proxy derived from a two-source energy balance model (TSEB) with direct assimilation of LST measurements. They found that assimilating soil moisture proxy based on surface energy flux estimations was superior, which was attributed to the fact that the relationship between root-zone soil moisture and LST was highly nonlinear and dependent on the accuracy of uncertain micrometeorological variables. Pipunic et al. (2008) reported a successful assimilation of evapotranspiration (ET) observations derived from TIR images into a land surface model, however Anderson et al. (2011) showed that TIR-based ratio of actual ET to potential ET \( f_{PET} = AET/PET \) was better correlated with soil moisture deficiencies in comparison with ET estimations. Based on this finding, Hain et al. (2012) recommended the use of RS-based soil moisture proxy (ET predictions of ALEXI normalized by potential ET) for assimilation rather than the direct use of RS-based ET.

Despite these positive examples, considerable uncertainty remains with regards to the appropriate level of model complexity required to effectively assimilate surface energy flux estimates into land surface models. Kalman filter-based data assimilation techniques work in two distinct steps: i) the background prediction step which estimates root-zone soil moisture using model dynamics and ii) the update step which corrects the estimations whenever a surface observation is available via the application of an observation operator (which relates the model states to the observed variables). Model complexity can
potentially impact both steps. During the prediction step, the exchange of water between the atmosphere, surface and root-zone is parameterized through model physics which describe the prognostic relationship between surface/root-zone soil moisture and surface energy fluxes. The update step calculates and applies a water increment to root-zone soil moisture based – in part – on model error covariance information. The estimation of this information relies on the accuracy of model physics – regardless of whether it is sampled from a Monte Carlo ensemble (as in ensemble Kalman filtering (EnKF)) or estimated via tangent-linear assumptions as in the extended Kalman filter (EKF). In an EnKF, the model ensemble is used to sample an error covariance matrix between the surface variable and root-zone soil moisture, which determines the strength and validity of the surface information to update the root-zone soil moisture estimations. Simply updating the surface information can also have a significant influence on the root-zone soil moisture, whether the update results in a more accurate analysis or not, when model physics predict strong vertical coupling between surface variables and root-zone soil moisture states. Since such coupling strength differs for various models, surface information is propagated differently for various background models (Kumar et al. 2009). Therefore, over-simplification of the relationship between surface variables and root-one soil moisture in the model may hamper the performance of system based on the assimilation of surface observations.

Instead of relying directly on background model predictions during the update step, previous attempts to assimilate land surface observations have typically assumed a simple ancillary relationship between RS-based flux products and soil moisture and applied it as the observation operator (e.g., Hain et al. 2012, Crow et al. 2008). However, assuming a linear relationship between soil moisture and $f_{P_{ET}}$ (Hain et al. 2011) can only provide a reasonable estimate of soil moisture when the soil is dry (moisture content below field capacity) and soil water vs. $f_{P_{ET}}$ follows the assumed linear trend (Hain et al. 2012). In this case, assimilation of soil moisture proxy may cause errors when the assumed relationship between the proxy and the actual soil moisture becomes no longer valid under wet soil condition. Results of Chapter 4 showed that, apart from soil wetness range, vegetation growth stage can also have an important effect on the relationship between soil moisture and surface fluxes. In particular, they demonstrated the suitability of a linear soil moisture vs. flux relationship is limited only to the period when plants are in their active growth
period. Also, the dynamic depth of plant roots may influence this relationship by enabling the plant to extract water from various soil layers. As a result, the required relationship between soil moisture and evaporative fluxes (or flux ratios like $f_{PET}$) is likely to be much more complex than assumed by past data assimilation studies.

Despite the apparent importance of this relationship, relatively little is currently known about its role in successful data assimilation systems. In this paper, two different model schemes are employed to investigate how the use of different model parameterization schemes affects the performance and results of a data assimilation system designed to ingest surface flux information gleaned from TIR remote sensing. In particular, we investigate the influence of employing more realistic coupling strength on the accuracy and validity of data assimilation method in transferring surface flux information into the root-zone. The experiment is conducted using both the simple water and energy balance-soil vegetation atmosphere transfer (SWEB-SVAT) model (Crow et al. 2008, Li et al. 2010) and the multi-layer WEB-SVAT with dynamic root distribution (MWSDR) model (Hashemian et al. 2015). These two models employ substantially different subsurface soil-vegetation schemes.

Considering this coupling, we assimilate the evaporative fraction (EF), which is a ratio of the latent heat flux (LE) to the sum of LE and the sensible heat (H) fluxes, to update deeper layer moisture content. Since energy fluxes are not observable directly from satellites, TIR-based instantaneous surface energy flux retrievals acquired from the TSEB land surface model (Norman et al. 1995) will be used in DA system. The soil moisture content estimations produced from data assimilation based on each of these two models will be analysed and compared with observed soil moisture data. In addition, simple empirical observation operators employed in previous studies (e.g. Crow et al. 2008, Hain et al. 2012) will be evaluated as a tool to correct for unrealistic model coupling. Finally, observed relationships between EF and soil moisture extracted from field observations will be utilised in a data assimilation system to evaluate the efficacy of the observation-derived EF-soil moisture coupling for data assimilation.
5.2. Materials and Methods

5.2.1. Land surface models

This section provides a brief description of various land surface models used in this work: (i) the simple water and energy balance (WEB) soil-vegetation-atmosphere transfer model (SWEBSVAT) (Crow et al. 2008), (ii) the multi-layer WEB-SVAT with dynamic root distribution (MWSDR) model (Hashemian et al. 2015) and (iii) the thermal remote sensing-based TSEB (Norman et al. 1995, Kustas & Norman 1999). The TSEB model is used to estimate state variables based on tower-based thermal infrared temperature observations, which are later assimilated into the SWEBSVAT and MWSDR models.

For all three models (SWEBSVAT, MWSDR and TSEB), partitioning of surface net radiation into sensible and latent heating is performed separately for the vegetation canopy (C) and soil surface (S):

\[ R_{N,C} = H_C + LE_C \]  \hspace{1cm} (5-1a)
\[ R_{N,S} = H_S + LE_S + G \]  \hspace{1cm} (5-1b)

The physically-based radiation model of Campbell & Norman (1998) is used to estimate net radiation incident on the canopy \( R_{N,C} \) and soil surface \( R_{N,S} \) based on observations of downward solar radiation \( S_{\downarrow} \):

\[ R_{N,C} = (1 - \tau_{long})(L_{\downarrow} + L_S - 2L_C) + (1 - \tau_{solar})(1 - a_l C)S_{\downarrow} \]  \hspace{1cm} (5-2a)
\[ R_{N,S} = \tau_{long}L_{\downarrow} + (1 - \tau_{long})L_C - L_S + \tau_{solar}(1 - a_l S)S_{\downarrow} \]  \hspace{1cm} (5-2b)

where \( \tau \) is the canopy transmissivity for short wave \( (solar) \) and long wave \( (long) \) radiations, \( L_{\downarrow}, L_C \) and \( L_S \) emitted long-wave radiation fluxes from the sky, soil and canopy calculated from air, soil and canopy temperatures and \( a_l \) the albedo of soil (S) and canopy (C), respectively.

Assuming soil surface and vegetation canopy fluxes to be in parallel to each other (Li et al. 2005), sensible heat fluxes from the vegetation \( H_C \) and soil surface \( H_S \) are calculated as:
\[ H_C = \rho C_p \frac{T_C - T_A}{R_A} \]  \hspace{1cm} (5-3a)

\[ H_S = \rho C_p \frac{T_S - T_A}{R_A + R_{AS}} \]  \hspace{1cm} (5-3b)

where \( \rho C_p \) is the volumetric heat capacity of air and \( T \) represents temperature of air \((A)\), soil \((S)\) and canopy \((C)\). \( R_A \) is the above-canopy aerodynamic resistance and \( R_{AS} \) the within-canopy soil aerodynamic resistance.

Ground heat flux \((G)\) in Eq. (5-1b) is calculated as a simple function of net radiation:

\[ G = c_g R_{N,S} \]  \hspace{1cm} (5-4)

where \( c_g \) is estimated based on leaf area index (LAI) and time of day (Kustas et al. 1998).

There are important structural differences between these models in their treatment of surface temperature, which are described below.

**Two-source energy balance model (TSEB)**

In the thermal remote sensing two-source energy balance (TSEB) model, observations of surface radiometric temperature are used as input for the diagnostic estimation of surface energy flux components at (sporadic) times when surface temperature observations are available.

