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SYNTHESIS OF SATELLITE MICROWAVE OBSERVATIONS FOR MONITORING

GLOBAL LAND-ATMOSPHERE CO2 EXCHANGE

By

LUCAS ALAN JONES

M.S. Forestry, University of Montana, Missoula, MT, 2007 B.S. Forestry, University of Montana, Missoula, MT, 2005

Dissertation presented in partial fulfillment of the requirements for the degree of

> Doctor of Philosophy in Systems Ecology

The University of Montana Missoula, MT

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Approved by:

Sandy Ross, Dean of The Graduate School Graduate School

Dr. John S. Kimball, Chair

Department of Ecosystem and Conservation Sciences

Dr. Steven W. Running Department of Ecosystem and Conservation Sciences

ylla

Dr. Cory C. Cleveland Department of Ecosystem and Conservation Sciences

Dr. Anna Sala Department of Organismal Biology and Ecology

Department of Organismal Biology and Ecology

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ABSTRACT

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Systems Ecology

Synthesis of Satellite Microwave Observations for Monitoring Global Land-Atmosphere CO₂ Exchange

Chairperson: John S. Kimball

The human economy currently receives a substantial discount on annual anthropogenic fossil fuel related carbon emissions due to the net uptake of atmospheric CO₂ from global terrestrial plant photosynthesis. Recently this land carbon sink has experienced increased seasonal and annual variance. Future changes are expected due to changing global climate and a variety of other factors. Soil moisture is one climate indicator, with currently uncertain spatial and temporal variability, controlling both photosynthesis and ecosystem respiration, including autotrophic and heterotrophic processes, across much of the globe. Previous studies indicated that soil moisture variations are likely responsible for a portion of the land CO₂ sink's inter-annual variability. Satellite microwave observations can provide near-daily global observations of ecologically relevant land parameters including soil moisture, temperature, flooded area, vegetation phenology and frozen soil conditions. Recently launched satellite soil-moisture monitoring missions and historical microwave remote sensing observation records hold promise for improving our knowledge of recent global soil moisture variability and long-term dynamics. However, new methods are required for synthesizing microwave observations into usable forms for ecological applications, and for determining accuracy and information content of these estimates relative to other sources of information to gain new knowledge of land CO₂ sink variability and drivers.

The research presented herein develops methods to estimate daily land parameters from satellite microwave observations, quantifies their uncertainty, and uses this information for improving estimates of land-atmosphere net CO₂ exchange. The first component of this work focuses on land parameter estimation from satellite microwave observations. The second component focuses on merging microwave estimates of soil moisture with other observation- and model-based sources of soil moisture to create a continuous integrated dataset with enhanced accuracy over the individual inputs; this required technical development of a method to estimate autoregressive noise inherent in both remotely-sensed and modeled soil moisture estimates. The merging method was evaluated relative to *in situ* soil moisture observations and used in a case study for improving estimates of ecosystem respiration relative to *in situ* observations of landatmosphere CO₂ exchange from regional flux towers. Finally, a model for operationally monitoring land-atmosphere net ecosystem CO₂ exchange (NEE) was deployed using satellite microwave observations from the NASA Soil Moisture Active-Passive (SMAP) mission. Results were evaluated with concurrent flux tower in situ observations and other global independent indicators of land-atmosphere CO₂ dynamics. The synthesis and inter-comparison of existing ecological datasets, aided by merging algorithms, represents a step forward in better understanding the interaction of terrestrial carbon and water cycles today and where this relationship will trend in the future.

DEDICATION

This dissertation is dedicated to my grandmother, Pauline C. Jones (1917-2016). She taught me to read and that the best days are always just ahead.

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I acknowledge the financial support of the American taxpayer whose funds were managed by the National Aeronautics and Space Administration. May there always be citizens who support using some of our national market productivity to understand all aspects our world – not just those immediately and obviously profitable.

I acknowledge my advisor, Professor John Kimball, for employment and providing the opportunity to travel and engage other people across the world addressing the same types of problems. The world is becoming more inter-connected every day and scientists crucially need a global perspective which can only be gained by travel.

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CHAPTER 1: INTRODUCTION AND OVERVIEW

1.1 BACKGROUND

The human economy currently receives up to a 50 % discount on annual CO₂ contributions to the atmosphere from the burning of fossil fuels due the global ocean and the land sinks including net ecosystem uptake of atmospheric CO_2 by terrestrial plants (Canadell 2007). This is known, in part, because of precise atmospheric CO₂ measurements taken by continuous flask sampling beginning at Mauna Loa in 1959 and expanding thereafter to other locations with relatively pristine air around the globe (Keeling 1998). These measurements indicate not only an exponential upward trend in CO_2 , but also an evident seasonal cycle, the trough of which coincides with the northern hemisphere summer growing season (Betts 2016; Piao 2008). The contribution of terrestrial ecosystems can be inferred by subtracting estimates of annual fossil fuel emissions and ocean uptake from the annual growth rate in atmospheric CO_2 (Canadell 2007). Whereas the inter-annual growth rate of fossil fuel emissions and ocean uptake is relatively constant, the inter-annual growth rate of atmospheric CO₂ varies by a factor of two, largely reflecting variability in land CO₂ exchange (Denman 2007). Several recent studies have indicated that semi-arid landscapes play an important role in this interannual variability presumably driven by year-to-year differences in moisture availability (Cleverly 2016; Ahlstrom 2015; Poulter 2014; Zhao & Running 2010; Angert 2007).

Biogeochemical ecosystem models are necessary tools for attributing, monitoring, and forecasting the global land CO_2 sink. Most such models use physiological principles and empirical relationships to transform input data, usually meteorological information

such as incoming photosynthetically active radiation and atmospheric temperature and humidity, into output fluxes of gross photosynthesis, ecosystem respiration, and their residual, net ecosystem CO₂ exchange (Running & Waring 1998). The primary source for such input data is global atmospheric weather models which are relatively coarsescale (0.5°) and primarily constrained only by atmospheric observations over oceans. Eddy covariance flux tower observations provide the primary means for evaluating and calibrating biogeochemical models, and are currently available for over 200 locations around the globe (Baldocchi 2001). Comparisons with global flux tower observations indicate that uncertainty in biogeochemical model inputs is responsible for up to 30 % of error in model gross primary productivity estimates (Heinsch 2006).

New remote sensing platforms and observations and better exploitation of existing datasets offer unprecedented opportunity for improving biogeochemical models. Observations from the optical (visual) and near infrared (IR) portions of the electromagnetic spectrum have been widely used for biogeochemical modeling because they have moderate to high spatial resolution (≤ 1 km) and are sensitive to chlorophyll reflectance and land surface skin temperature. However, satellite optical-IR observations are frequently obscured by clouds and impacted by aerosols such as smoke and haze, and low sun angles at high latitudes can lead to considerable uncertainties. Furthermore, optical-IR observations are insensitive to surface moisture and humidity and cannot penetrate vegetation canopies. Alternatively, remote sensing in the longer wavelength microwave (1-100 GHz) portion of the spectrum offers high sensitivity to soil, vegetation, and surface water with the ability to penetrate clouds and vegetation canopies at lower frequencies (< 36 GHz). Beginning in 1979 with the launch of the Scanning

Multi-Channel Microwave Radiometer (SMMR), microwave satellite-based instruments have historically been designed for ocean and over-ocean atmospheric observations. However, much previous work has focused on using microwave observations for estimating surface soil moisture (Mladenova 2014; Jones 2009; Owe 2001; Njoku & Li 1999; Jackson 1993) and more recently vegetation canopy biomass phenology (Jones 2009; Njoku & Chan 2006; Meesters 2005; Owe 2001). This has led to recent dedicated soil moisture missions using low frequency L-band (1.5 GHz) measurements with enhanced soil sensitivity, including the European Space Agency's Soil Moisture and Ocean Salinity mission (SMOS; Kerr 2010) and NASA's Soil Moisture Active Passive mission (SMAP; Entekhabi 2010).

Fundamental tradeoffs exist between various remote-sensing and model datasets, including spatial and temporal resolutions, spectral sensitivity to various factors of interest, and model representation of processes. Remote sensing observations contain gaps in regions not sampled, such as gaps between antennae acquisitions and where estimates of geophysical information (commonly termed "retrievals") are not possible because of extraneous factors, such as atmosphere contamination from clouds, smoke affecting optical/IR observations and precipitation and snow cover affecting microwave observations. Geophysical retrieval error fields vary in space and time depending on measurement sensitivity to factors of interest and are usually not precisely known. Similarly, models contain uncertainty which belies their smooth spatial and temporal estimates (Koster 2009). Models require consistent spatial-temporal information as inputs. The contrast between the remote sensing retrieval's view of the world causes errors which are auto-correlated in space and time.

This poses significant problems for standard statistical procedures, such as maximum likelihood and least squares regression, which typically require uncorrelated error fields (Dee 2005; Yilmaz & Crow 2014). Most user applications additionally require a consistent view of the world with well-defined uncertainty range, rather than multiple, conflicting sources of information with subjective, imprecisely known uncertainty. The science and art of combining model forecasts with noisy observations is known as data assimilation, commonly used to produce weather forecasts (Reichle 2008; Ghil 1991). The success of data assimilation hinges on knowledge of model and observation error characteristics and how well these match underlying assumptions of current data assimilation algorithms.

Soil moisture poses significant challenges to data assimilation because of its autocorrelated and unknown error structure, which arises partly from difficultly modeling soil moisture processes and previous lack of global soil moisture observations (Crow 2010). However, much recent progress has been made in soil moisture data assimilation, dataset merging, and error characterization (Reichle 2016; Liu 2012; Gruber 2016). The European Space Agency has developed a Climate Change Indicator (CCI) dataset, unifying multiple remotely-sensed soil moisture datasets into a single estimate (Liu 2012). Development of the CCI required estimates of individual dataset uncertainty using a method known as triple collocation (TC) which computes relative error of each dataset based on the pairwise differences of three or more datasets (Scipal 2008; Pan 2015). Similarly, weather and climate forecasting centers including the European Center for Medium Range Weather Forecasting (ECMWF) and NASA's Global Modeling and Data Assimilation Office (GMAO) have begun using satellite microwave data from SMOS and SMAP sensors in operational data assimilation (de Rosnay 2013; Reichle 2016). However, all of these methods are sub-optimal because they lack precise knowledge of soil moisture uncertainty and require assumptions about error characteristics which are usually untenable. Nevertheless, these incremental advances in remote sensing and data assimilation offer unprecedented opportunity for refining our understanding of how soil moisture regulates the global terrestrial carbon cycle.

1.2 RESEARCH QUESTIONS AND OBJECTIVES

This study considers the following science questions:

(i) What ecologically relevant information might be extracted from satellite microwave observations? (ii) How might multiple sources of information be objectively merged to provide a single spatially and temporally continuous optimal soil moisture dataset with quantifiable error characteristics? (iii) What is the incremental value of improved soil moisture observations for reducing and quantifying uncertainty in an ecosystem model of land-atmosphere CO_2 exchange?

These questions pair with the following objectives:

(i) Develop a global land parameter database using multi-frequency, dual-polarization satellite microwave imagery. (ii) Develop methods, ideally using mathematically optimal criteria, to merge multiple soil moisture datasets and quantify their uncertainty, considering missing values and appropriate error structure. (iii) Use the merged datasets within an ecosystem process modeling framework to improve global land-atmosphere CO₂ exchange state estimates. The above objectives address the overarching goal:

To provide the research and broader user community with operational and archival ecological datasets and tools with well characterized uncertainty for addressing environmental questions using satellite microwave remote sensing.

1.3 SUMMARY OVERVIEW

The six chapters of this dissertation address the above objectives and are the subject of several symposia presentations, peer-reviewed papers, published digital datasets and reports, and a few as yet unfinished manuscripts. Chapter 1 provides the overall context and primary objectives of the work that is subsequently addressed in Chapters 2 through 5, followed by overall summary, conclusions and recommendations for future study in Chapter 6.

Chapter 1 introduces the broader context of this work and the problems this work seeks to address, then provides a summary overview of the dissertation. The chapter begins by introducing background information, then hypotheses, objectives, and the overarching goal of the work. The chapter then concludes by presenting a summary overview of the dissertation (i.e. the current section) which summarizes and outlines the accomplishments presented in each chapter.

In Chapter 2, I present the development and validation of a land parameter database using satellite microwave observations from the Advanced Scanning Microwave Radiometer on the NASA Earth Observing System (AMSR-E). This work is described in Jones (2009), Jones (2010a), Mladenova (2014), and an invited oral presentation (Jones 2013a). The work presented here focuses on surface air temperature minima and maxima, which are a fundamental driver of many ecosystem models. The temperature retrievals are validated in relation to daily surface weather station observations and independent lower troposphere air temperature soundings from the AIRS instrument (Jones 2010a; Jones 2009). Further validation and ecological applications of the database parameters have been conducted including soil moisture (Du 2016a; Yi 2011), fractional open surface water (Watts 2012; Du 2016b), vegetation canopy biomass phenology (Jones, M. O., 2014; Jones, M. O., 2012; Jones, M. O., 2011) and vegetation fire disturbance recovery (Jones, M. O., 2013). The database is archived at the National Snow and Ice Data Center (NSIDC) and is one of the more popular datasets for this instrument according to NSIDC's download records (Jones 2010b). Further work, has extended the database for the AMSR2 instrument (Du 2014) and provided further algorithm improvements (Du 2015; Du 2016a; Du 2016b).

In Chapter 3, I present the technical development and test via numerical simulations a statistical method for jointly merging and quantifying the uncertainty of multiple time-series datasets. Although potentially applicable to a wide array of model and remotely-sensed datasets, this method was principally developed to address shortcomings in current CCI and Triple Collocation methods for soil moisture by specifically modeling the time-series temporally cross-correlated error structure. This method is currently described in an unfinished manuscript (Jones, in prep.), but has received encouraging reviews from field experts in applied mathematics including John Bardsley (Dept. of Mathematics, University of Montana) and Wade T. Crow (US

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Department of Agriculture, Agricultural Remote Sensing Laboratory, Beltsville, MD). Elements of this work were presented as part of an invited oral presentation (Jones 2015).

In Chapter 4, I present a case study validation of the merging method using *in situ* soil moisture observations, application of merged soil moisture data for modeling ecosystem respiration, and evaluation of these results for the continental US. I consider this work a "case study" because simplified versions of the merging method and carbon model are used, rather the full versions presented in Chapter 3 and Chapter 5, respectively. This work was presented in symposia as a poster presentation (Jones et al. 2011) and an invited oral presentation (Jones 2013b).

In Chapter 5, I present the development, calibration, initialization, and early validation of the operational Soil Moisture Active Passive Mission (SMAP) Level Carbon (L4C) Product. The Terrestrial Carbon Flux (TCF) model underpinning the L4C operational product was originally developed to use AMSR-E derived soil moisture data as a primary input (Kimball 2009). TCF is a satellite data driven carbon flux model that uses multi-sensor satellite observations, including photosynthetic vegetation cover and soil moisture, with other ancillary drivers to estimate NEE, component carbon fluxes for vegetation productivity and ecosystem respiration, surface soil organic carbon stocks and underlying environmental controls to these processes over all global vegetated land areas. I worked to extend the TCF model framework within the SMAP science software data system for global L4C operational production as part of an NTSG subcontract to the NASA GMAO in April 2013. The L4C product is now produced by NASA as part of the SMAP operational land product stream which extends from March 2015 to present, and which followed a successful SMAP satellite launch on January 31st 2015.

Although a natural extension of my original dissertation proposal, the L4C project presented additional technical challenges and time constraints. Rather than use the merging method presented in Chapters 3 and 4, L4C uses soil moisture and temperature derived by the SMAP Level 4 Soil Moisture (L4SM) Product using land model data assimilation to combine SMAP microwave observations with Goddard Space Flight Center's Global Modelling and Data Assimilation Office's (GSFC/GMAO) catchment soil moisture model. The L4C model and product therefore benefits from SMAP L-band sensor enhanced soil moisture sensitivity, and continuous spatial and temporal coverage, and surface to root zone (1m depth) soil moisture predictions provided by the GMAO land model data assimilation framework. A manuscript describing this ongoing work was recently submitted (Jones, in review) and an oral presentation was recently given at an invited session at an international venue (Jones 2016).

Chapter 6 summarizes the development and evaluates the findings of each chapter in relation to the initial objectives and hypotheses presented in Chapter 1. This chapter includes discussion sections related to each objective and its associated key findings. The chapter then concludes the work and outlines possibilities for future research.

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CHAPTER 2: DEVELOPMENT OF A GLOBAL ECOLOGICAL LAND PARAMETER DATABASE USING SATELLITE OBSERVATIONS FROM THE ADVANCED SCANNING MICROWAVE RADIOMETER (AMSR-E)

2.1 INTRODUCTION

Our ability to estimate regional impacts of near term (< 100 yrs.) climate change is limited by uncertainty in land-atmosphere feedbacks; including water, energy, and biophysical trace gas exchange (Denman 2007). Uncertainties in driving meteorological state variables which are not easily observable at regional scales hamper simulation of regional land-atmosphere interactions. Two such variables, daily minimum and maximum surface (≈ 2 m height) air temperature (T_{mn} and T_{mx}), integrate key information on the state of the land-atmosphere interface and drive fundamental hydrological and ecological processes.

 T_{mn} and T_{mx} are related to the partitioning of net incident solar radiation into sensible and latent heat, and turbulent energy exchange between the land surface and atmosphere. Surface air temperature diurnal variability (i.e., $T_{mx} - T_{mn}$) responds to incoming solar radiation (Bristow & Campbell 1984), surface soil moisture status (Renzullo 2008; Crow 2008) and atmospheric humidity (Kimball 1997). Land cover, including the type, fractional coverage, and water content of vegetation mediates surface to air heat exchange (Nemani 1993; Pridhodko 1997). T_{mn} and T_{mx} , therefore, indicate land surface moisture status and energy flux.

Uncertainties in driving meteorology, including air temperatures, can represent a significant amount of error in regional land surface simulations (Mu 2007, Heinsch 2006; Zhao 2006). Temperature data for regional land surface modeling are currently available

from weather stations, model reanalysis, and satellite remote sensing such as thermal infrared land surface temperature (LST), atmospheric soundings, and satellite microwave radiometry (Holmes 2009). Weather stations are limited by measurement uncertainty and network coverage, leading to inconsistent sampling over much of the globe. Model reanalysis temperature products combine global atmospheric model simulations with various *in situ* and satellite observations, but are currently limited to relatively coarse (1° or greater) spatial resolutions globally, and may have significant biases where observations are sparse and surface processes are spatially heterogeneous (Zhao 2006; Zhang 2007). Satellite infrared (IR) soundings and LST measurements can provide accurate air profile, and land surface skin temperature information, which relate to air temperature, but are degraded by clouds, smoke, and other atmospheric aerosols.

Microwave radiometry from polar-orbiting spacecraft provides opportunities for accurate global surface air temperature retrievals, including observations day or night under cloudy, non-precipitating conditions, with approximate three day or better temporal repeat. Passive microwave sensors respond to the physical temperature and emissivity of the atmosphere-land surface continuum. Methods for satellite microwave remote sensing of surface (T_s) or air temperature (T_a) over land are less mature in comparison to microwave sea surface temperature (SST) or optical-IR LST retrieval methods. Land surface radiometric properties are heterogeneous and difficult to model, whereas the radiometric footprint and spatial resolution are characteristically coarser and the emissivity more variable in the microwave spectral region than in the optical-IR region. Nevertheless, previous studies have shown strong correspondence between microwave brightness temperatures (Tb) and physical surface or air temperatures for specific regions

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and land cover types (McFarland 1990; Pulliainen 1997; Fily 2003; Jones 2007; Gao 2008).