TSEB estimates canopy latent heat flux \((LE_C)\) using the Priestly-Taylor formula as the first guess:

\[ LE_C = f_g \alpha_{PT} \frac{\Delta}{\Delta + \gamma} R_{N,C} \]  \hspace{1cm} (5-5)

where \( f_g \) is the green fraction derived from LAI (typically equal to 1), \( \alpha_{PT} \) the Priestley-Taylor constant (typically assumed to be 1.3 for unstressed vegetation condition), \( \Delta \) the slope of the saturation vapour pressure versus temperature curve and \( \gamma \) the psychrometric constant.

\( H_C \) is calculated as a residual of the surface energy balance from Eq. (5-1a), and Eq. (5-3a) is inverted to obtain \( T_C \).
TSEB expresses the observed surface radiometric temperature ($T_{rad}$) as a composite of soil and canopy temperatures using the local vegetation cover fraction ($f_c$) visible at the view angle of thermal sensor ($\theta$):

$$T_{rad} = [f_c T_C^4 + (1 - f_c) T_S^4]^{1/4}$$  \hspace{1cm} (5-6)

where $f_c$ is predicted as:

$$f_c = 1 - \exp\left(\frac{-0.5 \Omega LAI}{\cos(\theta)}\right)$$  \hspace{1cm} (5-7)

and $\Omega$ is a clumping factor correction for non-homogeneous canopy cover. $T_S$ is calculated from Eq. (5-6) using the estimated $T_C$, and the observed $T_{rad}$ is used to calculate $H_S$ via Eq. (5-3b). This leaves $LE_S$ as the residual of the soil surface energy balance in Eq. (5-1b).

Assuming $\alpha_{PT} = 1.3$ under soil moisture stress may lead to a negative $LE_S$ due to the overestimated $LE_C$. Therefore, negative instantaneous $LE_S$ upon an application of the TSEB to a sunny mid-afternoon condition can be considered an indication of a water-stressed vegetation canopy. The gradual adjustment of $\alpha_{PT}$ in an iterative manner until $LE_S$ becomes positive is employed to address problem (Kustas & Norman 1999).

### SWEB-SVAT model

The SWEB-SVAT model (Crow et al. 2008) is based on merging a force restore model (Noilhan & Planton 1989, Montaldo et al. 2001) with a two-layer vegetation/soil energy balance formulation in which vertical canopy structure is identical to parallel version of the TSEB model (Norman et al. 1995). The water balance approach of SWEB-SVAT model divides the soil profile into vertically-overlapping surface and root-zone layers parameterizing as:

$$\frac{d\theta_{sz}}{dt} = \frac{C_1}{d_{sz}} \left[P_g - LE_S (\rho \lambda)^{-1}\right] - \frac{C_2}{f_d} (\theta_{sz} - \theta_{eq})$$  \hspace{1cm} (5-8a)

$$\frac{d\theta_{rz}}{dt} = \frac{1}{d_{rz}} \left[P_g - LE_C (\rho \lambda)^{-1}\right] - LE_S (\rho \lambda)^{-1} - Q$$  \hspace{1cm} (5-8b)

where $\theta_{sz}$ and $\theta_{rz}$ are surface- and root-zone soil moisture contents, $d_{sz}$ and $d_{rz}$ surface- and root-zone depth, $P_g$ throughfall, $\rho$ the density of air, $\lambda$ the latent heat of vaporisation, $f_d$
the frequency of diurnal variations (24 hours), \( \theta_{eq} \) the equilibrium surface volumetric moisture content and \( Q \) the drainage from the bottom of the root-zone. \( C_1 \) and \( C_2 \) are force and restore coefficients for soil moisture.

In contrast to the TSEB model, the SWEB-SVAT model predicts \( LE_S \) and \( LE_C \) as:

\[
LE_S = \rho C_P \gamma^{-1} [e_S(T_S) - e_a] / (R_{AS} + R_A + R_S) \tag{5-9a}
\]

\[
LE_C = \rho C_P \gamma^{-1} [e_S(T_C) - e_a] / (R_C + R_A) \tag{5-9b}
\]

where, \( e_S \) and \( e_a \) are saturation and near-surface water vapour pressure, \( R_S \) and \( R_C \) are soil and canopy resistances which are a function of surface and root-zone soil moisture, respectively. The canopy resistance \( R_C \) is estimated by:

\[
R_C = \begin{cases} 
R_{C,\text{max}} & \theta_{rz} < \theta_w \\
(R_{C,\text{min}} - R_{C,\text{max}}) \frac{\theta_{rz} - \theta_w}{\theta^* - \theta_w} + R_{C,\text{max}} & \theta_w < \theta_{rz} < \theta^* \\
R_{C,\text{min}} & \theta_{rz} > \theta^*
\end{cases} \tag{5-10}
\]

where \( \theta^* \) and \( \theta_w \) are the volumetric soil moisture levels at the field capacity and the wilting point, respectively. Resistance extremes \( R_{C,\text{max}} \) and \( R_{C,\text{min}} \) are specified based on typical literature values considering the soil texture (Li et al. 2010).

In the computation order of SWEB-SVAT model, soil and canopy resistances are calculated based on the initial values of \( \theta_{sz} \) and \( \theta_{rz} \) as the first step. All fluxes in Eqs. (5-1) are expressed in terms of canopy and soil temperature \( (T_C \text{ and } T_S) \) and solved for \( T_C \) and \( T_S \) simultaneously using a Newton-Raphson approach. Final output of energy balance section includes soil evaporation \( (LE_S) \) and canopy transpiration \( (LE_C) \) fluxes, which are then employed in Eqs. (5-8) to provide temporally-continuous surface and root-zone soil moisture predictions.

**MWSDR model**

The SWEB-SVAT model was extended to a new multi-layer WEB-SVAT model with a dynamic root distribution (MWSDR) within additional soil layers (Hashemian et al. 2015). Apart from utilising a sophisticated root distribution model which considers the dynamic
nature of plant growth, MWSDR model also adapts a new parameterization of canopy resistance based on plant phenology. However, this model still shares a common set of energy balance equations with the SWEB-SVAT model (see above).

Within the MWSDR model, the water balance equation for the surface and root-zone layers is given as:

\[
\frac{d\theta_{sz}}{dt} = \frac{1}{d_{sz}} \left[ P_g - LE_S(\rho \lambda)^{-1} - q_{1 \rightarrow 2} \right]
\]

(5-11a)

\[
\frac{d\theta_{rz,i}}{dt} = \frac{1}{d_i} \left[ q_{l-1 \rightarrow l} - LE_{C,i}(\rho \lambda)^{-1} - q_{l \rightarrow l+1} \right]
\]

(5-11b)

where \( \theta_{rz,i} \) is moisture content of root-zone layers, \( d_i \) the depth of root-zone layer, \( LE_{C,i} \) the fraction of canopy water uptake of each layer, and \( q_{l \rightarrow l+1} \) denotes the water flux from layer \( i \) to layer \( i+1 \) (redistribution) utilising Darcy’s law (Campbell & Norman 1998).

Root-zone soil moisture (\( \theta_{rz} \)) is then calculated as:

\[
\theta_{rz} = \frac{d_{sz} \cdot \theta_{sz} + \sum_{i=1}^{n} d_i \cdot \theta_{rz,i}}{d_{sz} + \sum_{i=1}^{n} d_i}
\]

(5-12)

where \( n \) represents the number of layers. The transpiration contribution of each individual soil layer (\( LE_{C,i} \)) is calculated based on available soil water (\( \alpha \)) and the fraction of root density located in layer \( i \) (\( F_i \)) as:

\[
LE_{C,i} = \frac{\alpha_i^2 F_i^3 P_t}{\sum_{i=1}^{n} \alpha_i F_i^3 P_t}
\]

(5-13)

where \( P_t \) is potential transpiration and \( F_i \) is calculated by:

\[
F_i = \ln \left( \frac{1 + \exp(-bZ_i)}{1 + \exp(-bZ_{i+1})} \right) + 0.5[\exp(-bZ_i) - \exp(-bZ_{i+1})]
\]

\[
\cdot \ln \left( \frac{1 + \exp(-bZ_r)}{1 + \exp(-bZ_{r+1})} \right) + 0.5[1 - \exp(-bZ_r)]
\]

(5-14)

\( Z_i \) is soil depth of layer \( i \), \( Z_r \) is root depth, and \( b \) is an empirical extinction coefficient of root distribution. \( Z_r \) and \( b \) vary temporally during the vegetation growing period due to the time evolution of root depth and density. These variables can be estimated from ground-based observation or based on typical growth stage-based values reported in the past studies.
(e.g. Li et al. 2001, Dwyer et al. 1988). The fraction of root density ($F_i$) is then dynamically estimated using dynamic $Z_r$ and $b$.

Unlike the SWEB-SVAT model, the minimum canopy resistance (used in the calculation of potential transpiration) in the MWSDR model is estimated as a function of NDVI to relate the total canopy resistance to the plant phenology:

$$R_{C,\text{min}} = \frac{k}{NDVI} \quad (5-15)$$

In the overall computational stream of the MWSDR model, the minimum canopy resistance calculated using Eq. (5-15) is used for calculating potential transpiration. Then partial transpiration values for different layers calculated using Eq. (5-13) are summed up to obtain total $LE_C$. Next, $T_C$ and $T_S$ are estimated iteratively using the same method as the SWEB-SVAT. Final estimates of soil evaporation ($LE_S$) and canopy transpiration ($LE_C$) are then employed in Eqs. (5-11) to predict multi-layer variations in soil moisture over time.

### 5.2.2. Site description

This work is based on the data collected in a cornfield site developed for the US Department of Agriculture (USDA) Optimizing Production Inputs for Economic and Environmental Enhancement (OPE$^3$) program, located in Beltsville, Maryland, USA. The focus of this research is on the experimental campaign carried out in 2002, encompassing all the stages of the growing season from mid-April (planting) to the end of September (close to harvest).

Micrometeorological instrumentation positioned at 10 m above the ground level measured meteorological variables such as rainfall, air temperature, solar radiation, relative humidity and wind speed. Sensible and latent heat fluxes and radiometric surface temperature were also measured. All the data were stored as 10-minute averages.

Soil moisture was also monitored at the depths of 10, 30, 50, and 80 cm. Surface and subsurface soil water dynamics and ET observations show that 2002 growing season was relatively dry, with the profile volumetric soil moisture content ranging between 0.06 m$^3$m$^{-3}$ and 0.22 m$^3$m$^{-3}$. 

98
LAI was sampled periodically during the corn development in 2004. For 2002, the dynamics observed during the 2004 growing season were integrated with available sporadic LAI measurements at crop emergence and maturity stages in order to estimate the LAI time series using a piecewise linear model (Crow et al. 2008). Plant-canopy height is assumed to follow the same piecewise-linear model as LAI considering a minimum of 0.1 m and a maximum of 2 m.

This study is based on running the models on a 10-minute time step and through approximately 159 days of forcing data observations available at the site. SWEB-SVAT model soil layering includes one surface layer (0-10 cm) and one lumped root-zone layer (0-100 cm). MWSDR model is run with four soil layers with thicknesses 0–10 cm, 10–40 cm, 40–70 cm and 70–100 cm which are partly matched with soil moisture measuring depth at the field. Weighted average modelled soil moisture at 0-100 cm depth is considered as modelled root-zone soil moisture. Representation of the 1-m root-zone soil moisture needed for evaluation the model performance is obtained as a depth-based weighted average of available soil moisture observations.

Since the first several meters of soil texture is characterized as sandy loam (Crow et al. 2008), all soil parameters of the models were set equal to sandy loam lookup table values presented in Cosby et al. (1984) and Noilhan & Planton (1989). However, changing the default value of 4.34 for $b$ to 2.8 improves the soil moisture estimations of SWEB-SVAT model. Also calibrated values of $b$ were found and substituted for different layers of MWSDR model.

5.2.3. **Data assimilation approach**

The ensemble Kalman filter (EnKF) is a widely used assimilation technique which has been shown to be effective for land surface data assimilation (Hain et al. 2012, Crow & Reichle 2008, Zhou et al. 2006). Compared to the original Kalman filter (KF) presented by Kalman (Kalman 1960), the EnKF does not require linearization of the model and it provides a more flexible way to calculate error covariance between the variables (Reichle et al. 2002). The background prediction and the observation uncertainties are explicitly generated by a Monte Carlo simulation.
The EnKF is implemented in two distinctive steps: (i) an ensemble forecast step and (ii) a data assimilation update (analysis) step. In the forecast step, the land surface model propagates the ensemble of model state vector $X_k(n_{state} \times 1)$ forward in time. Model states and observations are assumed to be linked by:

$$Y = h(X) + \varepsilon$$  \hspace{1cm} (5-16)

where $\varepsilon(n_{state} \times 1)$ is a Gaussian noise vector with covariance $R(n_{obs} \times n_{obs})$ and $h$ is an observation operator that transfers the model state vector ($X$) to the variable ($Y$) compatible with the observed variable ($O$).

At times ($t$) in which an observation vector $O^t(n_{obs} \times 1)$ is available for assimilation, the forecast state vector associated with each model replicate ($i$) is updated as:

$$X_i^{t+} = X_i^{t-} + K^t[O^t + \varepsilon_i^t - Y_i^{t-}]$$  \hspace{1cm} (5-17)

where $t+$ and $t-$ refer to the state estimates before and after update respectively. The second term of Eq. (5-17) determines the correction applied to the forecast state vector. The Kalman gain $K (n_{state} \times n_{obs})$ represents the relative uncertainty of the predicted and actual observation based on the error covariance matrices as:

$$K = \frac{C_{ym}}{C_y + R}$$  \hspace{1cm} (5-18)

where $C_y$ is variance of model forecast of the observation states ($Y$), and $C_{ym}$ a vector containing the covariance between model states ($X$) and model forecast of the observation states ($Y$). $C_y$ and $C_{ym}$ can be statistically estimated from all individual ensemble realizations and calculated around the ensemble mean as:

$$C_{ym}^t = \frac{(X_i^{t-} - \bar{X}^{t-})(Y_i^{t-} - \bar{Y}^{t-})^T}{m - 1}$$  \hspace{1cm} (5-19a)

$$C_y^t = \frac{(Y_i^{t-} - \bar{Y}^{t-})(Y_i^{t-} - \bar{Y}^{t-})^T}{m - 1}$$  \hspace{1cm} (5-19b)

where $m$ denotes the number of ensemble members and $\bar{X}$ represents the ensemble mean across all members of $X$. Although 30 ensemble members has been proved by previous studies to be appropriate upon using one-dimensional land surface models (Crow & Wood
2003, Reichle & Koster 2005), a larger ensemble size of 150 is used here to ensure the optimal performance of sampling method.

Data assimilation results here are for the special case in which assimilated observations correspond to a flux estimates provided by the model. In this case, there are two options. First, the observation operator $h$ can be neglected and the error covariance and variance terms in Eqs. (5-19) are sampled directly from forecasted model states and model flux estimates to parameterize Eq. (5-18). The other option is that the model-based flux estimates are discarded and an empirical expression is utilized for $h$. Instead of using model flux estimates directly to calculate Eq. (5-18), state estimates are processed through an empirical observation operator $h$ to obtain states in $Y$. Such flux estimates are, in turn, sampled in Eqs. (5-19) and used to parameterize Eq. (5-18) (see Hain et al. 2012, Crow et al. 2008). Utilizing an external observation operator is potentially useful when the model-based predictions are not able to accurately capture the right coupling between soil moisture and surface fluxes. In this case, model-based coupling between surface fluxes and root-zone soil moisture has less influence in the update step. However, it still impacts model dynamics and thus the state forecast step within a DA system. The following sections explain how to implement DA based on these two strategies.

- **EnKF Implementation**

The following cases, detailed below, will be considered in the analysis of EF assimilation into SWEB-SVAT and MWSDR models with and without an empirically-based observation operator.

**SWEB-SVAT-based DA**

In the application of the SWEB-SVAT model for assimilation of evaporative fraction (EF) ($n_{obs} = 1$) to update soil moisture states, $n_{state}$ is set to 2 considering the two surface (0-10 cm) and root-zone (0-100 cm) layers of the model.

Ensemble spread is created through direct application of additive mean-zero Gaussian noise with a covariance matrix $S$ ($2 \times 2$) to soil moisture states at each individual 10-min model time step. The standard deviation $s$ for random perturbations is applied to the surface layer
and the standard deviation for the root-zone perturbations is rescaled by multiplying $s$ by $1.5 \times d_{sz}/d_{rz}$. Also, a cross-correlation of 0.5 is assumed between the soil moisture perturbations applied to the surface and the root-zone soil layers to reflect the hydraulic links between the individual soil layers.

EF retrievals are derived from the tower-based TIR measurements at the OPE$^3$ site applied as an input to TSEB. All EF retrievals are assumed to occur at 2pm local solar time (LST) assuming daily thermal infrared observations available from a polar orbiting satellite. The observation error covariance ($R$) is estimated by comparing EF estimations from TSEB with observed EF values and calculating the mean squared difference to determine the error range. Observation error expressed by $\varepsilon$ in Eq. (5-17) is introduced by perturbing the observation with a mean-zero Gaussian noise with the calculated standard deviation prior to the data assimilation. All model and observation perturbations are specified to be uncorrelated in time and mutually independent. In order to use the actual model structure for the update state, the Kalman gain is statistically estimated using Eq. (5-18) from individual ensemble realizations.