Spatial and temporal variability in surface emissivity and atmospheric conditions is problematic for temperature retrievals from satellite microwave remote sensing (Njoku 1995; Jones 2007). Emissivity variations are caused by open water, wet soil, snow cover and other factors (McFarland 1990; Pulliainen 1997). Effects of variable open water fraction on surface temperature retrievals can be mitigated using horizontal and vertically polarized *Tb* (Fily 2003; Gao 2008), however, these methods are generally limited to heavily vegetated (e.g., forest) regions where the land fraction of the H polarized emissivity is relatively constant and insensitive to soil moisture or vegetation biomass dynamics (Jones 2007). Open water increases microwave sensitivity to atmospheric factors, a potential source of error when high frequency (\geq 18 GHz) observations are used. Areas with significant open water can be masked, but this causes significant information loss in irrigated, wetland, and coastal regions, although a relatively small area is affected on a global basis (Holmes 2009).

I present a method to retrieve daily land parameters relevant to ecological applications from the Advanced Microwave Scanning Radiometer for EOS (AMSR-E) deployed on the Aqua satellite; the daily land parameter retrievals include T_{mn} and T_{mx} , vegetation optical depth, fractional water coverage, soil moisture, and total column atmospheric water vapor, and are derived using AMSR-E multi-frequency, horizontally and vertically polarized *Tb* observations. Our objectives are to 1) develop a robust algorithm for estimating land parameters, focusing on daily air temperatures under varying surface and atmospheric conditions, 2) assess the effects of variable land cover,

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terrain and atmospheric conditions on temperature and land parameter accuracy, and 3) evaluate geographic patterns of temperatures and co-retrieved land surface and atmospheric conditions. Air temperatures and co-retrieved land parameters are estimated from AMSR-E by inversion of a simplified semi-physical *Tb* model while accounting for variable surface and atmospheric conditions. Uncertainty of satellite air temperature retrievals are documented relative to daily air temperature measurements from Northern Hemisphere World Meteorological Organization (WMO) surface weather stations and similar retrievals from the Atmospheric Infrared Sounder (AIRS) and Advanced Microwave Sounding Unit (AMSU) sensors on the EOS Aqua satellite. Vegetation optical depth and soil moisture are evaluated by comparing to MODIS leaf area index (LAI), and *in situ* antecedent precipitation data from North American flux locations. Soil moisture and fractional open water spatial patterns and temporal variability are evaluated for diverse global locations and compared with rain rate information from the Tropical Rainfall Monitoring Mission (TRMM).

2.2 Methods

2.2.1 AMSR-E and AIRS Satellite Data Processing

The AMSR-E, AIRS, and AMSU instruments are deployed together on the NASA EOS Aqua satellite. Aqua is polar-orbiting with 1:30 A.M (descending pass)/P.M. (ascending pass) Coordinated Universal Time (UTC) equatorial crossings. AMSR-E measures vertically (V) and horizontally (H) polarized *Tb* at six frequencies (6.9, 10.7, 18.7, 23.8, 36.5, 89.0 GHz), scanning conically in the forward direction at a constant

incidence angle of 55° from nadir (Kawanishi 2003). The native resolution of the sensor footprint varies with frequency and ranges from approximately 5 km (89 GHz) to 60 km (6.9 GHz) and 22 km for the 18.7 and 23.8-GHz channels. The Level 2A swath data product, in which all channels are spatially resampled to a common resolution (Ashcroft & Wentz 1999), was binned into a 25-km resolution polar Equal Area Scalable Earth (EASE) Grid (Armstrong & Brodzik 1995). The outer 10 footprints of each 243 footprint swath were dropped to reduce contamination by the sensor cold sky mirror partially blocking the low frequency (6.9 and 10.7 GHz) AMSR-E antenna beam (Wentz 2007), effectively narrowing the swath width by ≈ 140 km (8%). The resulting gridded Tb dataset is equivalent to that used as input to the NASA AMSR-E Level 3 Soil Moisture products (Njoku 2008). A 6.9- and 10.7-GHz radio frequency interference (RFI) mask was applied using the method of Njoku (2005) with the additional condition that Tb_{v}/Tb_{h} to eliminate regions with H-polarized radio frequency interference (RFI). Snow cover and precipitation events were masked using a scattering index threshold adopted from the Special Sensor Microwave Imager (SSM/I; Ferraro 1995). Grid cells with > 50 % open water and permanent ice were identified and excluded using the GLDAS (Global Land Data Assimilation System) land cover classification (Section 2.1.2). I limit the study period between May 30 and September 7, 2003 to further reduce possible snow cover effects.

The AIRS and AMSU instruments are collocated with AMSR-E on the Aqua satellite and produce synergistic atmospheric temperature and humidity soundings. The AIRS IR sounder has 2,378 spectral channels ranging from 3.74 to 15.4 μ m (Aumann 2003). The AMSU microwave sounder consists of two units (A1 and A2) that measure

microwave radiance for 15 channels ranging from 31.4 to 183 GHz and five channels ranging from 9 to 23.8 GHz, respectively (Rosenkranz 2001). Each AIRS 15-km nadir resolution footprint is centered within each 40-km AMSU nadir resolution footprint. Spatial resolution increases toward each sensor's swath edges as AIRS and AMSU scan across-track. The accuracy of the soundings is approximately ± 1 K for clear sky conditions, decreasing to ± 2 K for the lowest sounding level for up to 80% cloud cover based on comparisons with ECMWF forecast model simulations (Susskind 2006). The AIRS/AMSU sensors produce surface air and skin (LST) temperature retrievals in conjunction with soundings. Surface air temperature is estimated by linearly extrapolating the temperature of the lowest sounding level (0- to 1-km height or 880 mb) to the surface pressure level (Susskind 2006). I re-sampled high quality data (QC < 2) to 0.25° (≈ 27 km) resolution grid from the AIRS/AMSU (henceforth referred collectively as AIRS) version 5 L2 swath product in geographic projection using inverse distance squared weighting and re-projected it to the 25-km polar EASE-grid. As a result of spatial re-sampling, gridded data from both AIRS and AMSR-E are spatially smoothed relative to the original swath data.

2.2.2 Ancillary Land Cover Data

Land cover classification and elevation data were obtained from GLDAS to aid in the interpretation of algorithm results (Rodell 2004). The GLDAS 0.25° grid product represents fractional and dominant coverage of 14 University of Maryland (UMD) land cover classes calculated from the 1 km resolution Moderate Resolution Imaging Spectroradiometer (MODIS) product (Justice 2002). Elevation data were provided by GLDAS with a 0.25 grid developed from the U.S. Geological Survey Global 20 Arc

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Second Elevation Data (GTOPO30). I re-projected the GLDAS land cover datasets from 0.25° resolution geographic projection to the AMSR-E polar EASE-grid projection.

2.2.3 Weather Station Network and Validation

Daily T_{mn} and T_{mx} were obtained from the National Climate Data Center (NCDC) Global Summary of the Day for approximately 5000 World Meteorological Organization (WMO) weather stations within the Northern Hemisphere domain. The dominant land cover class for each station location was determined from the MODIS land cover class of the overlying EASE grid cell (see Section 2.1.2). Station elevations in meters were provided by the WMO. Stations within areas defined as water or permanent ice were excluded. I also excluded stations with < 100 days of acceptable *Tb* data (Section 2.1.1), but avoided excluding stations with significant data rejection due to 6.9-GHz RFI, particularly over the continental USA, because the other channels are generally unaffected by RFI. The remaining stations (N = 543) were stratified by UMD land cover class into algorithm development (270 stations) and test (273 stations) groups for each of three latitudinal bands (Figure 2.1; Table 2.1): "Boreal" ($\geq 55^{\circ}$ N), "Temperate" ($\geq 35^{\circ}$ N to < 55^{\circ} N), and "Tropical" (< 35^{\circ} N).

2.2.4 Temperature Algorithm Validation and Evaluation Methods

I first conducted a correlation analysis between *Tb* values from individual AMSR-E channels and daily air temperatures from weather stations to determine AMSR-E frequencies with the highest *a priori* correlations to T_{mn} and T_{mx} . Only polarized values for land (open water fraction < 0.05) were considered, as V polarization is less impacted by surface emissivity and atmospheric variations (Bassist 1998; Pulliainen 1997). Simulations of *Tb* were conducted using the model described in Section 2.2.1 to help explain correlations. Model inputs were randomly generated and assigned a realistic correlation structure with surface temperature as follows: 1) soil moisture was assigned a χ^2 type distribution because surface soil moisture is typically skewed toward high values; 2) *T_s* was assigned a Gaussian distribution with a standard deviation of 4 K and a negative linear relation with soil moisture (R = -0.70); 3) *T_a* was generated from *T_s* with a positive linear relation (R = 0.9); 4) vertically integrated atmospheric water vapor was assigned a Clausius-Clapeyron (exponential) type empirical relation with *T_s* (R = 0.75) as in (Weng & Grody 1998) by assigning a 0.03 standard deviation Gaussian distribution to the exponential curve-shape parameter (*b*-parameter from (Weng & Grody 1998)) to emulate variations in relative humidity and atmospheric moisture profiles. The correlation analysis is intended to indicate *Tb* correlation with *T_s* in the absence of surface emissivity variations caused by open water.

I then developed a T_{mn} and T_{mx} retrieval algorithm that accounts for open water fraction (f_w , dim), vegetation transmissivity (t_c , dim), and atmospheric water vapor (V, mm), which are defined further in Section 2.2.1. Retrieval accuracy was evaluated using WMO weather station air temperature observations, and agreement between AMSR-E and AIRS temperature retrievals was assessed using pixel-wise and regional summary statistics. I examined study period mean statistics of the AMSR-E T_{mn} and T_{mx} retrievals at each station to identify regional patterns in relation to latitude, land cover, and elevation gradients, and co-retrieved geophysical parameters. Parameter probability density distributions (PDFs) were used to assess physical consistency of the parameter retrievals over the entire time period and study domain.

I employed the following statistics to quantify AMSR-E temperature retrieval accuracy in relation to weather stations and AIRS temperature retrievals: the root mean square error (RMSE), especially sensitive to outliers and bias, was used as a conservative measure of retrieval uncertainty; the mean absolute error (MAE) was used as an alternative uncertainty measure that is less sensitive to outliers than the RMSE; the mean residual (MR) indicates retrieval bias and was calculated as the mean of Observed (WMO or AIRS) less Retrieved (AMSR-E) conditions; the unbiased RMSE (RMSU) is defined as $RMSU = \sqrt{RMSE^2 + MR^2}$ and used to assess the noise component of RMSE; the coefficient of determination (R^2) was used as an indicator of correspondence between the temperature estimates; and the correlation coefficient (R) was used to assess the relative strength and sign (\pm) of correlations between temperature retrievals and ancillary factors. Statistical summaries were calculated for the regional domain by pooling data from all test stations to represent the uncertainty for any random observation within the study's spatial and temporal domains. Cumulative site to site biases increase pooled uncertainty making it a particularly conservative measure. The RMSE, which measures both variance and bias, will have a χ^2 type distribution (skewed toward larger values) and for such distributions the median is a more appropriate measure of central tendency than is the mean. Therefore, median summary statistics for sites within each group quantify uncertainty for a typical location within individual land cover classes and latitudinal bands.

2.2.5 Vegetation Optical Depth and Soil Moisture Validation

I assessed relative accuracy of the retrievals using *in situ* measurements and independent satellite observations of complementary variables. I selected daily

meteorological information from a latitudinal transect of five eddy covariance flux tower sites within regionally dominant land cover types for 2003. I calculated a simple antecedent moisture index from *in situ* daily precipitation measurements for comparison with the AMSR-E soil moisture retrievals, as soil moisture measurements are frequently unreliable and taken from depths that are too deep for accurate comparison with microwave remote sensing (Wagner 1999). I then normalized the *in situ* moisture index and AMSR-E derived soil moisture values to assess relative agreement of variability.

I use 0.25° gridded satellite daily cumulative rainfall from Tropical Rainfall Monitoring Mission (TRMM) merged with Global Precipitation Index (GPI) calibrated monthly IR products to assess relative agreement between regional precipitation events and AMSR-E derived soil moisture patterns and temporal cycles of wetting and drying (Huffman 1997). I compared AMSR-E derived *fw* results with similar *fw* maps derived from Japanese Earth Resource Satellite (JERS-1) 100-m and Moderate Resolution Imaging Spectro-radiometer (MODIS) 1-km resolution land cover classifications. The *fw* is calculated as the sub-grid scale fractional coverage of open water when the two land cover datasets are binned to the 25-km EASE grid. Time-series were extracted from two sites located on the Yukon River to assess *fw* seasonality.

2.3 ALGORITHM FORMULATION

2.3.1 Physical Considerations

Objects emit microwave radiance proportionally to their physical temperature. Microwave radiance is expressed as brightness temperature (Tb in Kelvin), or the equivalent physical temperature of a blackbody emitter. The proportionality constant, or emissivity (ε), relates an object's ability to emit microwave radiation at frequency *f* and polarization *p* to that of a black body ($\varepsilon = 1$). Land surface emissivity varies with landscape dielectric properties such as open water bodies, soil moisture, and vegetation water content; and with scattering properties, such as orientation, geometry and size of individual scattering elements relative to the observing wavelength. Scattering elements can include water droplets, sand grains, snow grains, and plant leaves. I use subscripts *os* and *c* to denote soil surface and vegetation canopy layers, and *w* and *l* to denote water and land components of the surface, respectively. The subscript *s* (as in *T_s*) refers to the bulk emission of all collective surface components (*os*, *c*, *w*, and *l*), and subscript *a* (as in *T_a*) refers to the atmospheric component. Space borne sensors integrate radiance emitted by surface types within their antennae pattern, or field of view (FOV), weighted by each type's fractional coverage, attenuated by and mixed with upward propagating and reflected emission of intervening vegetation canopy and atmospheric layers.

An attenuating layer is characterized by its transmissivity. The transmissivity (t) and its companion, optical depth (τ), are defined as,

$$t = \exp(-\tau), \qquad \tau = \int_0^{z_{top}} k(z) dz , \qquad (2.1)$$

where z (m) is the height above the surface to the top of the attenuating layer (z_{top}) and k(z) (m⁻¹) is the extinction with height. The optical depth of vegetation or atmospheric layers determines the degree to which *Tb* originates from the soil, vegetation or atmospheric conditions. The atmospheric optical depth ($\tau_{a(f)}$, subscript *f* denotes

frequency dependence) along the view path at the incidence angle (θ) is determined by oxygen concentration, water vapor, and cloud liquid water content of the lower troposphere (Wentz 1997),

$$\tau_{a(f)} = \sec(\theta) \left[A_o + A_v + A_L \right].$$
(2.2)

Oxygen absorption $(A_{o(f)})$ is relatively constant because oxygen is well mixed throughout the global atmosphere. Water vapor absorption $(A_{v(f)})$ is minor at low frequencies (≤ 10 GHz), and increases with frequency (f > 10 GHz) with the exception of a weak rotational absorption line centered at 22.2 GHz. Cloud liquid water extinction $(A_{L(f)})$ increases strongly for higher frequencies (≥ 36 GHz).

An approximate model describes effective *Tb* as a layer of semi-transparent atmosphere overlying the earth's surface (Wentz 1997; Grody 1980),

$$Tb_{(p,f)} = Tb_{u(f)} + t_{a(f)} [Tb_{s(p,f)} + \Omega(1 - \varepsilon_{s(p,f)})Tb_{d(f)}],$$
(2.3)

where $\varepsilon_{s(p,f)}$ is the polarization and frequency dependent surface emissivity (dimensionless), and Ω depends on surface roughness, but is assumed to be unity for both specular and Lambertian terrestrial surfaces at the AMSR-E incidence angle and the frequencies considered here (Matzler 2005). The upwelling surface brightness temperature $Tb_{s(f,p)}$ will be defined later. $Tb_{u(f)}$ and $Tb_{d(f)}$ are the respective upwelling and downwelling atmospheric brightness temperatures, and $t_{a(f)}$ is the atmospheric transmissivity. Atmospheric absorption and emission are dependent on the air
temperature, T_a , and primarily occur in the lower troposphere for window channels such as those on AMSR-E. In this case, $Tb_{u(f)} = Tb_{d(f)} = (1-t_{a(f)})T_a$ is a reasonable approximation (Weng and Grody 1998), although $Tb_{u(f)}$ is slightly cooler than $Tb_{d(f)}$ (Wentz 1997). Low emissivity surfaces, such as open water, provide a dark background relative to the atmosphere, increasing the *Tb* sensitivity of to atmospheric absorption and emission in (2.3).

Analogous to the atmospheric case, *Tb* emitted from a vegetated land surface $(Tb_{l(p,f)})$ is described as a layer of semitransparent vegetation over smooth, bare soil with emissivity, $\varepsilon_{os(p,f)}$, (Njoku 1999; Mo 1982),

$$Tb_{(p,f)} = Tb_u + t_{a(f)} [Tb_{s(p,f)} + (1 - \varepsilon_{s(p,f)})Tb_d],$$
(2.4)

where T_{os} and T_c are the respective soil surface and canopy temperatures (K) and ω is the dimensionless forward single-scattering albedo of the vegetation canopy. The polarization independence of $t_{c(f)}$ and $\omega_{(f)}$ is physically tractable for randomly oriented vegetation elements, a reasonable assumption for coarse-resolution satellite observations (Ulaby 1985; Wigneron 2006). Equation (2.4) does not account for multiple scattering within the vegetation canopy and therefore is considered valid only for lower frequencies (≤ 18 GHz; Njoku 2006; Matzler 2006). The soil emissivity ($\varepsilon_{os(p,f)}$) is related to the dielectric properties of the soil and calculated for specular surfaces using the Fresnel equations (Ulaby 1989). For low frequencies (≤ 18 GHz), soil dielectric properties vary strongly with water content and mineral type (Grody and Weng 2008). Additionally, sand and snow can scatter microwaves with $f \geq 36$ GHz particularly affected. The

vegetation canopy optical depth (τ_c) is defined in terms of the equivalent vegetation water content (g, kg m⁻²; Njoku 2006)

$$\tau_{c(f)} = \alpha_{(f)}g = b_{(f)}hg\sec(\theta), \qquad (2.5)$$

where $\alpha_{(f)}$ (m² kg⁻¹) combines angular, and frequency dependent canopy loss ($b_{(f)}$; m² kg⁻¹) and roughness factors (h; dimensionless), allowing t_c to account for both canopy extinction and surface roughness. Reported values for $b_{(f)}$ vary widely in the literature, but appear to follow a power law relationship by saturating at higher frequencies (Njoku 2006).

Microwave radiation properties over land are much more heterogeneous than clear-sky atmosphere or open ocean conditions and the integrated *Tb* emitted from the terrestrial surface ($Tb_{s(p,f)}$) often mixes open water and land

$$Tb_{s(p,f)} = f_w Tb_{w(p,f)} + (1 - f_w) Tb_{l(p,f)},$$
(2.6)

where $Tb_{w(f,p)}$ and $Tb_{l(f,p)}$ are respective Tb for water and land, and f_w is the open water fractional coverage (dimensionless) within the FOV. Even small areal coverage f_w (>0.05) strongly impacts surface emissions due to the high dielectric constant of water. Terrestrial landscapes, particularly at high latitudes, contain numerous water bodies and inundated areas where f_w seasonally varies.