In order to find an appropriate value for $s$ which is used to perturb model forecasts and provide forecast uncertainty, normalized filter innovations $\nu$ are derived as:

$$\nu^t = (O^t - Y^t)/\sqrt{C_y + R}$$  \hspace{1cm} (5-20)

where the angle brackets denote averaging across the ensemble members. This value can be used as a diagnostic tool to constrain the model and observations perturbations. If all the assumptions underlying the application of the EnKF filter such as the additive optimal Gaussian error specification are met, the resulting times series of $\nu$ should have mean zero and a variance of 1 (Crow & Reichle 2008). Following Crow & van den Berg (2010), given that an independent estimation of observation error ($R$) is available from comparing the TSEB predictions with measured fluxes, Eq. (5-20) is used to constrain $s$. In this study, optimal value of $s$ is selected by checking a range of pre-specified values to find the one that produces normalized innovations with a variance closest to unity and an average closest to zero.
MWSDR-based DA

In order to utilise MWSDR model in data assimilation system to update all four soil moisture states using TIR-based EF data, \( n_{\text{state}} \) should be set to 4.

Additive Gaussian noise with covariance matrix \( S (4 \times 4) \) is applied to soil moisture states at each 10 minutes time step to provide the ensemble spread. If the standard deviation of perturbations for the surface layer is defined as \( s \) (the first diagonal component of \( S \)), the \( n^{th} \) diagonal component of \( S \) is defined by multiplying \( s \) with the ratio \( d_1/d_n \) using \( d_n \) to refer to the thickness of the \( n^{th} \) soil layer. Also the cross-correlation matrix is applied to obtain off-diagonal terms in \( S \) following past researches (Reichle et al. 2007, Kumar et al. 2009) as listed in Table 5.1. The filter innovations constraint presented in Eq. (5-20) is utilized to find the optimal standard deviation of perturbations. However, the error parameters needed for perturbation of MWSDR ensemble are also tuned to yield comparable ensemble spreads as SWEB-SVAT. In order to take the most advantages from the MWSDR model structure, Kalman gain is also estimated using Eq. (5-18) independent from the predefined observation operator.

<table>
<thead>
<tr>
<th>Layer 1 SM (0–10 cm)</th>
<th>1.0</th>
<th>0.6</th>
<th>0.4</th>
<th>0.2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Layer 2 SM (10–40 cm)</td>
<td>0.6</td>
<td>1.0</td>
<td>0.6</td>
<td>0.4</td>
</tr>
<tr>
<td>Layer 3 SM (40–70 cm)</td>
<td>0.4</td>
<td>0.6</td>
<td>1.0</td>
<td>0.6</td>
</tr>
<tr>
<td>Layer 4 SM (70–100 cm)</td>
<td>0.2</td>
<td>0.4</td>
<td>0.6</td>
<td>1.0</td>
</tr>
</tbody>
</table>

**EnKF Implementation using an empirical observation operator**

Utilising an assumed simple ancillary relationship between RS-based flux products and soil moisture as the observation operator \( h \) instead of relying on the relationship existing in the model has been attempted in previous studies (Hain et al. 2012, Crow et al. 2008). When independent EF observations are available, the functional relationship between EF and root-zone soil moisture (RZSM) derived from observations may be useful for improving soil moisture via data assimilation. In this case the observation operator is empirically estimated from the relationship between the observed EF and root-zone soil moisture, not from the EF versus root-zone soil moisture relationship predicted by the
model. More specifically, $h$ is calculated empirically using a least square regression analysis to estimate the relationship between the variables. Instead of directly using model flux estimates in the update step in Eq. (5-17), predicted flux observations ($Y_{t^-}$) are obtained by processing the state estimates through an empirical $h$ relationship. These flux estimates are also sampled in Eqs. (5-19) to calculate $C_{ym}$ and $C_y$ which are required to parameterize Kalman gain using Eq. (5-18). In this case the new equation for the update step is introduced as:

$$X_{i^+} = X_{i^-} + K^t [O^t + \varepsilon_i^t - h(X_{i^-})] \quad (5-21)$$

$C_y$ and $C_{ym}$ are sampled as:

$$C_{ym}^t = \frac{(X_{t^-} - X_{\bar{t}^-})(h(X_{t^-}) - \text{Mean}(h(X_{t^-})))^T}{m - 1} \quad (5-22a)$$

$$C_y^t = \frac{(h(X_{t^-}) - \text{Mean}(h(X_{t^-})))^T(h(X_{t^-}) - \text{Mean}(h(X_{t^-})))}{m - 1} \quad (5-22b)$$

Figure 5.2a presents the relationship between observed root-zone soil moisture and EF clustered in three stages of growth period. Initial stage, mid-season and late season in the growing season are categorised based on the days after planting and NDVI range. Specifically, NDVI larger than its seasonal mean value is used to indicate the active growth (or mid-season) period. Conversely, NDVI smaller than this value indicates the initial growth stage after sowing or last stage close to maturity. Figure 5.1 illustrates the NDVI time series and the temporal partitioning into the various growth periods.

![Figure 5.1: NDVI time series and the temporal partitioning of growth stages](image-url)
Figure 5.2a indicates that the coupling between EF and root-zone soil moisture is significant only during dry portions \((\theta_{rz} < 0.10)\) of the active growth period. The efficacy of assimilating EF to improve RZSM prediction will be confined to the dry regime of soil wetness accordingly. Since there is no sensitivity between RZSM and EF during the initial and late season growth stages, the observed variables are filtered in Figure 5.2b to show the relationship between soil moisture states and EF only during the active growth period. Also an exponential function fitted on this relationship is represented in the figure. On the other hand, a linear relationship can be distinguished during the active growth period when the soil is dry (soil moisture less than 10%) as represented in Figure 5.2b. Linear and exponential function forms will both be used to define observation operator \((h)\).

\[
(5-21)
\]

(SWEB-SVAT-based DA)

Considering a linear relationship between root-zone soil moisture and EF during the dry active growth period, the relation between model state vector and observation can be assumed as:

\[
EF = q \cdot \theta_{rz}
\]

where \(q\) is a constant value.

Considering the exponential relationship during the entire active growth period, the relationship between EF and root-zone soil moisture is defined as:
\[ EF = q_1 \cdot \exp(q_2 \cdot \theta_{rz}) + q_3 \] (5-22)

**MWSDR-based DA**

Figure 5.2a represents the relationship between vertically-integrated RZSM value and EF which correlates high EF to high soil moisture content during the active growth period while the soil is relatively dry. However, high EF alone does not constrain the vertical distribution of soil moisture within the root-zone. Since surface soil moistens and dries very quickly, for some period of this time, EF may be sensitive to the surface moisture content (evaporation from the wet surface layer) but in other times even though the surface is dry high EF may still have driven by high latent heat flux due to plants transpiration. In this case EF is sensitive to moisture content of the deeper soil layers. EF decreases upon drying the root-zone layer; however, rainfall in this time may make the top layers very wet while the deeper zone is still dry; in this case EF is more correlated to the top layers.

Therefore, apart from the wetness of different layers of soil, plant transpiration activity also depends on the depth and density of the plant root. Plant water extraction scheme may vary based on the wetness of soil layers only if there is enough root in those layers (Li et al. 2001); therefore the relationship between EF and profile soil moisture may be influenced by considering the most effective layers of soil in transpiration activity and the contribution of each layer in the estimated EF. Knowing that MWSDR model simulate the root distribution in various layers of soil, weighting soil moisture based on the root density of the soil layers provides a more appropriate soil moisture state to be used in data assimilation method.

Weighted root-zone soil moisture (\( \theta_{wrz} \)) based on root availability of each layer is calculated as:

\[ \theta_{wrz} = \frac{d_{sz}}{d_{sz} + \sum d_i} \theta_{sz} + \frac{\sum d_i}{d_{sz} + \sum d_i} \left( F_1 \theta_{rz,2} + F_2 \theta_{rz,3} + F_3 \theta_{rz,4} \right) \] (5-23)

where \( F_i \) is the fraction of root density in each layer, \( \theta_{rz,i} \) root-zone soil moisture content and \( d_n \) depth of layer \( n \). Figure 5.3a shows the relationship between observed \( \theta_{wrz} \) and EF classified based on three stages of the growth period.
Given the NDVI-based various growth stages, the relationship between EF and weighted root-zone soil moisture can be figured out as a linear function when the soil is dry (soil moisture less than 12%) during active growth period, or an exponential function for the entire active growth period. Figure 5.3b represents these two kinds of relationships by fitting a linear and exponential function to the observed variables only during the active growth period.

Weighted root-zone soil moisture using the simulated root density appears to be similar with simple linear averaging of soil moisture presented in Figure 5.2, in this particular application. However, assuming that it may result in different relationship for other sites or other soil moisture conditions, this more sophisticated vertical weighting is utilised for this implementation.

Considering the linear relationship between EF and weighted root-zone soil moisture as:

$$EF = q \cdot \theta_{wrz} \quad (5-24)$$

Considering an exponential relationship between weighted soil moisture and EF as:

$$EF = q_1 \cdot \exp(q_2 \cdot \theta_{wrz}) + q_3 \quad (5-25)$$
5.3. Results and Discussions

5.3.1. Pre-analysis of models predictions

The open loop predictions of SWEB-SVAT and MWSDR, and the output of TSEB are compared with the ground-based observations of the OPE$^3$ site. Evaluation of daily evapotranspiration (ET) and evaporative fraction (EF) predictions presented in Figure 5.4 and Table 5.2 suggests slightly superior performance for TSEB.

The error statistics of daily and instantaneous (at 2pm) predictions of ET and EF are presented in Table 5.2. Although daily TSEB ET predictions demonstrate a positive bias, TSEB \textit{RMSE} and correlation coefficient results are superior to SWEB-SVAT and MWSDR (Table 5.2). In addition, instantaneous TSEB 2 pm ET estimates are relatively unbiased (while retaining the relatively good RMSE and correlation characteristics). Since all results here are based on the sequential assimilation of instantaneous flux predictions, the bias in TSEB daily ET is inconsequential.

Figure 5.4: (a) Daily EF and (b) daily ET estimations of MWSDR, WEB-SVAT and TSEB models comparing with observations
In addition to the statistics of the models for the whole growing season, error statistics from the active growing period are represented in this table. Active growth period is defined here as all days where NDVI is above the growing season mean (see Figure 5.1). Excluding the initial and late stages of the growing season based on this threshold provides even more reliable results of TSEB model compared with MWSDR and SWEB-SVAT. As shown in Table 5.2, the RMSE of TSEB EF and ET is much lower than two other models during this time. Also smaller bias and high correlation coefficient of the TSEB results demonstrate more accurate TSEB predictions during the active growth period.

<table>
<thead>
<tr>
<th></th>
<th>RMSE</th>
<th>R</th>
<th>Bias</th>
</tr>
</thead>
<tbody>
<tr>
<td>Daily-ET (mm/d)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>SWEB-SVAT</td>
<td>1.4233</td>
<td>0.4392</td>
<td>-0.4175</td>
</tr>
<tr>
<td>MWSDR</td>
<td>1.1064</td>
<td>0.6870</td>
<td>-0.3016</td>
</tr>
<tr>
<td>TSEB</td>
<td>0.9329</td>
<td>0.8459</td>
<td>0.4592</td>
</tr>
<tr>
<td>ET_2pm (mm)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>SWEB-SVAT</td>
<td>0.0411</td>
<td>0.4119</td>
<td>-1.41e-04</td>
</tr>
<tr>
<td>MWSDR</td>
<td>0.0338</td>
<td>0.6196</td>
<td>-1.17e-04</td>
</tr>
<tr>
<td>TSEB</td>
<td>0.0302</td>
<td>0.7031</td>
<td>-6.95e-05</td>
</tr>
<tr>
<td>ET_2pm (mm)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>(Active growth period)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>SWEB-SVAT</td>
<td>0.0577</td>
<td>0.3482</td>
<td>-2.89e-04</td>
</tr>
<tr>
<td>MWSDR</td>
<td>0.0475</td>
<td>0.4797</td>
<td>-2.27e-04</td>
</tr>
<tr>
<td>TSEB</td>
<td>0.0221</td>
<td>0.8578</td>
<td>-6.68e-05</td>
</tr>
<tr>
<td>Daily-EF</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>SWEB-SVAT</td>
<td>0.2688</td>
<td>0.0675</td>
<td>-0.1376</td>
</tr>
<tr>
<td>MWSDR</td>
<td>0.2168</td>
<td>0.3292</td>
<td>-0.1155</td>
</tr>
<tr>
<td>TSEB</td>
<td>0.1591</td>
<td>0.6847</td>
<td>0.0390</td>
</tr>
<tr>
<td>EF_2pm</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>SWEB-SVAT</td>
<td>0.3089</td>
<td>-0.2477</td>
<td>-0.1562</td>
</tr>
<tr>
<td>MWSDR</td>
<td>0.2328</td>
<td>0.1274</td>
<td>-0.1018</td>
</tr>
<tr>
<td>TSEB</td>
<td>0.2445</td>
<td>0.4495</td>
<td>-0.0370</td>
</tr>
<tr>
<td>EF_2pm</td>
<td></td>
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</tr>
<tr>
<td>(Active growth period)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>SWEB-SVAT</td>
<td>0.3963</td>
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<td>-0.3782</td>
</tr>
<tr>
<td>MWSDR</td>
<td>0.2756</td>
<td>0.6101</td>
<td>-0.2593</td>
</tr>
<tr>
<td>TSEB</td>
<td>0.0742</td>
<td>0.7089</td>
<td>0.0147</td>
</tr>
</tbody>
</table>

Figure 5.5 illustrates that TSEB results demonstrate a better fit ET observations during the active growth period (days 60-122) than other models predictions which is compatible with the statistics presented in Table 5.2.

On the other hand, soil moisture estimations derived from the WEB-SVAT and MWSDR models obtained at 2pm presented in Figure 5.6 show that the time series of root-zone soil moisture (\(\theta_{rz}\)) predictions of MWSDR are generally good comparing with observations.
while $\theta_{rz}$ estimations of SWEB-SVAT model demonstrate a large difference from the observed states especially from day 75 to day 120, which is a major portion of the active growth period.

Figure 5.5: Comparing daily ET estimations of TSEB with (a) SWEB-SVAT and (b) MWSDR models

Figure 5.7 presents the relationship between the root-zone soil moisture and EF for each of the three stages of growth period. Discrepancies between MWSDR and SWEB-SVAT illustrate different model parameterization of vertical coupling. Compared to the result of SWEB-SVAT, EF vs. RZSM reproduced by MWSDR exhibits much higher similarity with the observations. However, the observed EF vs. RZSM indicates that the coupling between EF and RZSM is significant only during dry portions ($\theta_{rz} < 0.10$) of the active growth period.

Figure 5.6: Soil moisture estimations of MWSDR and WEB-SVAT model comparing with observations

There are two major differences between the coupling of SWEB-SVAT model and the observed coupling; one is over-predicting coupling outside of the active growth period, that is, when soil moisture decreases, EF declines instantly regardless of the growth stage (e.g.
whether it is in the active growth or initial stage). The other difference is incorrect coupling (over-prediction) during the growing period when the soil is not dry. Observed coupling (Figure 5.7c) shows that during the active growth period EF and RZSM are correlated only when the soil moisture is lower than 10% while SWB-SVAT coupling (Figure 5.7b) shows that they are correlated even when the soil wetness is around 15%. On the other hand, improvements made to the MWSDR model, allow it to qualitatively match observed coupling patterns. In particular, the MWSDR model uses an NDVI-based canopy resistance, which tries to get maximum transpiration during the active growth period, but very low soil moisture in this period will finally result in low EF.

![Figure 5.7: Scatter plots of root-zone soil moisture versus EF at 2pm marked based on growth stages for (a) MWSDR model, (b) SWEB-SVAT model and (c) observations](image)

Although MWSDR-based soil moisture estimates present a good agreement with the observations, they may be further improved via the assimilation of TSEB-based EF estimates.

### 5.3.2. EF assimilation into SWEB-SVAT and MWSDR model

In this section, the results of using the inherent coupling of the models in both forecast and update steps of DA (section 2.2.1) are evaluated. The root-zone soil moisture predictions of EnKF implementation based on both SWEB-SVAT and MWSDR models are compared with vertically-integrated, top 1-m soil moisture observations for verification.
Figure 5.8: Daily time series of modeled root-zone soil moisture, observations, and results obtained from EF assimilation during the whole growing season into (a) SWEB-SVAT and (b) MWSDR models at 2pm. Dotted vertical lines indicate EF observation times.