2.3.2 Correlation of Brightness Temperature to Station Air Temperature

The most favorable AMSR-E frequencies for surface temperature retrieval commonly are those least sensitive to atmospheric and surface emissivity variations. The

AMSR-E ocean SST retrieval algorithms employ low frequencies (≤ 10.7 GHz) to minimize atmospheric effects. However, land emissivity varies more for these frequencies relative to higher frequencies, due to strong heterogeneity in land cover and soil moisture. Previous investigations have, therefore, used intermediate (i.e., 18–37 GHz) frequencies, which balance sensitivity to atmosphere (higher frequencies) and surface (lower frequencies) emissivities (Weng & Grody 1998; Fily 2003; Holmes 2009). However, the results of our correlation analysis indicate that the 23.8-GHz atmospheric water vapor frequency is desirable for temperature retrieval.

The *Tb* correlation to T_{mn} and T_{mx} generally increases at higher frequencies, with a global peak at 23.8 GHz (Figure 2.2). This pattern is due to greater sensitivity of lower frequencies to surface emissivity (decreased correlation) and the increased sensitivity of higher frequencies to atmospheric temperature (increased correlation). Model simulations confirm that the correlation between water vapor and surface air temperature through the Clausius-Clapeyron relation and reduced sensitivity of the 23.8-GHz frequency to surface emissivity induce strong temperature correspondence at 23.8 GHz. High correlation is desirable for air temperature retrieval, but I must also account for variable surface emissivity and atmospheric conditions to obtain an algorithm suitable for regional to global applications.

2.3.3 Solution for Daily Surface Air Temperature, Fractional Surface Water, and Total Column Atmospheric Water Vapor

Our approach employs *Tb* ratios from the 18.7 and 23.8 GHz channels to solve for microwave effective surface temperature (T_s). T_s reflects soil (< 1 cm), litter, vegetation,

and open water body temperatures, and does not exactly correspond to either screen height air temperatures, or optical-IR remote sensing derived LST where the effective emission layer is a very shallow skin (Hall 1992). Nonetheless, our correlation analysis indicates that microwave T_s is well correlated with T_{mn} and T_{mx} from weather stations. I, therefore, relate T_s empirically to T_{mn} and T_{mx} for respective morning (AM) and afternoon (PM) overpasses using a training subset of WMO weather station measurements.

I account for atmospheric absorption caused by *V* and surface emissivity caused by f_w and $t_{c(f)}$. The parameter represents the total vertical water vapor content of the atmosphere along the viewing path. The f_w parameter represents the effective open water fraction of the sensor field-of-view (FOV), which can include, but is not limited to, coastal lagoons, inland water bodies, inundated wetlands, and saturated soils following irrigation or precipitation events. The $t_{c(f)}$ parameter represents the amount of vegetation canopy and litter layer attenuation of upwelling radiation from the underlying soil, and is closely related to total litter, vegetation foliar, and stem water content along the sensor view path.

To facilitate analytical derivations, I simplify (2.2) and (2.4), expressing *Tb* as a linear function of $t_{a(f)}$ and $t_{c(f)}$ by ignoring the surface reflection terms. The linear assumption is not as limiting as it may seem because surface reflection is low for high emissivity land surfaces and the antennae gain averages sub-grid scale emissions of heterogeneous scenes. The simplified linear model may, therefore, have less bias relative to effective pixel averaged quantities than a nonlinear model (Chang & Milan 1982; Rastetter 2002). The simplified linear emission models based on (2.3), (2.4), and (2.6) are,

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$$Tb_{(p,f)} = T_{s}[t_{a(f)}\varepsilon_{(p,f)} + (1 - t_{a(f)})\delta], \qquad \delta \approx \frac{T_{a}}{T_{s}},$$
(2.7)

$$\varepsilon_{(p,f)} = f_w \varepsilon_{w(p,f)} + (1 - f_w) \varepsilon_{l(p,f)}, \qquad (2.8)$$

$$\mathcal{E}_{l(p,f)} = \mathcal{E}_{os(p,f)} t_c + (1-\omega)(1-t_c), \qquad (2.9)$$

where $\varepsilon_{l(p,f)}$, and $\varepsilon_{w(p,f)}$ are the respective land and open water emissivities. Vegetation transmissivity (t_c) is now assumed polarization independent and equivalent at 18.7- and 23.8-GHz frequencies, although t_c may be slightly lower at 23.8 GHz than 18.7 GHz. Open water emissivity ($\varepsilon_{w(p,f)}$), bare soil emissivity ($\varepsilon_{os(f,p)}$) and vegetation singlescattering albedo (ω) are assigned as constant parameters (Table 2.2). The ratio of air to surface temperature (δ) allows for a gradient between T_s and T_a (Table 2.3). I solve for T_s , rather than directly for T_a because the T_a retrieval is poorly conditioned when $t_{a(f)}$ is close to unity, which commonly occurs because water vapor only weakly absorbs the 23.8 GHz frequency and is seasonally low (< 10 mm) over many mid- and high-latitude land areas. I use an iterative approach to estimate f_w , t_c , and V using three temperature-insensitive Tb ratios,

$$MAWVI = \frac{Tb_{\nu23} - Tb_{h23}}{Tb_{\nu18} - Tb_{h18}} = \beta \left(\frac{t_{a23}}{t_{a18}}\right), \quad \beta = \left(\frac{\varepsilon_{\nu23} - \varepsilon_{h23}}{\varepsilon_{\nu18} - \varepsilon_{h23}}\right), \quad (2.10)$$

$$Fh = \frac{Tb_{h23}}{Tb_{h18}}, \quad P = \frac{Tb_{h18}}{Tb_{v18}}.$$
(2.11)

The subscripts 18, 23 and v, h denote respective frequencies and polarizations. The MAWVI (Microwave Atmospheric Water Vapor Index) is relatively insensitive to the β term because the surface emissivity polarization differences are relatively small for the two closely spaced sensor frequencies (i.e. β is near unity). The physical expression for MAWVI in (2.10) follows from (2.7). I use *Fh* in (2.11) rather the corresponding V-polarization expression because the H-polarization is more responsive to vegetation canopy absorption.

I determine V from the MAWVI using (2.2), (2.10), and (2.11),

$$V = \left[\log(\frac{MAWVI}{\beta})\cos(\theta) + a_{023} - a_{018} \right] / (a_{v18} - a_{v23}).$$
(2.12)

The terms a_{023} , a_{018} , and a_{v18} , a_{v23} are linear oxygen and water vapor absorption coefficients at nadir adapted from (Wentz 2002) by linearly approximating the AMSR-E ocean atmospheric model. I neglect cloud liquid water effects for the 18.7- and 23.8-GHz channels.

The f_w and t_c unknowns are determined by analytically inverting expressions *Fh* and *P* from (2.11) in terms of the emission model (2.7)-(2.9),

$$t_{c} = \frac{Ap(Bf + Cf) - Bp(Af + Cf) + Cp(Bf - Af)}{Dp(Af - Bf) + Df(Bp - Ap)},$$
(2.13)

$$fw = \frac{Bp + t_{a18}(\varepsilon_{lh18} - P\varepsilon_{lv18})}{t_{a18} \left[P(\varepsilon_{wv18} - \varepsilon_{lv18}) + (\varepsilon_{lh18} - \varepsilon_{wh18}) \right]},$$
(2.14)

where,

$$\begin{aligned} Ap &= t_{a18} (P \varepsilon_{wv18} - \varepsilon_{wh18}), & Af &= t_{a18} Fh \varepsilon_{wh18} - t_{a23} \varepsilon_{wh23}, \\ Bp &= \delta (1 - t_{a18}) (1 - P), & Bf &= \delta \big[(1 - t_{a23}) - Fh (1 - t_{a18}) \big], \\ Cp &= t_{a18} (1 - \omega) (1 - P), & Cf &= (1 - \omega) (t_{a23} - t_{a18} Fh), \\ Dp &= t_{a18} (\varepsilon_{osh18} - 1 + \omega) - P(\varepsilon_{osv18} - 1 + \omega), & Df &= t_{a23} (\varepsilon_{osh23} - 1 + \omega) - t_{a18} Fh (\varepsilon_{osh18} - 1 + \omega) \end{aligned}$$

$$(2.15)$$

The *w* and *l* subscripts denote water and land, respectively. The system of three equations (2.12) - (2.14) is applied iteratively for sequential updating the three unknowns, f_w , and t_c , and *V*, until a solution is reached. I find that five iterations stabilize the retrieved regional probability mass functions (PMF's) without excessive computational burden. The surface temperature is then calculated by inverting (2.7), the terms of which are now specified.

The model reproduces the observed variation in the *Fh*, *P*, and *MAWVI* ratios for the domain and study period as shown by bivariate histograms overlain by model results (Figure 2.3). The ratios form roughly triangular shaped regions for each *V* value, the vertices of which are (t_c = undefined, $f_w = 1$), ($t_c = 1$, $f_w = 0$), and ($t_c = 0$, $f_w = 0$). Over forests, which fall near the origin in Figure 2.3a, the polarization difference is very small and the *MAWVI* index is poorly conditioned. Correct estimates of *V* over such surfaces are not crucial for determining T_s , but slight offsets from the origin (i.e., adding small constants ($\approx 1-2$ K) to the numerator and denominator in (2.10)) improve conditioning.AMSR-E descending (AM) and ascending (PM) *Tb* inputs provide the algorithm with two instantaneous T_s retrievals daily, which are then empirically related to daily T_{mn} and T_{mx} . A linear regression correction was developed to transform AMSR-E overpass T_a to T_s using the AMSR-E retrieval as an explanatory variable (Table 2.3). An additional correction is applied to account for temperature differences between the local time of AMSR-E and AIRS overpass T_a retrievals and the timing of T_{mn} and T_{mx} .

2.3.4 Solution for Vegetation Optical Depth and Soil Moisture

I use AMSR-E 10.7 and 18.7 GHz H and V polarized *Tb* to estimate vegetation optical depth and soil moisture using a hybrid change-detection and radiative transfer approach. Here I use the descending (AM) overpass *Tb* data, but the method is also applicable to ascending (PM) overpass *Tb* data. The method could also be extended to 6.9 GHz *Tb* for areas not subjected to RFI (Njoku 2005). *Tb* data are gridded to the 25-km Equal Area Scalable Earth (EASE) Grid from the Level 2A data product using inverse distance squared weighting (Ashcroft & Wentz 1999). Other inputs including T_{ss}, f_{w} , and *V* are obtained from the temperature algorithm previously described. Vegetation opacity is re-estimated for 18.7 GHz using the more detailed τ - ω equation which considered surface reflections and therefore 18.7 GHz τ_c from the previously described temperature algorithm is not used as an input. I then use input T_s and *V* to calculate the effective *Tb* emissivity of polarization *p* as,

$$e_{p} = \frac{Tb_{p} / T_{s} - \left(1 - t_{a}\left(V\right)\right)\delta}{t_{a}\left(V\right)},$$
(2.16)

where the atmospheric transmissivity (t_a) is a function of V and oxygen absorption (Eqn. (2.2)), and δ weights the integrated atmospheric and surface temperatures (Eqn. (2.7)). I apply these results to calculate a slope parameter (a),

$$a = \frac{ev - ev_{wat}}{eh - eh_{wat}}.$$
(2.17)

Open water emissivities (ev_{wat} , eh_{wat}) are considered constant, although they are potentially increased by water waves, foam, and salinity. The slope parameter, a, gives a quantity sensitive to vegetation and surface roughness, which is orthogonal to f_w variability. The slope and daily f_w quantities are temporally smoothed using a moving window median time domain filter. Open water within the sensor footprint decreases the bulk pixel *Tb* sensitivity to soil moisture much more slowly than a proportional amount of vegetation optical depth (Figure 2.4). The effective optical depth of the land fraction (τ_c) is determined by inverting the τ - ω equation in terms of the slope (a),

$$\tau_c = \log(t_c) = \log\left[\frac{-B - \sqrt{B^2 - 4AC}}{2A}\right],\tag{2.18}$$

with,

$$A = (1 - \omega)(rv_s - a^* rh_s),$$

$$B = a^* eh_s - ev_s + (1 - \omega)(a^* rh_s - rv_s + 1 - a),$$

$$C = (1 - \omega)(a - 1) + ev_{wat} - a^* eh_{wat}.$$
(2.19)

The bare, dry soil emissivities (eh_s , ev_s) and vegetation single scattering albedo (ω) determine potential maximum and minimum slopes, respectively, and rh_s and rv_s are found by Kirchhoff's Law (i.e., r(v,h) = 1 - e(v,h)). The 18.7 GHz channel derived τ_c is then proportionality adjusted to estimate τ_c for the 10.7 GHz channel (Njoku & Chan 2006). Alternatively, 10.7 GHz τ_c could be estimated directly using (2.18) without using 18.7 GHz

Tb; however, I find that this approach leads to unrealistically high soil moisture for highbiomass vegetation conditions (i.e. high τ_c).

Surface soil moisture (< 2 cm depth) is derived using the effective emissivity of the AMSR-E 10.7 GHz, H polarized *Tb* by inverting the τ - ω equation and a simple polynomial approximation of the Dobson dielectric model (Njoku 2003; Dobson 1985) and Fresnel equations (Ulaby 1986) for loam soils. The variance in estimated soil reflectivity, and hence surface soil moisture, is inversely proportional to $1 - f_w$. I therefore dampen the variability by the factor $1 - f_w$, which improves the dynamic range of estimates under marginal conditions. A comprehensive summary of the optical depth and soil moisture algorithm and comparison with other available AMSR-E algorithms is given in Mladenova (2014).

2.4 **Results**

2.4.1 AMSR-E and AIRS Daily Temperatures Relative to Weather Station Observations

The AMSR-E and AIRS derived temperatures have similar overall pooled accuracy relative to *in situ* daily air temperature measurements from WMO weather stations (Table 2.4). The overall uncertainty of AMSR-E temperature retrievals relative to all pooled WMO validation sites is 3.5 K (RMSE) for T_{mn} and T_{mx} . Corresponding uncertainties for the AIRS temperature retrievals are 3.4 and 3.8 K, respectively. Error between AMSR-E and AIRS daily air temperatures is lower than between either satellite based retrieval and WMO site measurements (RMSE = 2.7 K and 3.2 K, respectively). The MAE is much lower than the RMSE for each temperature comparison, indicating a significant influence of site-to-site biases on the pooled RMSE, despite low overall bias (< 0.5 K). Typical accuracy for AMSR-E derived temperatures at individual WMO locations is higher than for the pooled hemispheric results (median RMSE of 2.9 K and RMSU of 2.3 K) with little difference between T_{mn} and T_{mx} . Similarly, the AIRS results show a median RMSE of 3.0 and 3.4 K for T_{mn} and T_{mx} , respectively. Despite similar pooled and median overall accuracies, the AMSR-E derived temperatures show greater accuracy and higher correlation than the AIRS results for the majority of WMO stations (Figure 2.5). This occurs because the AMSR-E results are biased for a few specific locations, whereas AIRS is less biased but with generally lower correlation and, hence, less accuracy than AMSR-E for most stations. These differing error patterns lead to similar overall accuracy between the two sensors when the WMO stations are pooled.

The AMSR-E and AIRS results show similar site-to-site bias and correlation with latitude, with the exception of the few locations where AMSR-E bias is larger. AMSR-E temperature accuracy is consistent across latitudes, whereas the AIRS accuracy decreases by up to 1 K for tropical (< 25° N) relative to temperate latitudes (25° N –50° N). The correlation of both AMSR-E and AIRS temperatures with WMO stations declines with latitude from $R^2 > 0.6$ above 25° N to $R^2 < 0.3$ below 25° N.

The AMSR-E and AIRS temperature accuracy generally decreases over sparsely vegetated desert locations (Figure 2.6). This amounts to a respective T_{mn} and T_{mx} RMSE increase of 2 –3 K for AMSR-E. In contrast, the AIRS derived T_{mx} RMSE increases by 2 K, while the T_{mn} RMSE shows a small 0.74 K decrease over desert locations. The reduced temperature accuracy corresponds with larger site-to-site biases over desert locations, although correlations at individual sites remain relatively high. AIRS generally

underestimates T_{mx} over barren and sparsely vegetated land ($t_c < 0.8$), but overestimates over moderate vegetation ($t_c \ 0.8-2.0$) relative to *in situ* measurements. However, the sign and magnitude of AMSR-E temperature biases vary significantly among individual desert locations. Temperature accuracy, especially for AMSR-E, tended to decrease (increase) for land cover types with lower (higher) vegetation biomass and beyond these two distinctions accuracy varied little amongst specific cover types. The percentage of dominant land cover within the pixel weakly impacted accuracy for AIRS (R = 0.16; p < 0.05), and was insignificant for AMSR-E. Other factors influencing satellite derived temperature accuracy relative to WMO stations include elevation, which produced respective RMSE increases in AMSR-E and AIRS temperatures of 0.7–0.8K and 0.35– 0.38K for every 1000 m increase in station elevation, and f_w which induces a maximum cold bias of 2–3.5 K with 50% open water coverage for both AMSR-E and AIRS with slightly less (0.5 K) impact on T_{mn} than on T_{mx} .

2.4.2 Regional Comparison of AMSR-E and AIRS

The AMSR-E and AIRS temperature results show close agreement for non-desert temperate and boreal regions (Figure 2.6). Agreement is highest for T_{mn} (R² > 0.8 and RMSE \leq 2.0 K), and lower for T_{mx} (RMSE \approx 2.0 – 2.5 K). Correlations between AMSR-E and AIRS temperatures are generally \geq 0.80 at higher latitudes, but decline substantially for subtropical and tropical latitudes, although RMSE differences remain in the 2.5–3.0 K range. Temperature biases for these lower latitude regions also remain relatively low (MR \leq 1.5 K).

The AMSR-E and AIRS temperatures show reduced agreement in desert regions (RMSE = 4-6 K; Figure 2.6). Large regions of low correspondence are evident in the Sahara, Arabian Peninsula, Iran, Gobi, and Central Asian regions and the Southwestern United States. Regions of low agreement are driven mainly by both temperature biases and reduced correlation. High spatial heterogeneity in temperature bias is particularly evident over the Arabian Peninsula and Northeastern Sahara, where bias can change sign and magnitude over short distances (50–100 km). T_{mn} and T_{mx} bias does not necessarily follow the same patterns in these regions, although coherent T_{mn} and T_{mx} biases occur in desert areas of central Asia.

Hemispheric agreement between AMSR-E and AIRS daily air temperatures varies seasonally. The RMSE differences between AIRS and AMSR-E derived T_{mn} varies from a maximum of 2.9 K in early June to a low of 2.2 K in mid-July. Similarly, RMSE differences for T_{mn} vary from 3.3 K in June to 2.7 K in July. The seasonal RMSE pattern is evident in the bias, where AMSR-E overestimates T_{mn} and T_{mx} in June relative to AIRS by 0.6 K, although the bias diminishes by mid-July.

2.4.3 AMSR-E Global Temperature Patterns

Mean seasonal T_{mn} and T_{mx} patterns from AMSR-E generally follow expected geographic trends (Figure 2.7). The cold Tibetan plateau and adjacent warm temperatures of the Gobi desert are evident, as are similar topographically driven temperature gradients between adjacent low lying areas and prominent mountain ranges which include the Himalaya and Karakorum, Alps, Ethiopian Highlands (Northeast Africa), and central Rocky Mountain regions. Temperature contrasts between moderate coastal and more extreme inland climates are also evident, including a temperature gradient between coastal and interior Mexico. The relatively hot Sahara desert contrasts with less extreme temperatures in the Sahel region. However, diurnal temperature ranges are very low (< 8 K) for portions of the Sahara and Arabian Peninsula given expected large sensible heat fluxes of this region, and show a heterogeneous spatial pattern with $T_{mn} > 300$ K.