Figure 5.8a compares EnKF results with the results of the open-loop SWEB-SVAT simulation (prior to data assimilation) and ground observations of RZSM at 2pm. Dotted vertical lines indicate EF observation times when updating occurs. Shaded region represents 2.5th to 97.5th percentile spread of ensemble members. Root-zone soil moisture predictions obtained from assimilating EF into SWEB-SVAT model show lower accuracy mostly during the active growth period comparing with the open loop. Since most of the difference between EF estimated from TSEB and SWEB-SVAT occurs during the active growth period (Figure 5.5a), the influence of DA during this period is more significant due to the larger innovations. Also based on Figure 5.7b, the strong correlation can be found between SWEB-SVAT-based EF and root-zone soil moisture during the active growth period even when the soil is not dry ($\theta_{rz} > 0.10$) while observed states (Figure 5.7c) are only correlated when the soil moisture is below 0.10. Since root-zone soil moisture analysis increments are computed based on the Kalman gain and the innovations ($K^t$ and $O^t - Y_i^t$) respectively in Eq. (5-17)), the size of the root-zone increment that results from a unit innovation is directly indicated by the Kalman gain. The Kalman gain includes the error covariance between the surface flux forecast and soil moisture in the root-zone layers ($C_{ym}$ in Eq. (5-18)) which is calculated from the ensemble at each update time. It shows that how much a surface observation can influence on the root-zone soil moisture through the assimilation update. Since the Kalman gain is calculated from the model ensembles, the spurious coupling of SWEB-SVAT model is reproduced and utilized in the DA system.
This excessive coupling leads to a high bias in the sampled $C_{ym}$ cross-covariance term obtained from the SWEB-SVAT forecast ensemble leading to large values of Kalman gain which makes the changes more significant during the active growth period. Consequently, the assimilation of EF fails to correct large underlying errors in SWEB-SVAT RZSM predictions.

Figure 5.9 represents the Kalman gain time series of SWEB-SVAT-based and MWSDR-based data assimilation. A 15-day moving window averaging was applied to original Kalman gain time series to produce a smoother graph. Comparing Kalman gain time series of both SWEB-SVAT- and MWSDR-based EnKF shows that the SWEB-SVAT model provides higher values of Kalman gain almost during the whole growing period. However, the Kalman gain produced from the MWSDR model is lower early and late in the season due to the reduced correlation between RZSM and EF in this period. Relatively large SWEB-SVAT-based Kalman gain between days 70 to 100 in Figure 5.9 justifies the large differences between open loop and updated soil moisture at the same period in Figure 5.8a. Although Kalman gain is also large at the end of the growing period, the innovations are almost small at the same time due to the small difference between EF derived from SWEB-SVAT and TSEB (Figure 5.5a); accordingly, they counteract each other’s influence on the results of EnKF and there is little difference between open loop and updated soil moisture late in the season as shown in Figure 5.8a.

![Figure 5.9: Kalman gain (low-pass filtered) time series of SWEB-SVAT- and MWSDR-based DA](image)

In addition to SWEB-SVAT DA results, MWSDR EnKF results also evaluated based on direct comparisons with the ground RZSM measurements at the OPE\textsuperscript{3} site. Figure 5.8b
compares the open-loop and updated RZSM of MWSDR with the ground observations. There is a noticeable improvement of the updated MWSDR RZSM during the active growth period (days 60-122) while the improvement appears to be insignificant during the other parts the season. This is likely the result of small correlation between EF and RZSM during the early and late seasons of growing period (Figure 5.7a). The other possibility is small difference between EF derived from MWSDR and TSEB (Figure 5.5b) leading to small innovation and trivial Kalman update. Relatively higher values of MWSDR-based Kalman gain between days 70 to 130 (Figure 5.9) comparing with other portions of the season in addition to large innovation values during this time (due to large difference between EF derived from MWSDR and TSEB showed in Figure 5.5b) make the differences between open loop and updated soil moisture more significant (Figure 5.8b); while both innovations and Kalman gain represent smaller values early and late in the season which provide very small updates in RZSM results.

Table 5.3 includes error statistics of data assimilation implementation using both MWSDR and SWEB-SVAT models. Comparing each data assimilation case with the open loop illustrates that assimilation of EF data in MWSDR model has a positive influence on the results of model while EF assimilation into SWEB-SVAT model reduces the accuracy of root-zone soil moisture predictions. Therefore, the benefits of modified MWSDR physics extend to both an enhanced background model and an enhanced EF assimilation. In other words, improved model physics has two separate benefits: i) it leads to a better open loop model (Table 5.2) and ii) it allows for the further improvement of the model via EF assimilation (Table 5.3).

Table 5.3: Error statistics of root-zone soil moisture predictions before and after EF assimilation into MWSDR and SWEB-SVAT models

<table>
<thead>
<tr>
<th></th>
<th>RMSE</th>
<th>R</th>
<th>Bias</th>
</tr>
</thead>
<tbody>
<tr>
<td>SWEB-SVAT</td>
<td>0.036</td>
<td>0.782</td>
<td>0.024</td>
</tr>
<tr>
<td>SWEB-SVAT-based DA</td>
<td>0.042</td>
<td>0.584</td>
<td>0.027</td>
</tr>
<tr>
<td>MWSDR</td>
<td>0.019</td>
<td>0.974</td>
<td>-0.016</td>
</tr>
<tr>
<td>MWSDR-based DA</td>
<td>0.013</td>
<td>0.957</td>
<td>-0.007</td>
</tr>
</tbody>
</table>

114
5.3.3. Implementation of data assimilation using an empirical observation operator

In this section the results of data assimilation based on the empirical observation operator (section 2.2.2) are evaluated. As it mentioned in section 2.3, this experiment aims to verify the effectiveness of an empirical observation operator for over-coming underlying model deficiencies. The root-zone soil moisture predictions of EnKF implementation based on both SWEB-SVAT and MWSDR models are compared with RZSM observations to estimate the error.

Figure 5.10 shows data assimilation results comparing with the results of SWEB_SVAT model (before data assimilation) and field measurements of root-zone soil moisture at 2pm. Since EF observations are assimilated only during the active growth period, the major change in the results can be seen between day 60 and 122. Generally, SWEB-SVAT-based DA fails regardless of which observation operator is used; as presented in the figure, linear-based DA estimates root-zone soil moisture worse than SWEB-SVAT model having higher difference with observed data whereas exponential-based DA does not change the results significantly. This is clear evidence showing that model physics deficiencies cannot be overcome by utilizing an empirically realistic observation operator.

![Figure 5.10: Daily time series of SWEB-SVAT root-zone soil moisture results, observations and results obtained from EF assimilation based on h from observed (a) linear, (b) exponential relationships at 2pm, dotted vertical lines indicate EF observation times](image)

Table 5.4 compares root mean square error (RMSE), correlation coefficient (R) and bias of SWEB-SVAT model with the results of assimilation using linear and exponential functions. While both methods illustrate worse results, linear method demonstrates considerable larger
error and lower correlation coefficient comparing with SWEB-SVAT estimations. Since the slope of fitted exponential function is less than the fitted linear function at higher EF range (Figure 5.2b), the unfavourable influence of linear-based DA is more significant.

Table 5.4: Error statistics of root-zone soil moisture predictions of EF assimilation into SWEB-SVAT model using linear and exponential functions based on observed correlation

<table>
<thead>
<tr>
<th></th>
<th>RMSE</th>
<th>R</th>
<th>Bias</th>
</tr>
</thead>
<tbody>
<tr>
<td>SWEB-SVAT</td>
<td>0.036</td>
<td>0.782</td>
<td>0.024</td>
</tr>
<tr>
<td>DA Results</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>(linear)</td>
<td>0.042</td>
<td>0.492</td>
<td>0.024</td>
</tr>
<tr>
<td>DA Results</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>(exponential)</td>
<td>0.037</td>
<td>0.657</td>
<td>0.021</td>
</tr>
</tbody>
</table>

Comparing the results of SWEB-SVAT-based DA method implemented based on observation operator (Table 5.4) with the results of DA implemented independent from $h$ (Table 5.3), indicates that both method provides worse results comparing with open loop case. The former method calculates the covariance matrices based on the model ensemble which concentrating more on the structure of the model. Since SWEB-SVAT model constructs a spurious linear relationship between EF and root-zone soil moisture (Figure 5.7b), its worse results is expected. Since the $h$-base data assimilation case provides the comparable results with this method, it shows that the impact of model structure is still high even when it is used just for the forecast state.

Figure 5.11 compares the root-zone soil moisture results of EF assimilation to MWSDR model with observations and MWSDR predictions. This figure includes the results of DA implemented using linear and exponential fitted functions to the relationship between observed EF and weighted soil moisture. Both methods provide similar results according to the error statistics represented in Table 5.5. According to the figure, first significant change to the soil moisture starts around day 70 for both cases while the start day of assimilated EF data is day 60 for the exponential case (start of active growth period based on NDVI). This period (between day 60 and 70) coincides with the time when EF is not sensitive to soil moisture due to non-stressed soil condition. Since there is no difference in the results of these two cases the only preference for exponential method is that there is no need to filter out EF data when the soil is wet. This is an important issue because finding the value of soil
moisture identifying the start of stress condition might be difficult; while applying an exponential function during the NDVI-based active growth period is easily applicable.