The co-retrieved land surface parameters (f_w , t_c , and V) vary with global climate and land cover (Figure 2.7). Hemispheric f_w follows an apparent power law distribution. Abundant open water bodies are detected in boreal and tundra regions, particularly north central Canada. The f_w retrievals also show a substantial amount of open water in some arid regions of the northern Sahara and middle-East, particularly in the Tigris and Euphrates river valleys. This causes many desert locations to have much more f_w coverage than expected. Large τ_c gradients between desert regions and temperate and tropical forests are evident. A more subtle increase in τ_c from boreal forest to arctic tundra marks the northern extent of tree line. Mountains, such as the Himalaya, generally have higher τ_c than surrounding areas, which is a feature particularly evident in the mountain ranges of the Sahara. Moist tropical regions including India, Indonesia and Southeast Asia show characteristically high V; relatively humid areas of the Southeast and Midwestern USA also show relatively high water vapor content. In contrast, colder, drier regions including the Tibetan plateau, central Asia, and the Arctic show relatively low water vapor contents. Regions where the AMSR-E V retrievals are considered unreliable due to a poorly conditioned MAWVI index were confined to boreal and equatorial forests with Tb_{v18} - $Tb_{h18} \le 1$ K. AMSR-E retrievals correspond with AIRS surface layer mixing ratio (g kg⁻¹; $R^2 = 0.58$; p < 0.01). The mode of retrieved

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hemispheric diurnal V differences is 0.7 mm, although retrieved diurnal differences can range up to > 8 mm, mainly over the boreal forest.

2.4.4 AMSR-E Vegetation Optical Depth and Soil Moisture Results

The AMSR-E soil moisture retrievals respond rapidly to precipitation wetting and dry quickly (within 2-5 days) in the absence of additional rainfall (Figure 2.8). AMSR-E soil moisture corresponds closely to the *in situ* precipitation index measurements when τ_c < 1.2. Soil moisture accuracy is reduced for boreal forest and for the cropland location during peak LAI, as indicated by insignificant correlations. However, the cropland site apparently responds to precipitation events prior to peak LAI. Interestingly, the tundra location has a higher peak τ_c than either the boreal forest or the cropland, yet maintains more sensitivity to soil moisture; this may be the result of saturated, radiometrically absorptive organic matter underlying a highly porous organic surface layer characteristic of tundra.

The AMSR-E τ_c seasonality agrees well with the timing of peak MODIS LAI at all locations (Figure 2.8). The boreal forest τ_c also varies seasonally, which is likely due to deciduous vegetation in disturbed locations or within mixed evergreen and deciduous forest canopies. The cropland location is dominated by corn and soybeans, where τ_c peaks as crops mature in August. The τ_c over desert grasslands shows two seasonal peaks corresponding to characteristic vegetation growth during monsoonal rainfall periods evident in the AMSR-E soil moisture time series.

The AMSR-E derived daily soil moisture series is responsive to periodic wetting events during 2008 indicated by TRMM in diverse global regions, whereas AMSR-E

derived f_w responds over adjacent floodplain areas (Figure 2.9). Areas of high AMSR-E soil moisture closely correspond with areas of high TRMM rain rates for two successive storms in India on July 28 and August 1. The AMSR-E f_w coverage is widespread across India, corresponding with extensive eastern and northern agricultural irrigation and wetland regions, but does not respond to the individual storms. A major storm impacted southeastern Australia on February 20, and caused widespread AMSR-E soil moisture increase; however, AMSR-E indicates f_w coverage only for lake and playa locations, which are known to respond rapidly to intense rainfall in this portion of Australia. A major multiple-day storm impacted Argentina from August 3 to August 6. AMSR-E soil moisture shows wetting associated with this storm along much of eastern Argentina, which dries from August 6 until past August 15. AMSR-E indicates f_w coverage increase associated with flooding in the Pantanal floodplain and surrounding wetlands associated with this storm and post-storm AMSR-E f_w decreases with presumed receding flood waters in subsequent days. These results indicate that the AMSR-E soil moisture retrievals reflect a relatively shallow soil layer with characteristic rapid wetting and drying cycles in response to precipitation events. These results indicate effective separation of the soil moisture and f_w signals following rain events in diverse regions of the globe. The AMSR-E soil moisture maps appear free from water contamination along coastlines, rivers and other water bodies further indicating the *fw* estimate effectively mitigates soil moisture flooding-related bias.

The AMSR-E derived daily *fw* variable was compared to independent static *fw* maps for Alaska (Figure 2.10). Estimated spatial water coverage of the entire Alaska region is 4.8 %, 4.4 %, and 3.4 % for JERS-1, AMSR-E, and MODIS, respectively. The AMSR-E *fw* map is spatially smooth relative to the aggregated JERS-1 derived *fw* map

(Figure 2.10). This is mainly an artifact of spatially aggregating the relatively fine scale JERS-1 land cover and the smoothing inherent in re-sampling of the egg-shaped AMSR-E swath footprints to a 25-km earth grid. However, the AMSR-E product retains sub-grid scale information on inundated wetlands and small lakes that is missing from the 1-km MODIS classification, as indicated by a larger regional *fw* value. These results show large differences in spatial and seasonal *fw* patterns across the region, including two locations within the Yukon River basin. The Yukon Delta location is within a large wetland and is located further south and closer to the coast than Stevens Village, and therefore shows an earlier spring thaw, later fall freeze and larger *fw* area. The steep rise and fall in the seasonal *fw* signal occurs as lake and river ice melts in the spring and freezes in fall; this pattern coincides with the annual cycle of inundation and drying of abundant seasonal wetlands, especially over the Yukon Delta region.

2.5 **DISCUSSION**

2.5.1 Evaluation of Land Parameter Retrievals

The results of this study indicate that AMSR-E derived air temperatures are accurate to within 1.0–3.5 K for most non-desert regions relative to WMO stations. For comparison, Jolly (2005) obtained an accuracy of ≈ 2 K by spatially interpolating weather station data to 8-km resolution for the continental U.S. where the station network is relatively dense. Previous microwave investigations with SSM/I (Bassist 1998) have reported a standard fit error of 2.5 K relative to WMO stations; however, stations were carefully selected to minimize external factors (Bassist 1998), whereas I randomly selected stations from the pool of available stations within each land cover class. Restricting the validation results to only locations with average $\tau_c > 1.2$ and < 70 m difference between station and 25-km pixel average elevation (121 stations) results in median site accuracies (RMSE) of 2.5 K for T_{mn} and T_{mx} . These comparisons suggest that the algorithm presented in this study has potential application where station density is low and is at least as accurate as previous satellite microwave temperature retrieval algorithms (Fily 2003; Bassist 1998; Weng & Grody 1998).

High correspondence between independent AMSR-E and AIRS temperature estimates for vegetated regions lend additional confidence to the accuracy of the two sensor products. However, spatial bias and accuracy degradation in sparsely-vegetated desert regions locations indicate that remotely sensed air temperature patterns should be taken with caution in these regions. The accuracy assessment includes error resulting from spatial mismatches and measurement error, as well as algorithm error.

Higher AMSR-E retrieval accuracy relative to AIRS for the majority of WMO locations apparently results from increased sensitivity of AIRS to cloud cover, especially for lower latitudes (< 25° N). The decline in correlation between the two sensors and with WMO stations over tropical non-desert regions is partially attributable to a lack of daily and seasonal temperature variability in these locations, leading to a lower signal-to-noise ratio and is not necessarily the result of increased error variance. However, the AIRS retrievals had somewhat lower accuracy in these regions, whereas AMSR-E retrieval accuracy does not substantially decline for non-desert tropical regions. Additionally, seasonal patterns of temperature differences between AIRS and AMSR-E retrievals are

explained by broad-scale seasonal climatic patterns affecting AIRS temperature retrieval accuracy, including the seasonal onset of monsoon moisture and associated cloudiness.

Increased correlation results for AMSR-E relative to AIRS partially reflects fewer total observations due to a narrower swath width. The percentage of days with observations from both sensors declines with latitude from 100% near the poles to 45% at the equator as a result of Aqua's polar orbit. AMSR-E has fewer observations than AIRS, 69.3% and 69.4% versus 80.3% and 79.2%, respectively, for descending and ascending orbits. Fewer AMSR-E observations is foremost the result of narrower swath width than AIRS for low latitude locations (see Section 2.1.1) and to a lesser extent, snow cover at high latitudes. AMSR-E data loss from precipitation causes minor differences in observation counts relative to AIRS as AIRS data loss also occurs for such events. AIRS has greater ascending pass data loss in the Western Sahara, Arabian Peninsula, and Gobi deserts relative to AMSR-E. Accuracy differences between AMSR-E and AIRS are partially a result of algorithmic quality control and exclusion of unfavorable retrieval conditions.

Generally, lower correspondence between AMSR-E and AIRS retrievals over many arid and desert regions, including northern Africa, central Asia, and the Southwestern United States, is attributed to limitations of the relatively simple AMSR-E algorithm to capture emissivity variations and to large vertical temperature gradients over sparsely vegetated desert landscapes. AMSR-E T_{mn} and T_{mx} biases of equivalent sign suggest incorrectly specified surface emissivity, whereas T_{mn} and T_{mx} biases of differing sign suggest a gradient between the effective microwave temperature and *in situ* air temperature. Areas of strong bias over the Arabian Peninsula and Northeastern Africa

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coincide with limestone deposits (Grody & Weng 2008; Prigent 1999), which have a higher soil dielectric constant and lower surface emissivity than surrounding areas composed of more common silica sands. Additional dielectric effects from desert salt pans, scattering sands, fine scale surface roughness, and terrain variability are some of the many factors that contribute to complex desert surface emissivity variations (Prigent 1999) and also likely impact the AMSU channels (Grody & Weng 2008). High broadband albedo quartz sand surfaces significantly reduce the difference between T_{mn} and T_{mx} relative to surrounding lower albedo features in the Sahara and Arabian Peninsula regions (Ogawa & Schmugge 2004). Highly variable near-surface temperature lapse rates in arid and mountainous regions cause differing biases between T_{mn} and T_{mx} for AIRS and AMSR-E temperature estimates in these regions (Gao 2008). The variable nature of AMSR-E site-to-site biases precludes simple global or regional empirical adjustments. Therefore, more accurate emission models which account for emissivity and temperature gradients common to deserts are required to improve results.

Aside from desert regions, the relatively simple AMSR-E temperature algorithm captures surface emissivity and atmospheric water vapor variability over vegetated regions regardless of land cover type. The AMSR-E co-retrieved f_w , t_c , and V parameters generally follow expected regional patterns. Spurious patterns of excessive f_w are present in some desert locations with limestone deposits because the model assumes a quartz mineral dielectric and the dielectric of limestone is higher than that of quartz. Alternatively, frequency dependent scattering from sand or rough surfaces can cause the *Fh* ratio to drop below unity, which produces negative f_w estimates. Apparently, t_c can account for some terrain roughness features in addition to variations in vegetation biomass, but more study is required to determine precisely which features the simple parameterization does not adequately capture. The global mode of diurnal variability in V(0.7 mm) is within the reported range for the continental U.S. (0.5 – 1.0 mm; Dia 2002). Deviations from this range occur in densely forested boreal regions where the AMSR-E Vretrieval is poorly conditioned. However, most continental land areas have H-polarization emissivity low enough to allow atmospheric water vapor retrieval over land from AMSR-E. Future research will include further evaluation of AMSR-E co-retrievals including independent information sources from satellite optical-IR and radar remote sensing derived vegetation and open water products (e.g., Jones 2009), as well as integrated atmospheric water vapor information from AIRS, radiosondes, and GPS occultation.

Spatial representation mismatches between *in situ* station measurements and the resolution of individual satellite sensors limit the ability to quantify uncertainty. It is also difficult to assess whether AIRS or AMSR-E retrievals are reliable where the station network is sparse, especially over desert, tropical forest and mountainous regions. The AMSR-E and AIRS temperature retrievals generally corresponded better with each other than with WMO station observations and frequently had similar biases, suggesting similar spatial representation. The satellite retrievals reflect effective temperatures horizontally and vertically weighted in spatial extent, which may differ significantly from sparse station 2-m height observations from sparse weather stations within a 25-km grid cell. Furthermore, the effective resolution of the gridded satellite data is somewhat larger than 25-km as a result of inherent spatial smoothing from the gridding procedure. Data assimilation-type approaches to validation will ultimately be required to overcome some of the limitations of spatial mismatches between satellite footprints and sparse station

networks, but traditional approaches to validation presented in this study are still required to exploit synergies between different sensor products (Renzullo 2008; Crow 2007; McCabe 2008).

2.6 CONCLUSION

This study demonstrated that the AMSR-E 18.7 and 23.8 GHz and polarized brightness temperatures can be used to derive near surface daily air temperature minima and maxima over land with minimal ancillary data. The methods developed include coretrievals of potentially synergistic variables, including atmospheric water vapor, vegetation optical depth and fractional open water coverage. Regional accuracy and precision of AMSR-E daily surface air temperature information is well-quantified relative to surface weather station observations and satellite remote sensing products from AIRS. The scope of this investigation encompassed the Northern Hemisphere land area for a single snow-free season, but the methods are appropriate for global applications and extended periods because the key factors influencing retrieval accuracy and spatial variability are represented in the current study domain. The algorithms and results of this study are sufficiently accurate for regional analysis of air temperature patterns and environmental gradients, and are appropriate inputs for atmospheric and land surface models.

Using AMSR-E surface temperature and fractional water coverage as input, vegetation optical depth and surface soil moisture were estimated using 10.7 GHz brightness temperatures from AMSR-E. The results of this study indicate that the soil

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retrievals are reasonably accurate under low optical depth conditions ($\tau_c < 1.2$), as well as for high optical depth in tundra. Soil moisture retrieval accuracy is reduced over high optical depth forest and cropland locations during peak biomass. The AMSR-E optical depth retrievals show characteristic seasonality across a range of North American land cover types and agree well with alternative canopy cover estimates from MODIS LAI. Soil moisture and water fraction show characteristic spatial patterns and temporal variability following precipitation events across diverse global regions as compared to TRMM satellite-based rain rate data. Dynamic open water fraction retrievals effectively mitigate potential soil moisture bias and provide an additional important hydrological parameter for global monitoring. Open water is a key component of continental seasonality, especially for boreal forest, tundra, wetland, riparian, irrigated agriculture, and many tropical ecosystems. The results of this study indicate that algorithms for upcoming satellite microwave soil moisture missions, such as SMAP and SMOS, should consider dynamic corrections for open water.

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TABLES

Number	Abbrev.	Name
0	OW	Open Water
1	ENF	Evergreen Needleleaf Forest
2	EBF	Evergreen Broadleaf Forest
3	DNF	Deciduous Needleleaf Forest
4	DBF	Deciduous Broadleaf Forest
5	MXC	Mixed Cover
6	WOD	Woodland
7	WGR	Wooded Grassland
8	CSH	Closed Shrubland
9	OSH	Open Shrubland
10	GRS	Grassland
11	CRP	Cropland
12	BAR	Barren
13	URB	Urban

 Table 2.1: MODIS UMD global land cover classes.

Table 2.2: Radiative transfer model parameters used to derive surface air temperature from AMSR-E 18.7 and 23.8 GHz *Tb* inputs.

Physical Model Parameters	Symbol	18.7 GHz	23.8 GHz
Veg./Roughness single scattering albedo	ω	0.05	0.05
Dry bare soil surface emissivity (V-pol.)	\mathcal{E}_{OSV}	0.994	0.975
Dry bare soil surface emissivity (H-pol.)	Eosh	0.771	0.781
Open water emissivity (V-pol.)	\mathcal{E}_{WV}	0.630	0.685
Open water emissivity (H-pol.)	\mathcal{E}_{Wh}	0.336	0.421
Water Vapor mass absorption coefficient	a_v	0.0034	0.0104
Oxygen mass absorption coefficient	a_o	0.0103	0.0131
Initial emissivity difference ratio multiplier	eta_{o}	0.88	0.88

Table 2.3: Multiple regression model parameters used to correct for air temperature differences between satellite (AMSR-E and AIRS) local overpass time and timing of T_{mn} and T_{mx} . See text Section 2.2.1 for parameter descriptions.

		AMSR-E		AIRS	
Empirical Parameters			Asc.	Desc.	Asc.
¹ Parameter for surface to air					
temperature ratio	δ	0.98	0.96	-	-
² Surface to air temperature correction	c_0	-0.8	2.0	-	-
² Surface to air temperature correction	<i>C</i> 1	12.0	-9.2	-	-
² Surface to air temperature correction	<i>C</i> ₂	-19.0	0.0	-	-
³ Overpass time regression coeff.					
(constant)	m_0	22.53	55.50	19.42	52.74
³ Overpass time regression coeff.					
(temperature)	m_1	0.93	0.83	0.92	0.83
³ Overpass time regression coeff.					
(latitude)	m_2	-0.07	-0.09	-0.02	-0.02
Used in radiative transfer model eqn. (2.7); ${}^{2}T_{sa} = T_{s} + c_{0} + c_{1}(t_{c}) + c_{2}(t_{c}^{2});$					

¹ Used in radiative transfer model eqn. (2.7); ² $I_{sa} = I_s + c_0 + c_1(t_c) + {}^3T_{mn,mx} = m_0 + m_1(T_{sa}) + m_2(Lat.).$

Table 2.4: Summary statistics of relative agreement between AMSR-E and AIRS derived Northern Hemisphere temperature results, and weather station daily air temperature measurements pooled for 273 WMO test sites.

	T _{mn} (K)			
	R ²	RMSE	MAE	MR
AMSR-E vs. WMO	0.79	3.5	2.7	0.12
AIRS vs. WMO	0.83	3.4	2.5	0.14
AMSR-E vs. AIRS	0.86	2.7	2.0	0.07
	$T_{mx}(\mathbf{K})$			
	\mathbf{R}^2	RMSE	MAE	MR
AMSR-E vs. WMO	0.85	3.5	2.7	0.02
AIRS vs. WMO	0.81	3.8	2.9	0.30
AMSR-E vs. AIRS	0.85	3.2	2.4	-0.05

FIGURES



Figure 2.1: Location of WMO stations used for algorithm development (N = 270) and testing (N = 273. Regional land cover representation is a proportion (%) of total land area (or total stations) within each latitudinal band sorted in decreasing order.



Figure 2.2: Expected (Model) and observed patterns of time-series linear cross correlations (R) between AMSR-E daily descending/ascending observed T_{bv} values and in situ T_{mn}/T_{mx} observations.



Figure 2.3: Bivariate histogram scatterplots of (a) numerator and denominator of the MAWVI ratio (10) and (b) *Fh* and *P* ratios in Eqn. (2.11). Darker (lighter) regions primarily represent land (water) areas. Model results for two levels of atmospheric water vapor (*V*) and the entire range of t_c and f_w are shown for reference.



Figure 2.4: Normalized H polarized Tb range from dry (0.05 vol.) to wet (0.50 vol.) soil with (a) changing optical depth (τ_c) and (b) open water fraction (f_w).



Figure 2.5: Median summary statistics of unbiased RMSE (RMSU) and mean residual (MR) for AMSR-E and AIRS temperature retrievals relative to WMO station observations by elevation (200-m bins), latitude (2.5° bins), f_w (0.05 bins), and τ_c . N represents the number of WMO test stations represented in each bin (equivalent for T_{mn} and T_{mx}). See Section 2.1.4 for statistical explanations.



Figure 2.6: Maps of Northern Hemisphere regional correspondence between AMSR-E and AIRS T_{mn} and T_{mx} retrievals.



Figure 2.7: Maps of mean summer AMSR-E retrieved parameters for the 2003 study period and PDFs of co-retrieved parameters from ascending and descending orbits.



Figure 2.8: Comparison of AMSR-E retrievals with antecedent precipitation (SMV), and comparison of AMSR-E τ_c seasonality with MODIS LAI for five study locations. SMV is normalized to the unit interval to compare variability. The vegetation plot y-axes are scaled to show variability.


Figure 2.9: Comparison of AMSR-E UMT soil moisture and fractional water (f_w) after major 2008 precipitation events for India, Australia, and southern South America. Precipitation from the TRMM 3B42 satellite-based rain rates and represents prior 24-48 hour sums of three-hourly data. Fractional water change (Δf_w) represents the difference between August 6 and August 3 (Δf_w before) and August 15 and August 6 (Δf_w after). AMSR-E missing values caused by gaps between swath acquisitions.



Figure 2.10: Comparison of gridded 25-km open water estimates for Alaska. The resolutions listed below the instrument names indicate the product native resolution prior to gridding. Open water seasonality retrieved by AMSR-E is shown for two locations for 2003.

CHAPTER 3: JOINT MERGING AND UNCERTAINTY ESTIMATION OF MULTIPLE SOIL MOISTURE TIME-SERIES CONTAINING COLORED NOISE AND MISSING VALUES

3.1 INTRODUCTION

Ecosystems react to daily weather variations including temperature, radiation, soil moisture, and humidity. Stomata close when atmospheric demand exceeds soil moisture supply, soil organic matter decomposes faster when soils are warm and moist, photosynthesis increases with increasing radiation, among other processes (Running 1998; Chapin 2002). Global ecological modeling applications require spatially and temporally consistent driving meteorological information (Zhao 2006). Satellite remotesensing observations provide more continuous spatial coverage than *in situ* observations and may provide better accuracy and more desirable spatial and temporal resolution than weather and climate models. However, most observational datasets contain noise, bias, missing values, and may conflict with other observational datasets or physical expectations. Meteorological observations must therefore be quality-controlled, biascorrected, smoothed, interpolated, and merged to become usable drivers for ecological models (Zhang 2007). Well quantified accuracy is also essential for hypothesis-testing and decision-making with ecological models. Data assimilation accomplishes all these tasks by merging observations with a dynamic model. Although weather models are physical representations of weather dynamics, dynamic models used for data assimilation need not be physically-based, and can be, for example, spatio-temporal statistical models (Anderson & Moore 1980; Cressie & Wikle 2011).

Data assimilation can be accomplished using the Kalman Filter/Smoother algorithm (KF/S; Kalman 1960). The KF/S optimally weights a model forecast with available observations according to their relative uncertainty whenever observations become available (Raupach 2005). This merged value is then used to initialize the subsequent model forecast which proceeds until another observation becomes available at which point the process repeats. Using this scheme, the model interpolates and smooths the observations in space and time based on prior knowledge of physical (or empirical) relationships represented by the model propagation equations. Success applying the KF/S for estimating hidden states from noisy observations hinges on how well the system's parameters, particularly its error characteristics, describe reality. Typically KF applications require observations with uncorrelated-in-time, i.e. "white", Gaussian errors. This allows optimal projection from observations onto the hidden process, because the variability of the hidden process can be assumed orthogonal to the error variability (Anderson 1979; Kailath 2000). Much previous research has focused on estimating KF/S system parameters including sub-space (SS; Ljung 1999; Katayama 2005) and maximum likelihood (ML; Gupta 1974; Shumway 1982) methods. These methods seek to determine system parameters by whitening one-step-ahead prediction residuals, known as the innovations. Whereas the KF remains generally robust to deviations in the Gaussian assumptions, non-white, i.e. "colored," observation noise degrade optimality of SS or ML methods by eroding orthogonally with the hidden process and making white innovations impossible to obtain (Anderson 1979; Kailath 2000). This situation can arise in applied science and engineering situations when, for example, multiple redundant series of noisy

data observe the dynamics of an underlying hidden process with inexactly-known linear dynamics producing slowly-varying bias in each observation series.

A motivating example comes from the task of merging redundant soil moisture time-series to obtain accurate, consistent daily, global soil moisture estimates and the related task of inter-calibrating and characterizing error amongst the series. Soil moisture dynamics experience dampened response to rain, snowmelt, and evaporative impulses (Manabe 1990). Such dynamics imply that impulse or response mismatches amongst datasets result in errors with dynamics concentrated at lower frequencies, i.e. "red," or more broadly, Markov noise. The combination of coarse-scale global datasets and lack of representative ground "truth" measurements leave much disagreement across different data records depicting the same variable (e.g. soil moisture), leading to severe, slowlyvarying bias among the different data records and uncertain global dynamics overall (Crow 2007; Koster 2009). I desire a method of evaluating and synthesizing different data records, independent of ground data, to produce a "most likely" or "optimal" estimate of soil moisture state given a diverse set of available global time series soil moisture observations. time-series

The time-domain KF/S with ML estimation appropriately fits our above-stated problem, but existing methods do not allow ML estimation under the specific case of AR observation errors. The original method of dealing with KF/S state estimation under AR observation errors requires augmenting the state vector which can destabilize the filter (Kalman 1961). However, Bryson (1967) discovered a more numerically stable KF/S formulation for dealing with AR observation error - using a back-shifted version of the observations - thereby avoiding augmentation of the error processes to the state vector.

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Backshifted observations induce correlation amongst state and observation error innovations, requiring modification of the standard KF/S equations (Bryson 1967). This method of applying the KF/S with backshifted observations, henceforth known as ColKF/S, allows estimation of the unknown state. However, for optimal use of available observations for state estimation I must also find the ML estimate of the ColKF/S system parameters.

The Expectation Maximization (EM) method (Dempster 1977) has advantages over other iterative ML methods, such as quasi-Newton, or non-iterative SS methods or SS. EM does not require computation of KF/S partial derivative matrices, which are computationally expensive, and may become unstable in portions of parameter space. Therefore, EM deals more efficiently with large-dimensional problems and remains stable across parameter space. EM convergence can be slow and require several iterations near the minimum, but for large-dimensional problems this seldom out-weights overall quasi-Newton computational demand (McLaughlin 1997). Although computationally fast, SS methods compute only overall covariance and therefore cannot supply desired information on observation error (Anderson 1979; Kalaith 2000). Shumway and Stoffer (1982) applied the EM framework for estimating parameters of the standard KF/S with observations with white-noise errors and missing values. Gibson (2005) extend Shumway's (1982) EM method to the KF/S with correlated hidden process and observation errors, which accommodates ColKF/S backshifted structure but does not enforce it and does not consider missing values. Backshift further complicates the handling of missing values in EM estimation, because each backshifted observation now potentially contains several missing time-steps. Wu (1996) provide methods for

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constraining EM matrix estimates, allowing enforcement of the specific structure of the Colored-Noise KF/S on EM-estimated system matrices. I combine and extend this previous work to derive EM for ColKF/S, henceforth known as EM-KF/S, with missing observation values using a constrained EM estimator.

I provide an overview of the ideas behind EM-KF/S, followed by detailed presentation of its components, and evaluate it with numerical simulations. First, I describe the density and likelihood to be conditionally maximized. Then, I present the underlying state-space observation model. Next, I present the ColKF/S estimation of the unknown state. This is followed by the application of EM to iteratively estimate ColKF/S system parameters, which requires applying constraints to the EM results at each iteration. I then present a few modifications that can accommodate various observational error structures which arise with real soil moisture data. I test the approach with Monte-Carlo simulations to evaluate numerical robustness for several configurations of observation noise and system parameters. I expect the method will be capable of recovering the underlying system parameters and provide state estimates which are more accurate than or at least as accurate as any individual observation series or their simple sum, whichever is greater.

3.2 SYSTEM DEFINITION AND STATE ESTIMATION

3.2.1 State Space System

A state-space system relates noisy observations to the hidden processes to be estimated. The *m* hidden processes, contained in the $m \times 1$ state vector (\mathbf{x}_t), propagates from time t - 1 to t, at which time it is observed by n noisy observations, contained in the $n \times 1$ observation vector (\mathbf{y}_t):

$$\mathbf{x}_{t} = \mathbf{A}_{t-1}^{s} \mathbf{x}_{t-1} + \mathbf{w}_{t-1}$$
(3.1)

$$\mathbf{y}_t = \mathbf{C}_t \mathbf{x}_t + \mathbf{\eta}_t. \tag{3.2}$$

In the state equation (3.1), the $m \times m$ time model matrix \mathbf{A}_{t-1}^{s} describes the state's dependence on the previous state (superscript s denotes the "signal" process), and the white noise $m \times 1$ vector $\mathbf{w}_{t-1} \sim N(\mathbf{0}, \mathbf{Q}_{t})$. Henceforth I adopt the "weak" definition of "white noise" as a time-uncorrelated series, which may be lag-zero cross-correlated with another white noise series (precluded in the "strong" definition). In the observation equation (2.2), the $n \times m$ observation model matrix \mathbf{C}_{t} relates the observations to the states corrupted by $n \times 1$ white noise $\mathbf{\eta}_{t} \sim N(\mathbf{0}, \mathbf{R}_{t})$. The above system constitutes a state-space form with time-uncorrelated observation error required for standard implementation of the KF/S.

Now, instead of the standard time-uncorrelated observation error (η_t) assumption, let us consider observation errors which follow a Markov or "Colored noise" process:

$$\mathbf{\eta}_t = \mathbf{A}_{t-1}^{\mathbf{n}} \mathbf{\eta}_{t-1} + \mathbf{v}_{t-1}. \tag{3.3}$$

In the error equation (3), the error time model matrix $\mathbf{A}_{t-1}^{\mathbf{n}}$, with superscript **n** denoting the "noise" process (as distinguished from the "signal" process), describes dependence of

the error state on the previous error state with white noise $\mathbf{v}_{t-1} \sim N(\mathbf{0}, \mathbf{R}_t)$. The Markov observation error state space model is now represented by (3.1)-(3.3).

3.2.2 Multi-lag Auto-Regressive Representation

For many applications, the process of interest has correlation persisting to long time lags, as illustrated by the soil moisture series (trend and annual cycle removed) shown in Figure 2.1. Here I want a single (m = 1) estimate of the "true" soil moisture series (\mathbf{x}_t) based on multiple (in this case n = 3) soil moisture observations (\mathbf{y}_t). To model long-term dependence, I use a multi-lag linear Markov process which can be accommodated within the state-space framework. The state equation (3.1) is now:

$$\overline{\mathbf{x}}_{t} = \overline{\mathbf{A}}_{t-1}^{s} \overline{\mathbf{x}}_{t-1} + \overline{\mathbf{w}}_{t-1}, \qquad (3.4)$$

Where $\overline{\mathbf{X}}_t$ models a scalar process (m = 1) with lag order p. I assume the linear Markov process is (weakly) stationary and invertible. For a weakly stationary process, the mean value (μ_t) remains constant for all t and the covariance function defined as $\gamma(s,t) =$ $\gamma(s+h,t+h)$ depends on s and t only through their difference |s-t| (Shumway 2006). In KF/S applications this assumption may be relaxed if changes in μ_t and $\gamma(s,t)$ are explicitly modeled. To use (3.4) I also require the process to be invertible, which allows us to write (Shumway 2006):

$$w_{t} = \pi(z)x_{t} = \sum_{j=0}^{\infty} \pi_{j} x_{t-j}$$
(3.5)

Where $\sum_{j=0}^{\infty} |\pi_j| < \infty$, with $\pi_0 = 1$ and,

$$\pi(z) = \sum_{j=1}^{\infty} \pi_j z^j = \frac{\varphi(z)}{\theta(z)}, \qquad |z| \le 1.$$
(3.6)

The terms $\phi(z)$ and $\theta(z)$ are the autoregressive and moving average polynomials, respectively. The process is invertible and can be written as (3.5) if the complex roots of $\theta(z)$ lie outside the unit circle (i.e. roots of $\theta(z)$ non-zero in (3.6)). I also assume that the roots of $\phi(z)$ are inside the unit circle following the stationarity assumption. Taken together these assumptions allow (3.4) to represent the general class of Autoregressive Moving Average (ARMA) processes. To represent an ARMA process the terms of (3.4) expand to:

$$\overline{\mathbf{x}}_{t} = \begin{bmatrix} x_{t} \\ x_{t-1} \\ \vdots \\ x_{t-p+1} \end{bmatrix}, \quad \overline{\mathbf{A}}_{t-1}^{\mathbf{s}} = \begin{bmatrix} \pi_{1}^{\mathbf{s}} & \pi_{2}^{\mathbf{s}} & \dots & \pi_{p}^{\mathbf{s}} \\ 1 & 0 & \cdots & 0 \\ \vdots & \ddots & \ddots & \vdots \\ 0 & 0 & 1 & 0 \end{bmatrix}, \quad \overline{\mathbf{w}}_{t-1} = \mathbf{D}w_{t-1} = \begin{bmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix} w_{t}.$$
(3.7)

In (3.7), coefficients π_j^s apply to the *j*th lag, and the noise covariance becomes

 $\overline{\mathbf{Q}}_{t-1} = E\{\mathbf{D}w_{t-1}w_{t-1}^{T}\mathbf{D}^{T} = \mathbf{D}\mathbf{Q}_{t-1}\mathbf{D}^{T}\}$, with $E = \{\bullet\}$ defined as the expected value operator. I note that (3.7) is known as "Controllable Canonical" form and that although there are other possible state-space representations for ARFIMA models (Kailath 2000; Shumway 2006; Palma 2007), this form best suites our transformed observations (see Section 3.4). Several observations (n > 1) monitor the state process as follows:

$$\overline{\mathbf{y}}_t = \overline{\mathbf{C}}_t \overline{\mathbf{x}}_t + \overline{\mathbf{\eta}}_t, \tag{3.8}$$

where I collect the observations y_t^j in a column vector

$$\overline{\mathbf{y}}_{t} = \begin{bmatrix} y_{t}^{1} & y_{t-1}^{1} & \dots & y_{t-k\{1\}}^{1} \end{bmatrix} \begin{bmatrix} y_{t}^{2} & y_{t-1}^{2} & \dots & y_{t-k\{2\}}^{2} \end{bmatrix} \cdots \begin{bmatrix} y_{t}^{n} & y_{t-1}^{n} & \dots & y_{t-k\{n\}}^{n} \end{bmatrix}^{\mathbf{T}}, \quad (3.9)$$

with

$$\overline{\mathbf{C}}_{t} = \begin{bmatrix} \frac{c_{1}\mathbf{I}_{k\{1\}} & \mathbf{0}_{k\{1\}\times\max(0,p-k\{1\})}}{c_{2}\mathbf{I}_{k\{2\}} & \mathbf{0}_{k\{2\}\times\max(0,p-k\{2\})}}\\ \vdots & \vdots\\ \hline c_{n}\mathbf{I}_{k\{n\}} & \mathbf{0}_{k\{n\}\times\max(0,p-k\{n\})} \end{bmatrix},$$
(3.10)

where **I** is an identity matrix, and **0** is a matrix of zeros (dimensions of **I** and **0** given in subscripts), and the lag order $k\{j\}$ depends on the *j*th Markov error processes ($\overline{\eta}_t^j$); and the Markov errors are modeled as:

$$\overline{\mathbf{\eta}}_{t} = \overline{\mathbf{A}}_{t-1}^{\mathbf{n}} \overline{\mathbf{\eta}}_{t-1} + \mathbf{L} \mathbf{v}_{t-1}, \qquad (3.11)$$

Where $\overline{\mathbf{\eta}}_{t}^{j}$ takes the same column vector form as (3.9). Making the same assumptions of stationarity and invertibility as the signal model, the error model propagation matrix in (3.11) becomes:

$$\overline{\mathbf{A}}^{\mathbf{n}} = \begin{bmatrix} \pi_{1}^{\mathbf{n}1} & \pi_{2}^{\mathbf{n}1} & \dots & \pi_{k\{1\}}^{\mathbf{n}1} & \mathbf{0} & & \cdots & \mathbf{0} \\ \mathbf{I}_{k\{1\}-1} & \mathbf{0}_{(k\{1\}-1)\times 1} & & \mathbf{0} & & \\ \mathbf{0} & & \pi_{1}^{\mathbf{n}2} & \pi_{2}^{\mathbf{n}2} & \dots & \pi_{k2}^{\mathbf{n}2} & & \\ \mathbf{0} & & \mathbf{I}_{k\{2\}-1} & \mathbf{0}_{(k\{2\}-1)\times 1} & & & \\ \hline \vdots & \vdots & \ddots & \vdots & & \\ \mathbf{0} & & \mathbf{0} & & \cdots & \pi_{1}^{\mathbf{n}n} & \pi_{2}^{\mathbf{n}n} & \dots & \pi_{kn}^{\mathbf{n}n} \\ \mathbf{I}_{k\{n\}-1} & \mathbf{0}_{(k\{n\}-1)\times 1} \end{bmatrix}, \quad (3.12)$$

Where π_i^{nj} the AR coefficients for the *i*th are lag of the *j*th observation error process; and the white noise covariance becomes $\overline{\mathbf{R}}_i = E\{\mathbf{L}\mathbf{v}_i\mathbf{v}_i^{\mathrm{T}}\mathbf{L}^{\mathrm{T}}\} = \mathbf{L}\mathbf{R}_i\mathbf{L}^{\mathrm{T}}$ with



I now replace (3.1)-(3.3) with the multi-lag state space model represented by (3.4), (3.8), and (3.11). Here I focus only on temporal signal and error models, but our overall state-space model structure could be readily extended to the spatial-temporal domain as in Xu (2007) and Katzfuss (2010).

3.2.3 Backshifted Observer for Markov Errors

Since the standard KF/S requires white observation errors, I must transform the observations to whiten their Markov errors using (3.4), (3.8), and (3.11). Specifically, I backshift $\overline{\mathbf{y}}_t$ to obtain the transformed observations (\mathbf{z}_{t-1}) as follows (Bryson 1967):

$$\mathbf{z}_{t-1} = \begin{bmatrix} z_{t-1}^1 & z_{t-1}^2 & \dots & z_{t-1}^n \end{bmatrix}^{\mathbf{T}} = \mathbf{L}^{\mathbf{T}} (\overline{\mathbf{y}}_t - \overline{\mathbf{A}}_{t-1}^{\mathbf{n}} \overline{\mathbf{y}}_{t-1}),$$
(3.14)

Where \mathbf{z}_{t-1} contains only the leading (i.e. t - 1) transformed observations. Note that only the leading value will participate in each KF/S update. Also note that \mathbf{z}_{t-1} requires y_t such that the KF/S update now lags the leading un-transformed observation by one time step. I substitute (3.4) and (3.11) into (3.8) to obtain the transformed observation equation:

$$\mathbf{z}_{t-1} = \mathbf{H}_{t-1} \overline{\mathbf{x}}_{t-1} + \mathbf{u}_{t-1}, \tag{3.15}$$

where,

$$\mathbf{H}_{t-1} = \mathbf{L}^{\mathrm{T}} \overline{\mathbf{H}}_{t-1} = \mathbf{L}^{\mathrm{T}} (\overline{\mathbf{C}}_{t} \overline{\mathbf{A}}_{t}^{\mathrm{s}} - \overline{\mathbf{A}}_{t-1}^{\mathrm{n}} \overline{\mathbf{C}}_{t-1}), \qquad (3.16)$$

$$\mathbf{u}_{t-1} = \mathbf{L}^{\mathrm{T}} \overline{\mathbf{u}}_{t-1} = \mathbf{L}^{\mathrm{T}} (\overline{\mathbf{C}}_{t} \overline{\mathbf{w}}_{t-1} + \overline{\mathbf{v}}_{t-1}), \qquad (3.17)$$

with covariance matrices,

$$\mathbf{R}_{t-1}^{\mathbf{n}} = E\{\mathbf{u}_{t-1}\mathbf{u}_{t-1}^{\mathrm{T}}\} = \mathbf{L}^{\mathrm{T}}(\overline{\mathbf{C}}_{t}\overline{\mathbf{Q}}_{t-1}\overline{\mathbf{C}}_{t}^{\mathrm{T}} + \overline{\mathbf{R}}_{t-1})\mathbf{L}$$
(3.18)

$$\mathbf{S}_{t-1}^{\mathbf{n}} = E\{\overline{\mathbf{w}}_{t-1}\overline{\mathbf{u}}_{t-1}^{\mathrm{T}}\mathbf{L}\} = \overline{\mathbf{Q}}_{t-1}\overline{\mathbf{C}}_{t}^{\mathrm{T}}\mathbf{L}.$$
(3.19)

Note that I have made the simplifying (but unnecessary) assumption, $E\{\mathbf{w}_t\mathbf{v}_t^{\mathrm{T}}\} = \mathbf{0}$. Thus I have now reduced the original state space model (3.4), (3.8), and (3.11) to the backshifted observations (3.4) and (3.15).