Figure 5.11: Daily time series of MWSDR root-zone soil moisture results, observations and results obtained from EF assimilation based on h from observed (a) linear, (b) exponential relationships at 2pm, dotted vertical lines indicate EF observation times

Table 5.5 shows no improvement in the correlation coefficient between estimated and observed soil moisture after applying data assimilation method. However, since the correlation coefficient of MWSDR model is quite high, DA is not able to further improve it, instead due to the error perturbation it is more likely to lose the correlation. However, on the other hand assimilation of EF observations improves RMSE of root-zone soil moisture around 40 percent and reduced the bias around 75 percent during the whole growing season. Comparing these results with Table 5.3 indicates that DA implemented based on the observed sensitivity between EF and soil moisture is more favourable than implementing DA based on the correlations calculated from the model structure. However, very close and similar results show that MWSDR model structure is good enough to be used in DA case regardless of the correlation in observed variables, because it can simulate similar correlation to the one provided from observations.
Table 5.5: Error statistics of root-zone soil moisture predictions of EF assimilation into MWSDR model using linear and exponential functions based on observed correlation

<table>
<thead>
<tr>
<th></th>
<th>RMSE</th>
<th>R</th>
<th>Bias</th>
</tr>
</thead>
<tbody>
<tr>
<td>MWSDR</td>
<td>0.019</td>
<td>0.974</td>
<td>-0.016</td>
</tr>
<tr>
<td>DA Results (Linear)</td>
<td>0.011</td>
<td>0.964</td>
<td>-0.004</td>
</tr>
<tr>
<td>DA Results (Exponential)</td>
<td>0.011</td>
<td>0.973</td>
<td>-0.006</td>
</tr>
</tbody>
</table>

5.4. Discussion and Conclusions

Using data assimilation technique is very popular in the field of root-zone soil moisture estimation, but it is very important to use it correctly to improve the estimations. Observations of surface variables are propagated into deeper soil layers using the land dynamic model of a data assimilation system. Since the parameterisation of subsurface dynamics of LSMs differs significantly, the selection of a proper model as the system’s model component plays a critical role in the propagation of surface information through data assimilation system. In this study, the effect of two land surface model physics on root-zone soil moisture estimations derived from assimilation of EF surface flux is investigated.

In order to evaluate the contribution of the observed EF surface flux in the data assimilation system, having a closer look at how surface flux is connected to the root-zone soil moisture in the model can help. Verifying changes of EF versus soil moisture reproduced by the model and comparing them with the relationship between observed EF and soil moisture can show the validity of the model overground-underground coupling. Comparing different subsurface schemes of two models through evaluation of this relationship demonstrates an exponential or piecewise linear relationship between MWSDR estimates of EF and soil moisture during the active growth period, while a strong linear relationship can be found between the SWEB-SVAT model estimations. On the other hand, OPE \(^3\) observations show that this relationship is highly conditional and changes based on the overall wetness of soil, vegetation biomass and plant phenology. Very close similarity between the correlations found in MWSDR model estimations and observations illustrates that this model parametrization is successful in capturing the right relationship by employing dynamic vegetation components. Adding dynamic root growth, non-uniform root distribution and
NDVI-based canopy resistance to the model have improved the dependency of evapotranspiration to both crop phenology and water stress in MWSDR model.

The comparison of the performance of different land surface models in response to the assimilation of surface flux observations presented in this study clearly demonstrates that the assimilation of EF flux provides improvements in MWSDR root-zone estimates. Using MWSDR model we find that EF assimilation improves the agreement of the simulated soil moisture to observed soil moisture from RMSE of 0.019 (without assimilation) to 0.013 (with assimilation). Even though SWEB-SVAT model illustrates a stronger relationship between surface variables and soil moisture, DA results based on this model do not show any improvement relative to the open loop.

Different structure of the prognostic models in terms of surface fluxes to root-zone states coupling, propagates the surface information differently into the root-zone layer. This propagation occurs in both the forecast and update steps of the data assimilation system. Improving model physics therefore enhances both the background forecast and the responsiveness of the model to data assimilation (see Table 5.3).

The importance of utilised model becomes more explicit when instead of inherent model coupling, empirical observation operators are applied in the update step. Using an observation-based empirical observation operator \( h \) in DA system in order to undermine the role of model physics with possible spurious coupling does not improve the results significantly. Regardless of what observation operator is employed, the superior vertical physics of the MWSDR model leads to better DA performance than the (less vertically accurate) SWEB-SVAT model. This shows that propagating the surface observations into the root-zone layer through the model physics even only in the forecast stage has a great role in the DA system. In the other words, although inherent coupling of the model does not contribute in calculating error covariances of the update step, its great influence on propagating the surface observations into the root-zone layer in the forecast stage does not let the DA system to improve the results.

It should be mentioned that although using an observation-based observation operator \( h \) in DA system does not provide better estimations using SWEB-SVAT-based DA, it prevents the system to provide worse results with high estimations error. MWSDR-based DA also
represents very slight improvement in the results when more accurate observation-based $h$ is used. However, these modest benefits must be weighed against the practical difficulties of obtaining such an operator.

Overall, utilising a systematically accurate background model is an importance component of a data assimilation system tasked with updating unobserved system states. Systematic errors in the assimilation model can prevent assimilation of surface information from having a beneficial impact on unobserved variables. Comparing the model-predictions relations with the observed ones can provide insights into the optimal choice of system’s model for data assimilation when the closeness of model subsurface physics to the truth is essentially unknown. Based on the results of this study the potential for improvement in DA estimations is generally higher if the subsurface physics exhibits the appropriate relationship between the modelled surface variables and root-zone soil moisture.

As a summary the results of this study show that TIR-based instantaneous surface energy flux estimations of a two-source energy balance-based land surface model (TSEB) are able to improve soil moisture through DA only upon a choice of an appropriate assimilation model.
6. CHAPTER 6: SUMMARY AND CONCLUSIONS

6.1. Overview

The aim of this thesis was to improve root-zone soil moisture estimation by integrating remotely sensed thermal and optical observations into land surface models. Evaporative fraction (EF), which was derived from thermal infrared (TIR) measurements used as input to the TSEB model, was assimilated into a WEB-SVAT model to improve the root-zone soil moisture predictions.

The core part of this research focused on quantifying the influence of the connection between the surface variables and root-zone soil moisture of the model on the efficiency of assimilation surface observations to update the root-zone moisture states. In order to find the sources of incorrect coupling between the surface variables and the root-zone states, several aspects of the model schemes were explored.

Firstly, the representation of root growth including dynamic rooting depth and distribution was incorporated to a simple WEB-SVAT model to improve the soil water processes of the model. An exponential root water uptake model with water stress compensation was adopted and incorporated to the model to establish a more appropriate soil-biophysical linkage between root-zone moisture content and above-ground states. The original model was modified to include more (4 or 5) layers to implement the vertical profile of root distribution.

In addition, phenological variation in canopy resistance was incorporated to the original model to investigate the impact of new parameterization of plants specifications on model performance.

In order to evaluate the impact of new parameterization of plants specifications (each proposed change) on model performance, three different cases were defined including: adding RS-based dynamic canopy resistance, adding multiple soil layers, adding dynamic root depth and distribution. The new developed model included all three of these changes. Soil moisture and latent heat flux estimations of each case were then compared with the original and new model and they were also evaluated against field observations.
Transpiration rate, soil evaporation rate and water uptake distribution of the original model and new-developed model were analysed to investigate the potential merits of considering the dynamic nature of plant growth in the modelling.

In the next step, this study examined the sensitivity of surface energy fluxes to soil moisture reproduced by the models. Ground observations are used to verify the relationship between root-zone soil moisture and observed evapotranspiration and evaporative fraction. The relationship captured by new model was compared with predictions obtained from the conventional simple WEB-SVAT model (lacking dynamic rooting) and evaluated against the ground observations. The effects of incorporating dynamic vegetation components to the model on the coupling between ET/EF and the root-zone soil moisture and the realism of biophysical and hydrological processes were explored by these comparisons.

The second part of this research was built on the first part and focused on the influence of reproducing more realistic coupling between root-zone soil moisture and surface variables on updating root-zone soil moisture through data assimilation technique. Both models were used and compared to investigate the influence of coupling on the efficacy of assimilating EF. Results of assimilating EF to both models were validated using independent ground-based profile soil moisture measurements.