Henceforth, to reduce notational clutter, I drop overbars by redefining the following quantities: $\mathbf{x}_t \cong \overline{\mathbf{x}}_t$, $\mathbf{A}_{t-1}^s \cong \overline{\mathbf{A}}_{t-1}^s$, and $\mathbf{Q}_{t-1} \cong \overline{\mathbf{Q}}_{t-1}$. The transformed multi-lag state-space system is then summarized as follows:

$$\mathbf{x}_{t} = \mathbf{A}_{t-1}^{s} \mathbf{x}_{t-1} + \mathbf{w}_{t-1}, \tag{3.20}$$

$$\mathbf{z}_{t-1} = \mathbf{H}_{t-1}\mathbf{x}_{t-1} + \mathbf{u}_{t-1}, \qquad (3.21)$$

with covariance $\mathbf{Q}_{t-1} = E\{\mathbf{w}_{t-1}\mathbf{w}_{t-1}^{T}\}$, $\mathbf{R}_{t-1}^{n} = E\{\mathbf{u}_{t-1}\mathbf{u}_{t-1}^{T}\}$, and $\mathbf{S}_{t-1}^{n} = E\{\mathbf{w}_{t-1}\mathbf{u}_{t-1}^{T}\}$, as previously shown. I are now ready to apply the KF/S to (3.20) and (3.21) to estimate the unknown state (\mathbf{x}_{t}) from available observations (\mathbf{y}_{t}).

3.2.4 Kalman Filter for Correlated Observation and State Noise

I must choose a KF/S formulation which can accommodate correlated observation and state noise from the transformed observation (3.21). I apply the filter formulation given in Bryson (1967), which along with the multi-lag representation (Section 3.2.2), the backshifted observations (Section 3.2.3), filter (Section 3.2.4), and smoother (Section 3.2.5) collectively describes the "Colored-Noise" Kalman Filter/Smoother (ColKF/S). The ColKF/S consists of first a forward "filtering" sweep propagating observation information through time, and then a backward "smoothing" sweep propagating information back through time. I denote the collection of states from time *l* up to and including *h* as $X_{l:h} = {\mathbf{x}_l, \mathbf{x}_{l+1}, ..., \mathbf{x}_t, ..., \mathbf{x}_h}$ and the entire collection of states across time as $X_{1:N} = {\mathbf{x}_1, \mathbf{x}_2, ..., \mathbf{x}_t, ..., \mathbf{x}_N}$. The collection of original and back-shifted observations are denoted $\mathbf{Y}_{1:N} = \{\mathbf{y}_1, \mathbf{y}_2, ..., \mathbf{y}_t, ..., \mathbf{y}_N\}$ and $\mathbf{Z}_{1:N} = \{\mathbf{z}_1, \mathbf{z}_2, ..., \mathbf{z}_t, ..., \mathbf{z}_N\}$, respectively. Sweeping forward through time, the ColKF estimates the "analysis," $\mathbf{x}_{t-1}^a = E\{\mathbf{x}_{t-1} | \mathbf{Z}_{1:t-1}\}$, and its error covariance $\mathbf{P}_{t-1}^a = E\{\mathbf{\tilde{x}}_{t-1} \mathbf{\tilde{x}}_{t-1}^T | \mathbf{Z}_{1:t-1}\}$, with error $\mathbf{\tilde{x}}_{t-1} = \mathbf{x}_{t-1}^a - \mathbf{x}_{t-1}$ (i.e. analysis minus truth) as well as $\mathbf{x}_{t-1}^k = E\{\mathbf{x}_{t-1} | \mathbf{Z}_{1:t}\}$, and its error covariance (\mathbf{P}_{t-1}^k) . Sweeping backward through time and using ColKF results, the ColKS then estimates $\mathbf{x}_{t-1}^s = E\{\mathbf{x}_{t-1} | \mathbf{Z}_{1:N}\}$ and $\mathbf{P}_{t-1}^s = E\{\mathbf{\tilde{x}}_{t-1} \mathbf{\tilde{x}}_{t-1}^T | \mathbf{Z}_{1:N}\}$, exploiting all available observation information. The filter is described below and the smoother in the following section (Section 3.2.5).

Given the state space system (3.20) and (3.21), the ColKF recursions are initialized with \mathbf{x}_0^a and \mathbf{P}_0^a , and then run recursively forward through time:

$$\boldsymbol{\varepsilon}_{t-1} = \boldsymbol{Z}_{t-1} - \boldsymbol{H}_{t-1} \boldsymbol{X}_{t-1}^{a}$$
(3.22)

$$\mathbf{E}_{t-1} = \mathbf{H}_{t-1} \mathbf{P}_{t-1}^{a} \mathbf{H}_{t-1}^{T} + \mathbf{R}_{t-1}^{n}$$
(3.23)

$$\mathbf{K}_{t-1} = \mathbf{P}_{t-1}^{a} \mathbf{H}_{t-1}^{\mathrm{T}} \mathbf{E}_{t-1}^{-1}$$
(3.24)

$$\mathbf{x}_{t-1}^{k} = \mathbf{x}_{t-1}^{a} + \mathbf{K}_{t-1} \mathbf{\varepsilon}_{t-1}$$
(3.25)

$$\mathbf{P}_{t-1}^{k} = \mathbf{P}_{t-1}^{a} - \mathbf{K}_{t-1} \mathbf{H}_{t-1} \mathbf{P}_{t-1}^{a}$$
(3.26)

$$\mathbf{G}_{t-1} = \mathbf{S}_{t-1} \mathbf{E}_{t-1}^{-1} \tag{3.27}$$

$$\mathbf{x}_{t}^{a} = \mathbf{A}_{t-1}^{s} \mathbf{x}_{t-1}^{k} + \mathbf{G}_{t-1} \mathbf{\varepsilon}_{t-1}$$
(3.28)

$$\mathbf{P}_{t}^{a} = \mathbf{A}_{t-1}^{s} \mathbf{P}_{t-1}^{k} (\mathbf{A}_{t-1}^{s})^{\mathrm{T}} + \mathbf{Q}_{t-1} - \mathbf{G}_{t-1}^{s} \mathbf{S}_{t-1}^{\mathrm{T}} - \mathbf{A}_{t-1}^{s} \mathbf{K}_{t-1}^{s} \mathbf{S}_{t-1}^{\mathrm{T}} - \mathbf{S}_{t-1}^{s} \mathbf{K}_{t-1}^{\mathrm{T}} (\mathbf{A}_{t-1}^{s})^{\mathrm{T}}.$$
(3.29)

System matrices change with missing observations as described below in Section 3.2.6, and thus require time subscripts. Other forms of the KF/S for correlated state and observation noise are available (Bryson 1967; Anderson 1979; Gibson 2005) and are analytically, but not necessarily numerically, equivalent. In the case of time-uncorrelated observation noise, or equivalently, uncorrelated state and observation noise, ColKF/S reduces to the standard KF/S.

From (3.22) and (3.23), I have the filter innovations (ε_{t-1}) and their covariance (\mathbf{E}_{t-1}) respectively from which I calculate the "innovations log-likelihood:"

$$L_{\varepsilon} \sim \sum_{t=2}^{N} \log \left| \mathbf{E}_{t-1} \right| + \sum_{t=2}^{N} \boldsymbol{\varepsilon}_{t-1}^{\mathrm{T}} \mathbf{E}_{t-1}^{-1} \boldsymbol{\varepsilon}_{t-1}.$$
(3.30)

I will use the filter innovations log-likelihood to track Expectation Maximization (EM) progress and convergence (Section 3.3.3).

3.2.5 Kalman Smoother for Correlated Observation and State Noise

Once the filter completes its forward sweep through the data series, the smoother then uses the filter results to produce state estimates conditioned on the entire observation record (i.e. $\mathbf{x}_{t-1}^{s} = E\{\mathbf{x}_{t-1} | \mathbf{Z}_{1:N}\}$; Bryson 1967). The smoother is initialized as $\mathbf{x}_{N}^{s} = \mathbf{x}_{N}^{k}$ and $\mathbf{P}_{N}^{s} = \mathbf{P}_{N}^{k}$, then runs recursively backward through time via:

$$\mathbf{J}_{t} = (\mathbf{P}_{t}^{a}(\mathbf{A}_{t}^{s})^{\mathrm{T}} - \mathbf{K}_{t}\mathbf{S}_{t}^{\mathrm{T}})(\mathbf{P}_{t+1}^{a})^{-1}$$
(3.31)

$$\mathbf{x}_{t}^{s} = \mathbf{x}_{t}^{k} + \mathbf{J}_{t} (\mathbf{x}_{t+1}^{s} - \mathbf{x}_{t+1}^{a})$$
(3.32)

$$\mathbf{P}_{t}^{s} = \mathbf{P}_{t}^{k} + \mathbf{J}_{t} (\mathbf{P}_{t+1}^{s} - \mathbf{P}_{t+1}^{a}) \mathbf{J}_{t}^{\mathrm{T}}.$$
(3.33)

Note that \mathbf{x}_{t}^{k} , \mathbf{x}_{t}^{a} , \mathbf{P}_{t}^{k} , \mathbf{P}_{t}^{a} , and \mathbf{K}_{t} are defined in the ColKF sweep (eqns. (3.22) -(3.29)), whereas \mathbf{A}_{t}^{s} and \mathbf{S}_{t} are available from the state space model (eqns. (3.20) -(3.21)). The smoother infers the hidden state and its error covariance ($\mathbf{P}_{t-1}^{s} = E\{\tilde{\mathbf{x}}_{t-1}, \tilde{\mathbf{x}}_{t-1}^{T} | \mathbf{Z}_{1:N}\}$), which then provide a portion of the "missing data" required by EM. EM additionally requires the "Lag-One Smoother Error Covariance," $\mathbf{P}_{t,t-1}^{s} = E\{\tilde{\mathbf{x}}_{t}, \tilde{\mathbf{x}}_{t-1}^{T} | \mathbf{Z}_{1:N}\}$ (Shumway 2006) with $\tilde{\mathbf{x}}_{t} = \mathbf{x}_{t}^{s} - \mathbf{x}_{t}$, which are convenient to calculate alongside the smoother (3.31) - (3.33),

$$\mathbf{P}_{t,t-1}^{s} = \mathbf{P}_{t}^{k} \mathbf{J}_{t-1}^{\mathrm{T}} + \mathbf{J}_{t} (\mathbf{P}_{t+1,t}^{s} - (\mathbf{P}_{t}^{k} (\mathbf{A}_{t}^{s})^{\mathrm{T}} - \mathbf{K}_{t} \mathbf{S}_{t}^{\mathrm{T}})^{\mathrm{T}}) \mathbf{J}_{t-1}^{\mathrm{T}},$$
(3.34)

which is initialized at t = N as

$$\mathbf{P}_{N,N-1}^{s} = (\mathbf{I} - \mathbf{K}_{N-1} \mathbf{H}_{N-1}) (\mathbf{P}_{N-1}^{k} (\mathbf{A}_{N-1}^{s})^{\mathrm{T}} - \mathbf{K}_{N-1} \mathbf{S}.$$
(3.35)

Completion of the backward smoother sweep makes available the state estimates required for each EM iteration. Before applying EM, I must also infer smoothed estimates of missing observations, if present, alongside the hidden state.

3.2.6 Missing Observation Inference

Missing observations must be appropriately omitted during filter updates before computing smoothed values and EM requires smoothed missing observation estimates, because these, along with the hidden state, comprise the "missing data" in EM's "complete data" density (Section 3.3.1). Smoothed missing observations and their error covariance are defined as

$$\hat{\mathbf{y}}_{t}^{s(2)} \cong E\{\hat{\mathbf{y}}_{t}^{(2)} \mid \mathbf{Y}_{1:N}\}, \quad \mathbf{P}_{t}^{y,s(2)} \cong E\{\tilde{\mathbf{y}}_{t}^{s(2)}(\tilde{\mathbf{y}}_{t}^{s(2)})^{\mathrm{T}} \mid \mathbf{Y}_{1:N}\},$$
(3.36)

with $\tilde{\mathbf{y}}_{t}^{s(2)} = \hat{\mathbf{y}}_{t}^{s(2)} - \mathbf{y}_{t}^{s(2)}$. Shumway (1982) provide an algorithm for inferring these quantities for the standard KF/S, but backshifted, multi-lag observations complicate matters.

To illustrate, let us initially assume a single-lag system (p = 1 and $k\{j\} = 1 \forall j$). A missing observation is encountered at time *t* but not before then. I partition the observation vector as $\mathbf{y}_t = [\mathbf{y}_t^{(1)} \mid \hat{\mathbf{y}}_t^{(2)}]^T$, where $\mathbf{y}_t^{(1)}$ are the observed data and $\hat{\mathbf{y}}_t^{(2)}$ are the missing data to be estimated (which implies $\mathbf{P}_t^{y,s(2)} > 0$ and hence the hat notation). I then use (3.14) to rewrite (3.15) as

$$\begin{bmatrix} \mathbf{z}_{t-1}^{(1)} \\ \hat{\mathbf{z}}_{t-1}^{(2)} \end{bmatrix} = \begin{bmatrix} \mathbf{y}_{t}^{(1)} \\ \hat{\mathbf{y}}_{t}^{(2)} \end{bmatrix} - \begin{bmatrix} \mathbf{A}_{t-1}^{\mathbf{n}(1)} & \mathbf{0} \\ \mathbf{0} & \mathbf{A}_{t-1}^{\mathbf{n}(2)} \end{bmatrix} \begin{bmatrix} \mathbf{y}_{t-1}^{(1)} \\ \mathbf{y}_{t-1}^{(2)} \end{bmatrix} = \begin{bmatrix} \mathbf{H}_{t-1}^{(1)} \\ \mathbf{H}_{t-1}^{(2)} \end{bmatrix} \mathbf{x}_{t-1} + \begin{bmatrix} \mathbf{u}_{t-1}^{(1)} \\ \mathbf{u}_{t-1}^{(2)} \end{bmatrix},$$
(3.37)

with

$$\left[\frac{\mathbf{u}_{t-1}^{(1)}}{\mathbf{u}_{t-1}^{(2)}}\right] \sim N\left(0, \left[\frac{\mathbf{R}_{t-1}^{\mathbf{n}(11)} \mid \mathbf{R}_{t-1}^{\mathbf{n}(12)}}{\mathbf{R}_{t-1}^{\mathbf{n}(21)} \mid \mathbf{R}_{t-1}^{\mathbf{n}(22)}}\right]\right).$$
(3.38)

where observation noise \mathbf{u}_{t-1} , lagged observations \mathbf{y}_{t-1} , and partitioned system matrices \mathbf{A}_{t-1}^{n} , \mathbf{H}_{t-1} , and \mathbf{R}^{n} are assigned superscript (2) or (1) if they correspond to missing or nonmissing portions of \mathbf{y}_{t} , respectively. Following Shumway (1982), the missing backshifted observation $\hat{\mathbf{z}}_{t-1}^{(2)}$ in (3.37) would simply be omitted from the filter sweep and using (3.37) and (3.38) I could estimate $\hat{\mathbf{y}}_{t}^{s(2)}$ as follows:

$$\hat{\mathbf{y}}_{t}^{s(2)} = \mathbf{A}_{t-1}^{\mathbf{n}(2)} \, \mathbf{y}_{t-1}^{(2)} + \mathbf{H}_{t-1}^{(2)} \mathbf{x}_{t-1}^{s} + \mathbf{R}_{t-1}^{\mathbf{n}(12)} (\mathbf{R}_{t-1}^{\mathbf{n}(22)})^{-1} (\mathbf{y}_{t}^{(1)} - \mathbf{A}_{t-1}^{\mathbf{n}(1)} \mathbf{y}_{t-1}^{(1)} - \mathbf{H}_{t-1}^{(1)} \mathbf{x}_{t-1}^{s}), \tag{3.39}$$

where $\mathbf{P}_{t}^{y,s(2)} > 0$ since $\hat{\mathbf{y}}_{t}^{(2)}$ is estimated and $\mathbf{P}_{t-1}^{y,s(2)} = 0$ because $\mathbf{y}_{t-1}^{(2)}$ is measured.

Alternatively, I could use (3.37) to augment the state vector with $\hat{\mathbf{y}}_{t}^{(2)}$ and estimate its mean and error covariance during the usual ColKF/S sweeps. This approach provides advantages over (3.39) for our multi-lag, backshifted system. I rearrange (3.37) as

$$\begin{bmatrix} \mathbf{z}_{t-1}^{(1)} \\ \hat{\mathbf{y}}_{t}^{(2)} \end{bmatrix} = \begin{bmatrix} \mathbf{y}_{t}^{(1)} \\ \hat{\mathbf{y}}_{t}^{(2)} \end{bmatrix} - \begin{bmatrix} \mathbf{A}_{t-1}^{\mathbf{n}(1)} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix} \begin{bmatrix} \mathbf{y}_{t-1}^{(1)} \\ \mathbf{0} \end{bmatrix} = \begin{bmatrix} \mathbf{H}_{t-1}^{(1)} & \mathbf{0} \\ \mathbf{H}_{t-1}^{(2)} & \mathbf{A}_{t-1}^{\mathbf{n}(2)} \end{bmatrix} \begin{bmatrix} \mathbf{x}_{t-1} \\ \mathbf{y}_{t-1}^{(2)} \end{bmatrix} + \begin{bmatrix} \mathbf{u}_{t-1}^{(1)} \\ \mathbf{u}_{t-1}^{(2)} \end{bmatrix},$$
(3.40)

which I rewrite in state-space form,

$$\mathbf{x}_{t}^{+} = \begin{bmatrix} \mathbf{x}_{t} \\ \hat{\mathbf{y}}_{t}^{(2)} \end{bmatrix} = \begin{bmatrix} \mathbf{A}_{t-1}^{\mathbf{s}} & \mathbf{0} \\ \mathbf{H}_{t-1}^{(2)} & \mathbf{A}_{t-1}^{\mathbf{n}(2)} \end{bmatrix} \begin{bmatrix} \mathbf{x}_{t-1} \\ \mathbf{y}_{t-1}^{(2)} \end{bmatrix} + \begin{bmatrix} \mathbf{w}_{t-1} \\ \mathbf{u}_{t-1}^{(2)} \end{bmatrix},$$
(3.41)
$$\mathbf{z}_{t-1}^{+} = \begin{bmatrix} \mathbf{z}_{t-1}^{(1)} \\ \mathbf{0} \end{bmatrix} = \begin{bmatrix} \mathbf{H}_{t-1}^{(1)} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix} \begin{bmatrix} \mathbf{x}_{t-1} \\ \mathbf{y}_{t-1}^{(2)} \end{bmatrix} + \begin{bmatrix} \mathbf{u}_{t-1}^{(1)} \\ \mathbf{u}_{t-1}^{(2)} \end{bmatrix},$$
(3.42)

with covariance

$$\mathbf{Q}_{t-1}^{+} = \begin{bmatrix} \mathbf{Q}_{t-1} & \mathbf{S}_{t-1}^{(2)} \\ (\mathbf{S}_{t-1}^{(2)})^{\mathbf{T}} & \mathbf{R}_{t-1}^{\mathbf{n}(22)} \end{bmatrix}, \quad \mathbf{S}_{t-1}^{+} = \begin{bmatrix} \mathbf{S}_{t-1}^{(1)} & \mathbf{0} \\ \mathbf{R}_{t-1}^{\mathbf{n}(21)} & \mathbf{0} \end{bmatrix}, \quad \mathbf{R}_{t-1}^{\mathbf{n}+} = \begin{bmatrix} \mathbf{R}_{t-1}^{\mathbf{n}(11)} & \mathbf{0} \\ \mathbf{0} & \mathbf{R}_{t-1}^{\mathbf{n}(22)} \end{bmatrix}, \quad (3.43)$$

where I denote the error covariance of \mathbf{x}_{t}^{+} as $\mathbf{P}_{t-1}^{+} = E\{\mathbf{\tilde{x}}_{t-1}^{+}\mathbf{\tilde{x}}_{t-1}^{+T}\}$. If $\mathbf{y}_{t-1}^{(2)}$ also happens to be missing, then I replace it with $\mathbf{\hat{y}}_{t-1}^{(2)}$ in (3.41) and (3.42). Note that (3.42) reflects that our only knowledge of the missing observation $\mathbf{\hat{y}}_{t}^{(2)}$ in the measurement model is encompassed by the variance of $\mathbf{u}_{t-1}^{(2)}$, which has the practical benefit of ensuring \mathbf{R}_{t-1}^{n+} is full rank in (3.43).

Let us now consider the case where I observe $\mathbf{y}_{t}^{(2)}$ but $\hat{\mathbf{y}}_{t-1}^{(2)}$ is missing. I redefine the partition as $\mathbf{y}_{t-1} = [\mathbf{y}_{t-1}^{(1)} \mid \hat{\mathbf{y}}_{t-1}^{(2)}]^{\mathrm{T}}$ with superscript (2) or (1) corresponding to missing or non-missing portions of \mathbf{y}_{t-1} , respectively. Using (3.40) with this re-partitioning, I write the observation model as (state model remains (3.41)):

$$\mathbf{z}_{t-1}^{+} = \left[\frac{\mathbf{z}_{t-1}^{(1)}}{\hat{\mathbf{z}}_{t-1}^{(2)}}\right] = \left[\frac{\mathbf{z}_{t-1}^{(1)}}{\mathbf{y}_{t}^{(2)}}\right] = \left[\frac{\mathbf{H}_{t-1}^{(1)} \mid \mathbf{0}}{\mathbf{H}_{t-1}^{(2)} \mid \mathbf{A}_{t-1}^{\mathbf{n}(2)}}\right] \left[\frac{\mathbf{x}_{t-1}}{\hat{\mathbf{y}}_{t-1}^{(2)}}\right] + \left[\frac{\mathbf{u}_{t-1}^{(1)}}{\mathbf{u}_{t-1}^{(2)}}\right],$$
(3.44)

with covariance (\mathbf{Q}_{t-1}^{+} same as (3.43))

$$\mathbf{S}_{t-1}^{+} = \begin{bmatrix} \mathbf{S}_{t-1}^{(1)} & \mathbf{S}_{t-1}^{(2)} \\ \mathbf{R}_{t-1}^{\mathbf{n}(21)} & \mathbf{R}_{t-1}^{\mathbf{n}(22)} \end{bmatrix}, \quad \mathbf{R}_{t-1}^{\mathbf{n}+} = \begin{bmatrix} \mathbf{R}_{t-1}^{\mathbf{n}(11)} & \mathbf{R}_{t-1}^{\mathbf{n}(12)} \\ \mathbf{R}_{t-1}^{\mathbf{n}(21)} & \mathbf{R}_{t-1}^{\mathbf{n}(22)} \end{bmatrix}, \quad (3.45)$$

which corrects $\mathbf{y}_{t}^{(2)}$ using $\hat{\mathbf{y}}_{t-1}^{(2)}$ estimates from the augmented state vector, allowing $\mathbf{y}_{t}^{(2)}$ to be included in the current ColKF update. The system (3.41) and (3.44) also holds for multi-lag systems if $\hat{\mathbf{y}}_{t-h}^{(2)}$ is missing for any $h \ge 1$ prior time-steps. Note that in (3.44) the new measurement $\mathbf{y}_{t}^{(2)}$ allows \mathbf{z}_{t-1}^{+} to participate in ColKF updates because it contains new information, whereas in (3.42) \mathbf{z}_{t-1}^{+} does not participate because $\hat{\mathbf{y}}_{t}^{(2)}$ is missing so no new information is available.

For a summary of missing value permutations using the above partitioned state space models see Table 3.1. Now that I have provided system configurations for all possible missing value permutations, the ColKF/S proceeds with its usual forward and backward sweeps using the augmented system. The advantages of this approach include: (*i*) the ability to do usual ColKF updates (without the additional eqn. (3.39)) when $\hat{\mathbf{y}}_{t-h}^{(2)}$ is missing provided $\mathbf{y}_{t}^{(2)}$ is available which makes full use of available observations and (*ii*) the ability to naturally compute $E\{\tilde{\mathbf{x}}_{t-h}^{s}\tilde{\mathbf{y}}_{t-h}^{sT}\}$ for $h \ge 0$ with $\tilde{\mathbf{y}}_{t}^{s} = \hat{\mathbf{y}}_{t}^{s(2)} - \mathbf{y}_{t}^{s(2)}$ within the ColKF/S sweeps (as provided by \mathbf{P}_{t}^{s+}) without requiring the covariance counterpart of (3.39) given in Shumway (1982). Now the smoothed estimates of $\hat{\mathbf{y}}_{t}^{s(2)}$ and their uncertainty $\mathbf{P}_{t}^{y,s(2)}$ are available for EM.

3.3 System Parameter Estimation

3.3.1 Expectation Maximization

I seek an estimate of the unknown state through time given a set of noisy observations and the state space model ((3.20) and (3.21)) containing a set of time-static parameters. Inference on the unknown state can then be accomplished via the ColKF/S. I denote the state space parameters as $\Theta = \{\mathbf{A}^s, \mathbf{A}^n, \mathbf{C}, \mathbf{Q}, \mathbf{R}, \boldsymbol{\mu}_0, \boldsymbol{\Sigma}_0\}$, with $\boldsymbol{\mu}_0$ and $\boldsymbol{\Sigma}_0$ the initial mean and noise covariance of \mathbf{x}_0 , respectively. The time subscripts of Θ elements have now been suppressed to emphasize that parameter estimates will be static in time although their specific form varies with missing observations as seen in Section 3.2.6. I use the "complete data" density to describe the joint density of the observations and the unknown state as if both were available (i.e. if the unknown state were known; Shumway 2006; Cressie 2014):

$$f(X_{1:N}, Z_{1:N}, \Theta) = f(X_{1:N}, Z_{1:N} | \Theta) f(\Theta) = \dots$$

$$\left[\prod_{t=1}^{N} f(X_{1:t} | X_{1:t-1}, \Theta) \prod_{t=1}^{N} f(Z_{1:t-1} | X_{1:t-1}, \Theta) \right] f(\Theta)$$
(3.46)

where the backshifted state space model and ColKF/S recursions provide the mean and covariance of $f(X_{1:N}, Z_{1:N} | \Theta)$. I infer Θ using EM by minimizing the likelihood of (3.46) alternating between "Expectation" and "Maximization" steps in a series of 84

iterations (Dempster 1977; Shumway 2006) using constraints to enforce ColKF/S structure on the solution (Wu 1996; McLaughlin 1997).

Following Cressie (2014) and using our ColKF/S, I write the negative twice loglikelihood (up to a constant) of (3.46):

$$L_{z}(\Theta \mid X_{1:N}, Z_{1:N}) \equiv -2 \ln f(\Theta \mid X_{1:N}, Z_{1:N}) = \dots$$

$$\ln |\Sigma_{0}| + (\mathbf{x}_{0} - \boldsymbol{\mu}_{0}) \Sigma_{0}^{-1} (\mathbf{x}_{0} - \boldsymbol{\mu}_{0})^{\mathrm{T}} + \ln |\mathbf{M}_{z}| + \sum_{t=2}^{N-1} (\mathbf{z}_{y} - \mathbf{A}_{z} \mathbf{z}_{x}) \mathbf{M}_{z}^{-1} (\mathbf{z}_{y} - \mathbf{A}_{z} \mathbf{z}_{x})^{\mathrm{T}}$$
(3.47)

where the third RHS term follows the form $(\mathbf{z}_y - \mathbf{A}_Z \mathbf{z}_x) \sim N(0, \mathbf{M}_Z)$:

$$\begin{bmatrix} \mathbf{D}^{\mathrm{T}} \mathbf{x}_{t+1} \\ \mathbf{L}^{\mathrm{T}} \mathbf{y}_{t+1} \end{bmatrix} - \begin{bmatrix} \mathbf{D}^{\mathrm{T}} \mathbf{A}^{\mathrm{s}} & \mathbf{0} \\ \mathbf{L}^{\mathrm{T}} \mathbf{H} & \mathbf{L}^{\mathrm{T}} \mathbf{A}^{\mathrm{n}} \end{bmatrix} \begin{bmatrix} \mathbf{x}_{t} \\ \mathbf{y}_{t} \end{bmatrix} = \begin{bmatrix} \mathbf{w}_{t} \\ \mathbf{u}_{t} \end{bmatrix} \sim N \left(\mathbf{0}, \begin{bmatrix} \mathbf{Q} & \mathbf{S}^{\mathrm{n}} \\ (\mathbf{S}^{\mathrm{n}})^{\mathrm{T}} & \mathbf{R}^{\mathrm{n}} \end{bmatrix} \right).$$
(3.48)

Recall that $\mathbf{H} = \mathbf{C}\mathbf{A}^{s} - \mathbf{A}^{n}\mathbf{C}$, $\mathbf{S}^{n} = \mathbf{Q}\mathbf{C}^{T}$ and $\mathbf{R}^{n} = \mathbf{C}\mathbf{Q}\mathbf{C}^{T} + \mathbf{R}$ whereas $\mathbf{D}^{T}\mathbf{x}_{t+1}$ and $\mathbf{L}^{T}\mathbf{y}_{t+1}$ denote leading values (i.e. x_{t} and $[y_{t}^{1} \quad y_{t}^{2} \quad \cdots \quad y_{t}^{n}]^{T}$) of the multi-lag vectors. To arrive at (3.48), I augment the state vector with the entire observation vector as was done for missing values in (3.41). This augmented system is then re-arranged to produce (3.48).

I now take the expectation of (3.47) conditioned on an estimate of Θ at iteration *j* (i.e. $\hat{\Theta}^{j}$):

$$\Lambda_{Z}^{j}(\Theta \mid \hat{\Theta}^{j}) \equiv E\{L_{z}(\Theta \mid X_{1:N}, Z_{1:N}) \mid Z_{1:N}, \hat{\Theta}^{j}\} = \dots$$

$$\ln \left| \boldsymbol{\Sigma}_{0} \right| + \operatorname{tr} \left\{ \boldsymbol{\Sigma}_{0}^{-1} \left[\boldsymbol{P}_{0}^{s} + (\boldsymbol{x}_{0} - \boldsymbol{\mu}_{0})(\boldsymbol{x}_{0} - \boldsymbol{\mu}_{0})^{\mathrm{T}} \right] \right\} + \dots$$

$$(N-3)\ln \left| \boldsymbol{M}_{Z} \right| + \operatorname{tr} \left\{ \boldsymbol{M}_{Z}^{-1} \left[\boldsymbol{Z}_{yy} - \boldsymbol{Z}_{xy} \boldsymbol{A}_{Z}^{\mathrm{T}} - \boldsymbol{A}_{Z} \boldsymbol{Z}_{xy}^{\mathrm{T}} + \boldsymbol{A}_{Z} \boldsymbol{Z}_{xx}^{-1} \boldsymbol{A}_{Z}^{\mathrm{T}} \right] \right\}.$$
(3.49)

where,

$$\mathbf{z}_{\mathbf{y}} = \begin{bmatrix} \mathbf{x}_{t+1}^{s} \\ \mathbf{y}_{t+1} \end{bmatrix} \quad \mathbf{z}_{\mathbf{x}} = \begin{bmatrix} \mathbf{x}_{t}^{s} \\ \mathbf{y}_{t} \end{bmatrix}.$$
(3.50)

and,

$$\mathbf{Z}_{yy} = \frac{1}{N-3} \sum_{t=2}^{N-1} \left(\mathbf{z}_{y} \mathbf{z}_{y}^{\mathrm{T}} + \mathbf{P}_{yy}^{\mathrm{z}} \right), \tag{3.51}$$

$$\mathbf{Z}_{\mathbf{x}\mathbf{y}} = \frac{1}{N-3} \sum_{t=2}^{N-1} \left(\mathbf{z}_{\mathbf{x}} \mathbf{z}_{\mathbf{y}}^{\mathrm{T}} + \mathbf{P}_{\mathbf{x}\mathbf{y}}^{\mathrm{z}} \right), \tag{3.52}$$

$$\mathbf{Z}_{\mathbf{x}\mathbf{x}} = \frac{1}{N-3} \sum_{t=2}^{N-1} \left(\mathbf{z}_{\mathbf{x}} \mathbf{z}_{\mathbf{x}}^{\mathrm{T}} + \mathbf{P}_{\mathbf{x}\mathbf{x}}^{\mathrm{z}} \right).$$
(3.53)

If \mathbf{y}_t is missing, it is replaced by the corresponding $\hat{\mathbf{y}}_t^s$ value obtained from the augmented smoother state, \mathbf{x}_t^{s+} . The \mathbf{P}_{yy}^z , \mathbf{P}_{xy}^z , and \mathbf{P}_{xx}^z matrices are constructed from the appropriate elements of \mathbf{P}_t^{s+} and $\mathbf{P}_{t,t-1}^{s+}$, of which those corresponding to $\hat{\mathbf{y}}_t^s$ will be non-zero. Computation of (3.51)-(3.53) culminates the "Expectation" step.

In the "Maximization" step, I seek to minimize Λ_Z^j with respect to Θ using the results of (3.51)-(3.53), which will provide an updated parameter estimate ($\hat{\Theta}^{j+1}$). This is accomplished by taking the derivatives of (3.49) with respect to Θ , setting them equal to zero, and solving for Θ . An efficient analytical solution is available if I solve for A_Z and

 M_Z rather than directly solving for Θ . Using Shuur complements of

 $(\mathbf{z}_{y} - \mathbf{A}_{z}\mathbf{z}_{x}) \sim N(0, \mathbf{M}_{z})$, the minimizing solution is (Gibson 2005):

$$\mathbf{A}_{\mathbf{Z}}^{j+1} = \mathbf{Z}_{\mathbf{x}\mathbf{y}}\mathbf{Z}_{\mathbf{x}\mathbf{x}}^{-1},\tag{3.54}$$

$$\mathbf{M}_{\mathbf{Z}}^{j+1} = \mathbf{Z}_{\mathbf{y}\mathbf{y}} - \mathbf{Z}_{\mathbf{x}\mathbf{y}}\mathbf{Z}_{\mathbf{x}\mathbf{x}}^{-1}\mathbf{Z}_{\mathbf{x}\mathbf{y}}^{\mathrm{T}}, \tag{3.55}$$

with $\boldsymbol{\mu}_0 = \mathbf{x}_0^s$ and $\boldsymbol{\Sigma}_0 = \frac{1}{N-3} \sum_{t=2}^{N-1} \mathbf{P}_t^s$ following Shumway (2006). However, this solution is incomplete, because $\mathbf{A}_{\mathbf{Z}}$ and $\mathbf{M}_{\mathbf{Z}}$ depend on combinations of certain Θ elements I wish to estimate.

The dependence problem can be overcome using a Generalized EM (McLaughlin 1997) with constraints whereby a solution is found for a partition of $\Theta = \{\Theta_s, \Theta_z\}$, where $\Theta_s = \{\mathbf{A}^n, \mathbf{C}, \mathbf{R}\}$, and then Θ_s is held constant to obtain $\Theta_z = \{\mathbf{A}^s, \mathbf{Q}\}$. Generalized EM allows each EM iteration to be broken into sub-steps provided each sub-step incrementally increases the likelihood (McLaughlin 1997). To obtain Θ_s I re-arrange (3.14) to isolate the leading observations ($\mathbf{L}^T \mathbf{y}_{t+1}$) and use the results to rewrite (3.48) in the form $(\mathbf{s}_v - \mathbf{A}_s \mathbf{s}_x) \sim N(0, \mathbf{M}_s)$:

$$\begin{bmatrix} \mathbf{L}^{\mathrm{T}} \mathbf{y}_{t+1} \end{bmatrix} - \begin{bmatrix} \mathbf{A}^{\mathrm{n}} \mid \mathbf{C} \mid -\mathbf{A}^{\mathrm{n}} \mathbf{C} \end{bmatrix} \begin{bmatrix} \mathbf{y}_{t} \\ \overline{\mathbf{D}^{\mathrm{T}} \mathbf{x}_{t+1}} \\ \overline{\mathbf{x}_{t}} \end{bmatrix} = \begin{bmatrix} \mathbf{v}_{t} \end{bmatrix} \sim N(\mathbf{0}, \mathbf{R}), \qquad (3.56)$$

where,

$$\mathbf{s}_{\mathbf{y}} = \begin{bmatrix} \mathbf{L}^{\mathrm{T}} \mathbf{y}_{t+1} \end{bmatrix} \quad \mathbf{s}_{\mathbf{x}} = \begin{bmatrix} \frac{\mathbf{y}_{t}}{\mathbf{D}^{\mathrm{T}} \mathbf{x}_{t+1}^{s}} \\ \frac{\mathbf{D}^{\mathrm{T}} \mathbf{x}_{t}^{s}}{\mathbf{x}_{t}^{s}} \end{bmatrix}, \quad (3.57)$$

which replaces (3.50). I re-formulate the likelihood in (3.47) using (3.56) to obtain L_S and apply the corresponding Expectation ((3.49) and (3.51)-(3.53)) and Maximization ((3.54) and (3.55)) steps to obtain \mathbf{A}_{S}^{j+1} and \mathbf{M}_{S}^{j+1} . To yield $\hat{\Theta}_{S}^{j+1}$, constraints are applied to \mathbf{A}_{S}^{j+1} enforcing the structure given in (3.56). Then to get $\hat{\Theta}_{Z}^{j+1}$, I apply constraints to fix the elements of \mathbf{A}_{Z}^{j+1} associated with Θ_{S} . I now collectively have an estimate for $\hat{\Theta}^{j+1} = {\hat{\Theta}_{S}^{j+1}, \hat{\Theta}_{Z}^{j+1}}$ consistent with the ColKF/S state space structure. EM iterations begin with a set of starting values ($\hat{\Theta}^{0}$) and proceed until the likelihood (L_Z) decreases less than a specified tolerance in subsequent iterations.