Within this stage, in order to explore the role of dynamic model and its inherent coupling in the data assimilation system, two different experiments were implemented. In one experiment, model structure was used in both forecast and update steps of DA. In this case model structure and the coupling of the model had the greatest role in the DA system. The second scenario to run DA system was the use of an empirical observation operator estimated from the correlation between the observed surface fluxes and root-zone soil moisture. In this case coupling between surface fluxes and root-zone soil moisture in the model has less influence but still determinant role in the forecast state of the DA system.

6.2. Conclusions

The main findings of this thesis can be summarized as follows:
- TIR-based instantaneous evaporative fraction (EF) estimations of a two-source energy balance based land surface model (TSEB) are able to improve soil moisture through data assimilation only upon a choice of appropriate system’s model.

- Since the parameterisation of subsurface dynamics of LSMs differs significantly, the selection of a proper model as the system’s model component has an important role in the way of propagating surface information through data assimilation system.

- Overestimation of the coupling between surface variables and root-zone states (such as in the SWEB-SVAT model) does not guarantee higher efficiency for the data assimilation system. It forces the system to update the model state even when there is no real sensitivity between the model state and observed variable. This update will not always provide an improvement, on the contrary it may add more errors and inconsistency. As a result, a more accurate representing of the true coupling between surface fluxes and profile soil moisture can be more beneficial even if it shows a weaker surface flux–root-zone coupling.

- Comparing the correlation between model products with the correlation between observed variables can provide insights into the optimal choice of system’s model for data assimilation when the closeness of model subsurface physics to the truth is essentially unknown. The potential for improvement in DA estimations is generally higher if the subsurface physics exhibits a right correlation between the modelled surface variables and root-zone soil moisture. In other words, a land surface model with a coupling strength similar to the observations is perhaps a more robust choice for the system.

- Using an observation-based empirical observation operator \( (H) \) in DA system in order to undermine the role of model physics with spurious coupling does not improve the results significantly. Although inherent coupling of the model does not contribute in calculating error covariances of the update step, its great influence on propagating the surface observations into the root-zone layer in the forecast stage does not let the DA system to improve the results. However, this strategy may prevent the system to provide worse results with high estimations error. Overall, The Kalman gain is primarily determined by the model physics however the
parametrisation of DA system to calculate the error covariances may have a slight effect on it.

- More realistic coupling between root-zone soil moisture and surface energy fluxes in the model (like MWSDR) is attributed to the adequate representation of soil-vegetation-atmosphere processes in the model. Further details in the representation of vegetation dynamics and interactions between root depth and distribution with soil water content in the model leads to improvements in the root-zone estimations through the data assimilation technique.

- Although the overestimation of correlation between surface fluxes and soil moisture content is common in land surface modelling (like SWEB-SVAT), field observations show that this relationship is highly conditional on the vegetation biomass, plant phenology and net radiation. Also the overall wetness of soil at different stages of plant growth is very determinative for this correlation. Employing dynamic vegetation components such as dynamic root growth, non-uniform root distribution and NDVI-based canopy resistance can improve the dependency of evapotranspiration to both crop phenology and water stress which makes the model to be successful in capturing the right correlation resembling the observed correlation.

- Adding more sophisticated vegetation components to the conventional land surface models provides a substantial improvement in model estimates of profile soil moisture and evapotranspiration under high water stress conditions. It may not represent superior estimations when the overall soil wetness remains high during the growing period. On the other words, these modifications may lead to a consistent model performance under all conditions.

- Parameterization of root water uptake based on water stress compensation (which is applicable with dynamic root distribution) makes the crop root system capable of extracting more water from the wetter layers during the dry season; whereas in most land surface models, utilizing a lumped root layer with uniform redistribution of soil water – due to the assumption of uniform plant root distribution – may hamper the
simulation of soil water movement. These models just rely on the overall wetness of the whole depth and reduce water extraction under water-stressed condition.

- Although stratifying the soil profile to various soil layers is inevitable when adding a root growth component to the model, having multiple root layers in the model does not affect the final simulation of soil moisture unless the assumption of uniform root – and water uptake – distribution changes. It should be mentioned that this is a broad conclusion of this experiment in a particular study site that has to be quantified for different land cover, vegetation type and climate. On the other hand, this simulation of profile soil moisture using various soil layers is necessary for investigation of plant functioning at different stages of the plant growth.

- Estimating a dynamic canopy resistance based on the crop phenology and as a function of RS vegetation index, has a remarkable influence on the water extraction simulation of the model. This part of the model scheme enables the model to extract water and maintain high level of canopy transpiration in spite of the overall dryness of the soil profile. However, parameterising the canopy resistance solely as a function of profile soil moisture and neglecting the effect of crop phenology on transpiration strength may lead to spuriously high sensitivity of evapotranspiration to the root-zone soil moisture.

In summary, this thesis presents a significant contribution to the understanding of the needs for additional novel physics in the conventional land surface models to adequately capture the right relationship between surface fluxed and profile soil moisture across a range of crop growth stages. Results also show the importance of having an adequate representation of vegetation-related transpiration process for an appropriate simulation of water transfer in a complicated system of soil, plants and atmosphere. The developed model in this research could potentially be used either to predict root-zone soil moisture by itself or be utilised in a data assimilation system as a dynamic model to provide more accurate soil moisture prediction.
6.3. Challenges and recommendation for future work

There were a variety of the key challenges which can be discussed for the ways to improve the approaches and methods used in this thesis. One of the challenges found throughout this research comes from the general limitation of estimating root-zone soil moisture from thermal infrared data. Since surface temperature of vegetated area is affected by the moisture content available in the rooted layers of soil profile, if there is no growing or live vegetation, there is no way to estimate root-zone moisture content using surface temperature. On the other hand, verifying the correlation between surface fluxes and root-zone soil moisture under active growing season demonstrates enough sensitivity only under a certain level of water stress condition of this period. It means that root-zone soil moisture estimations can only be updated efficiently when surface flux products of RS methods or any other resources are supplied at critical range of soil moisture and vegetation activity. Sensitivity at a short range of soil moisture is a fundamental limitation for the applications of this relationship, however, the limited timespan of the sensitivity may represent the period when the root-zone soil moisture information is most needed. However, in the period of low or no vegetation, microwave remote sensing can fill the gap nicely, even though the resolution would be coarser comparing with thermal-based methods.

Another key challenge was concerns about simplifying the biophysical processes involved in the model. Development of a computational model for simulating a system describing ecological, hydrological, atmosphere and surface processes requires simplification of the processes involved in the system. In this research a land surface model was selected to be extended to incorporate dynamic vegetation root growth and density. Simulating the interaction of root depth and distribution with soil water content can be very complicated as some specific crop models have been developed for this purpose. In these models, vegetation growth such as root depth and density is dynamically simulated as a function of various parameters including soil moisture and temperature, crop and soil characteristics, climate and management variables such as irrigation and fertilizer application. However, incorporating such complicated root growth models to a land surface model which is a compound system of soil, plants and atmosphere, will make the original model more complex and some unexpected outcomes may be encountered. Accordingly, a relatively
simple exponential root water uptake model with water stress compensation was incorporated to the model which simulates the effects of soil properties and crop characteristics on root growth using an exponential equation as well as simulating soil water extraction by plant root. Although this model simplifies the whole process, it takes most of the key factors influencing on the plant root growth and distribution providing a satisfactory root water extraction scheme. More sophisticated biophysical models can be utilised instead; however, although these models may provide more detailed plant growth components, they include a higher demand for vegetation/crop-specific parameters, which is an important and challenging trade-off.

The new developed model in this work was evaluated for field-scale soil moisture estimates using tower-based input data. However, most applications in environment and hydrology require soil moisture estimates over larger spatial extents such as regionally or even globally. In order to apply the model at broader spatial scales, it needs to be implemented and verified at larger spatial support under diverse climatic and vegetation conditions. Incorporating the metrological data from data assimilation systems may resolve this limitation to examine a broader scale application. However, when the model is implemented at the spatial support scale, extra uncertainties originating from input forcing error and sub-grid-scale heterogeneity (in crop types and soil textural properties) can cause a significant degradation of the model performance. Moreover, the proposed methods including crop-specific root-growth and other general phenological characteristics utilised in MWSDR model need to be evaluated more rigorously over diverse crop, field and climatic conditions.

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Author/s:
Hashemian Rahaghi, Mahboobeh Sadat

Title:
Estimating root-zone soil moisture by assimilating remotely sensed biophysical states into modelling

Date:
2016

Persistent Link:
http://hdl.handle.net/11343/116016

File Description:
Estimating root-zone soil moisture by assimilating remotely sensed biophysical states into modelling