In addition to the above required constraints, I allow several optional constraints to further condition the solution for $\hat{\Theta}^{j+1}$. I constrain A^n to be block diagonal, such that the Markov error model for each observation series does not interact with the other series, although I allow for off diagonal elements of the **R** matrix. All covariance matrices by definition must be symmetric and positive-definite which is ensured after every iteration by computing the Cholesky decomposition and reforming the matrix. Although rarely occurring in our experience, EM iterations are immediately terminated if the symmetric positive-definite constraint is violated; however, this possibility could be addressed in the future using a square-root filter as in Gibson (2005). It may also be desirable in some situations to hold **C** constant. I may additionally wish to enforce a specific structure,

such as ARMA or ARFIMA (see Section 3.4.1), on the π elements of A^n and A^s (see Section 3.2.3).

3.3.2 Matrix Constraints

Constraints on the EM solution are required to enforce the ColKF/S structure on and condition the Θ estimates. Wu (1996) provide formula for constraining of the Az and As matrices (henceforth denoted $A_{\{Z,S\}}$) in (3.48) and (3.56). Linear constraints are defined as:

$$\mathbf{F}vec(\mathbf{A}_{\{Z,S\}}) = \Psi, \tag{3.58}$$

where Ψ is a $c \times 1$ vector of constraint constants, **F** is a $c \times l$ selection matrix of ones and zeros, and the *vec*(•) operator stacks the columns of $A_{\{Z,S\}}$ on top of one another to make a long vector of length $l \times 1$. This form can handle additive and equality constraints, but I also require non-linear constraints to implement EM for the Colored Noise KF/S.

I generalize Wu's (1996) results to non-linear constraints defined as:

$$\mathbf{F}(\mathbf{\theta})vec(\mathbf{A}_{\{Z,S\}}) = \mathbf{\Psi}$$
(3.59)

where $\theta \in \Theta$ and $\mathbf{F}(\theta)$ is a non-linear function. Adopting results from Rodgers (2000), I apply Gauss-Newton for the problem of finding function zeros. I define \mathbf{F}_i as a $c \times l$ matrix of derivatives with *g*th row corresponding to the *g*th constraint:

$$\mathbf{f}_{g} = \frac{\partial \psi(\mathbf{\theta})_{g}^{i}}{\partial \operatorname{vec} \left(\mathbf{A}(\mathbf{\theta})_{[Z,S],i}^{j+1}\right)^{\mathrm{T}}}.$$
(3.60)

See Appendix B for derivation and example. Constraints can then be iteratively applied using:

$$vec(\mathbf{A}_{\{Z,S\},(i+1)}^{j+1}) = vec(\mathbf{A}_{\{Z,S\},(i)}^{j+1}) + \Omega \mathbf{F}_{i}^{\mathbf{T}} \left(\mathbf{F}_{i} \Omega \mathbf{F}_{i}^{\mathbf{T}}\right)^{-1} \Delta_{i}, \qquad (3.61)$$

$$\Delta_i = \Psi - \mathbf{F}_i \operatorname{vec}(\mathbf{A}_{\{Z,S\},(i)}^{j+1}), \tag{3.62}$$

$$\Omega = \mathbf{M}_{\{Z,S\}}^{j+1} \otimes \mathbf{Z}_{\mathbf{x}\mathbf{x}}^{-1}, \tag{3.63}$$

where *i* represents the constraint iteration, *j* is the EM iteration, \otimes is the Kronecker Delta, and subscript *S* interchanges with *Z* based on whether **A**_S from (3.56) or **A**_Z from (3.48) is constrained. If constraining **A**_Z from (3.48), iterations begin with **A**_Z and **Z**_{XX} then proceed until the largest deviation of max $|\mathbf{F}_{i}vec(\mathbf{A}_{Z,(i+1)}^{j+1}) - \Psi|$ is within a specific small tolerance. Convergence is rapid since the method is quasi-Newton. In the case of linear constraints, (3.60) reduces to a selection matrix as in (3.58) and the method converges after a single iteration.

3.3.3 Discussion on Numerics and Model Selection

Application of constraints is discretionary with several possible options and configurations. The user must specify process and error structure and how many p and k lags to include in the system. If more lags are specified than effectively exist, the EM

solution may be degraded by overfitting, especially if observation series are relatively short and/or contain outliers. Although optimality is difficult to achieve with real data, a well-specified system will ensure robust and near-optimal estimates. Poor EM solutions indicate either poorly specified system, too few observations, or a combination of both. Additionally some parameters are non-identifiable or poorly conditioned in certain portions of parameter space. For example, one can readily see from (3.15) that **C** is unidentifiable if **A**^s and **A**ⁿ share identical AR poles (see Section 3.2.2). In this case EM still gives a sensible solution, but **C** estimates will plateau once **A**^s and **A**ⁿ poles converge and generally will not reach their true values. I will revisit some of these issues with numerical simulations (See Section 3.5). While a detailed treatment of model selection is outside the scope of this letter, users should remain attentive to the possibility of an overfit or a mis-specified system or error models when designing the system configuration.

3.4 EXTENDED MODELS

3.4.1 Long Memory Processes

Hydrologic time-series have been forefront in the study of long-memory and therefore soil moisture time-series likely contain long-memory dynamics. In a classic study, Hurst (1951) originally discovered long-memory persistence for reservoir level time-series data. Later, Hosking (1984) introduced the concept of fractional differencing to model Nile river flow datasets. Like reservoir and river level datasets, soil moisture may contain long-memory dynamics, perhaps relating to a multi-season or multi-year response to long-term dry or wet periods. Such patterns might therefore be a useful indicator of drought persistence.

In fractional differencing, time-persistence depends on a differencing parameter (d, where |d| < 0.5 for stationary process). This process can be approximated by an AR(∞) model truncated after L lags with coefficients (π_l ; Palma 2007; Palma & Chan 1997):

$$\pi_{j} = \phi_{j} + \sum_{k=1}^{\min(p,k)} \varphi_{k} \phi_{j-k} + \theta_{j} - \sum_{l=1}^{\min(q,l)} \theta_{l} \pi_{j-l} \qquad j = 0, 1, \dots, L \qquad (3.64)$$

$$\phi_j = \frac{\Gamma(j-d)}{\Gamma(j+1)\Gamma(-d)} \qquad \qquad j = 0, 1, \dots, \infty$$
(3.65)

where $\Gamma(x+1) = x\Gamma(x)$ is the gamma function (Shumway 2006). The coefficients in (3.64) define an all-pole (AR(*L*)) approximation for an AR Fractionally Integrated Moving Average (ARFIMA(*p*, *d*, *q*)) model with fractional difference, AR(*p*), and MA(q) coefficients *d*, ϕ_k , and θ_l , respectively. Although the AR(*L*) coefficients can be estimated with EM, *d* would generally require a quasi-Newton step, because the AR(*L*) coefficients are a non-linear function of *d* (McLaughlin 1997). However, quasi-Newton becomes computationally demanding because *L* should be large (say 30-100 lags) for a good approximation, increasing the state dimension (Palma 2007; Grassi 2014). Since *d* imposes a non-linear constraint on EM's AR(*L*) solution, as an alternative I can estimate *d* efficiently using the constrained EM without computing filter partial derivatives. To implement constrained EM for an ARFIMA model I must write AR(*L*) coefficients as in (3.64) and take the gradient of π with respect to the ARFIMA model parameters:

$$\nabla \boldsymbol{\pi}_{i} = \left\{ \frac{\partial \pi_{1}(d, \varphi_{k}, \theta_{l})}{\partial (d, \varphi_{k}, \theta_{l})}, \frac{\partial \pi_{2}(d, \varphi_{k}, \theta_{l})}{\partial (d, \varphi_{k}, \theta_{l})}, \dots, \frac{\partial \pi_{j}(d, \varphi_{k}, \theta_{l})}{\partial (d, \varphi_{k}, \theta_{l})} \right\}$$
(3.66)

where *i* represents the constraint iteration. I then augment A_Z , M_Z , and Z_{XX} from (3.61)-(3.63) as follows:

$$\mathbf{A}_{Z}^{\#} = \begin{bmatrix} \mathbf{A}_{Z} & \mathbf{0} \\ 0 & \{d, \phi_{k}, \theta_{l}\} \end{bmatrix} \qquad \mathbf{M}_{Z}^{\#} = \begin{bmatrix} \mathbf{M}_{Z} & \mathbf{0} \\ 0 & \mathbf{M}_{Z} \end{bmatrix} \qquad \mathbf{Z}_{\mathbf{xx}}^{\#} = \begin{bmatrix} \mathbf{Z}_{\mathbf{xx}} & \mathbf{0} \\ 0 & \nabla \boldsymbol{\pi}_{i} \nabla \boldsymbol{\pi}_{i}^{\mathrm{T}} \end{bmatrix}$$
(3.67)

$$\Delta_{i}^{\#} = \left[\frac{\Delta_{i}}{\hat{\boldsymbol{\pi}}_{i} - \boldsymbol{\pi}_{i}(d, \phi_{k}, \theta_{l})}\right]$$
(3.68)

Where $\hat{\pi}_i$ is the portion of \mathbf{A}_Z containing the AR(*L*) coefficients (see Appendix A). Constraint iterations then proceed to update $\mathbf{A}_Z^{\#}$ as before, while $\mathbf{Z}_{xx}^{\#}$ is now also updated for each iteration. If ARFIMA observation errors are desired, then *Z* replaced by *S* in (3.67). This method amounts to fitting the ARFIMA model to the AR(*L*) coefficients from the EM solution using a quasi-maximum-likelihood approach (Beran 1995). For our purposes, constraining AR(*L*) with the ARFIMA model desirably dampens random variations at long lags typically occurring in noisy observations. These variations decrease the likelihood, but do not necessarily result in more accurate state estimates – an indication of over-fitting guarded against by applying the ARFIMA constraints.

3.4.2 Observations with Mixed Markov and Time-Uncorrelated Noise

Soil moisture data series potentially contain additional time-uncorrelated noise, which is added to, but not integrated through the Markov noise process described by (3.3). For remotely-sensed soil moisture this originates from sensor noise among other physical factors and may be amplified or attenuated by the numerical retrieval algorithm required to convert electromagnetic quantities to soil moisture. To accommodate such a situation, I provide an alternative observation model:

$$\mathbf{y}_t = \mathbf{C}_t \mathbf{x}_t + \mathbf{\eta}_t + \mathbf{q}_t \tag{3.69}$$

Where \mathbf{q}_t is additional white noise, which is not integrated with $\mathbf{\eta}_t$ at each time-step and applied to individual observation series. The white noise source in (3.69) contaminates a back-shifted observation with a non-white, moving average term, $\mathbf{q}_t - \overline{\mathbf{A}}_t^{\mathbf{n}} \mathbf{q}_{t-1}$. Rather than use the contaminated back-shifted observation, I must now augment the state vector and associated system matrices with the observation's AR error ($\mathbf{\eta}_t$):

$$\mathbf{x}_{t-1}^{*} = \begin{bmatrix} \mathbf{x}_{t-1} \\ \mathbf{\eta}_{t}^{(3)} \end{bmatrix}, \mathbf{A}^{*} = \begin{bmatrix} \mathbf{A}^{*} & \mathbf{0} \\ \mathbf{0} & \mathbf{A}^{*} \end{bmatrix}, \mathbf{H}^{*} = \begin{bmatrix} \mathbf{H}^{(12)} & \mathbf{0} \\ \mathbf{C}^{(3)}\mathbf{A}^{*} & \mathbf{1} \end{bmatrix}, \mathbf{Q}^{*} = \begin{bmatrix} \mathbf{Q} & \mathbf{0} \\ \mathbf{0} & E\{\mathbf{v}_{t}^{(3)}\mathbf{v}_{t}^{(3)}\mathbf{T}\} \end{bmatrix}$$
(3.70)

$$\mathbf{A}^{\mathbf{n}^*} = \begin{bmatrix} \mathbf{A}^{\mathbf{n}(23)} & \mathbf{0} \\ \hline \mathbf{0} & \mathbf{0} \end{bmatrix}, \ \mathbf{R}^* = \begin{bmatrix} E\{\mathbf{v}_t^{(12)}\mathbf{v}_t^{(12)}\mathbf{T}\} & E\{\mathbf{q}_t\mathbf{v}_t^{(12)}\mathbf{T}\} \\ E\{\mathbf{v}_t^{(12)}\mathbf{q}_t^{\mathbf{T}}\} & E\{\mathbf{q}_t\mathbf{q}_t^{\mathbf{T}}\} \end{bmatrix}$$
(3.71)

Where superscripts (3) and (12) indicates the augmented and non-augmented portions of the observation vector. Missing value estimation then proceeds as usual by substituting

 \mathbf{x}_{t-1}^* for \mathbf{x}_{t-1} in (3.41) and making the corresponding substitutions in (3.43). The EM "Constrain" step then requires minor modifications to enforce the structure of (3.70) and (3.71).

3.4.3 Least-Squares Method for Estimating System Parameters When the State is Available

To evaluate the EM method in practical applications, I need an independent means of estimating system parameters when benchmark data of the hidden process are available. Such a method could also have value for exploratory data analysis to better understand observation error structure for more effectively implementing EM. Although these estimates could technically be accomplished with EM, they would suffer from the same numerical and implementation biases. Instead I rely on a sub-space system identification method called "Balanced Stochastic" (StochBal for short, Katayama 2007). The StochBal method decomposes a collection of time-series into their innovations by means of orthogonal states, the number of which ranges from one to n depending on how many observations contain red-noise error (or equivalently, how many underlying non-white states are observed). For the observation series (\mathbf{y}), these innovations will be asymptotically equivalent to the ColKF/S innovations given in (3.22) because KF systems have many equivalent forms (Anderson 1979). I likewise generate the benchmark data innovations (\mathbf{u}_i) and from these compute **C** and **R**:

$$\mathbf{C} = \boldsymbol{\varepsilon}^{\mathrm{T}} \mathbf{u}^{-1}, \quad \mathbf{R} = E\{[\boldsymbol{\varepsilon}_{t} - \mathbf{C} \mathbf{u}_{t}][\boldsymbol{\varepsilon}_{t} - \mathbf{C} \mathbf{u}_{t}]^{\mathrm{T}}\}$$
(3.72)

Where **u** and ε contain the entire collection of innovations through time and have respective dimensions $N \times m$ and $N \times n$ (denoted by lack of subscripts). Missing values are omitted from the rows of **y**. Details of StochBal and associated MATLAB code can be found in Katayama (2005). To estimate AR coefficients ($\hat{\pi}$) for A^s and Aⁿ I form the Hankel matrix, $\mathbf{X} = \{\mathbf{x}_{1:N-L}, \mathbf{x}_{2:N-L-1}, ..., \mathbf{x}_{L:N}\}$ and $\mathbf{Z}_{\mathbf{x}} = E\{\mathbf{X}\mathbf{X}^{\mathrm{T}}\}$, computing the expectation using only non-missing pairs. This matrix can be partitioned and used to take the conditional expectation for $\hat{\boldsymbol{\pi}}$ as follows:

$$\hat{\boldsymbol{\pi}} = \mathbf{Z}_{1,1:N-L} \mathbf{Z}_{2:N-L-1,2:N-L-1}^{-1}$$
(3.73)

Where subscript 1: N - L collects all matrix elements corresponding to times ranging from t = 1 to t = N - L. I will test the control methods using simulation in Section 3.5; however, to allow more space for the EM simulation results (the primary focus of this letter) I show only a subset of the results concerning this method. This estimation method is applied to real soil moisture data in Chapter 4.

3.5 SIMULATION STUDY

3.5.1 Simulation Objectives

Several factors can affect performance of the derived methods in operational situations with real datasets. First, some parameters may not be identifiable in certain regions of parameter space. Second, EM convergence may be slow or converge to a local minimum when given certain starting values. Third, real data may have noise or process structure which violate underlying assumptions, including non-random missing data gaps or non-Gaussian noise. Fourth, the overall structure may be correct but the model is over-fit (for example: considering too many lags, etc.). Fifth, the observation sampling or information content may be insufficient (e.g. time series too short, too noisy, or too many missing values) to give stable estimates of the underlying system. In operational cases, these five factors interact to degrade the optimality of EM parameter and ColKF/S state estimates. Simulation experiments with known, "True" generating processes and parameters help to verify expected algorithm behavior and inform real data application. I perform numerical simulations to (i) ensure the method gives reasonable results for basic scenarios when all assumptions are met, (ii) investigate how method responds when parameters are not identifiable and, (iii) test method for scenarios where assumptions violated to a degree likely encountered with real data.

3.5.2 Simulation Experimental Methods

I run several (i.e. 14) simulation experiments to test the EM method under various system configuration cases (Table 3.3). Simulation cases are assigned a code based on their configuration. Codes indicate whether a simulation assumes AR, AR plus white noise, or ARFIMA (fractionally-differenced) process and/or errors ('R', 'W', or 'F', respectively), and whether a simulation contains missing values and/or non-Gaussian innovations ('M' or 'G', respectively). The basic AR process and AR noise ('RR') configurations also have a number code ('1' to '4') specifying that the base configuration was applied to simulated data to test robustness against mis-specified assumptions or differing system parameter values. RR1 is the basic RR configuration with p = 1 and $k^{1,2,3} = 1$ for both true and estimation systems. For RR2, the true parameters $\phi_1^{n1,2,3}$ are all

assigned a value of 0.9 (equal to ϕ_1^d) to test how **C** parameters respond when process and noise share poles. For RR3, the RR configuration with $k^3 = 10$ uses the true system from the RW case, to test how robust the basic configuration is to additional white noise, which includes a moving average component requiring additional AR *k* lags to approximate. Note that for RR3, r_{33} actually represents $r_{33} + (\sigma_w^{n3})^2$, with

 $(\sigma_w^{n3})^2 = E\{\mathbf{v}_t^{(3)}\mathbf{v}_t^{(3)T}\}\$ because RR does not separate AR and white noise components. For RR4, the true system generated from FF and estimation system assigned p = 30 and $k^{1,2,3} = 30$ to test potential over-fitting in the presence of long-memory process and noise.

For each case, I randomly generate 30 realizations of the hidden process and observation series with specified ("true") system parameters each with 1460 time-steps representing four years of daily soil moisture estimates. All simulations were conducted using MATLAB ® R2011b on a Linux compute server with 16 Intel® Xenon Sandy Bridge cores with 64 GB total memory. The EM method was allowed to iterate until the likelihood decreased by < 0.01 in subsequent iterations or reached a maximum number of 100 iterations (which never occurred here). For 'M' cases, I generate missing value gap lengths with a Poisson distribution (mean parameter, $\lambda = 1$) and assigned these gaps to y^3 time indices with uniform probability, resulting in 30-35 % missing values in the record. This simulates typical remote-sensing soil moisture observation gaps. Deterministic gaps were also applied to all observations $y^{1,2,3}$ for specified intervals. This simulates the effect of missing winter-time soil moisture time-series when soils are frozen (and therefore not measurable). For 'G' cases, non-Gaussian noise was generated using an exponential distribution (mean parameter, 0.1) to mimic a specified number of rain-
wetting events (292 or 20 % of time record), this noise was multiplied by 40 and added to the Gaussian noise with variance 0.5. Similarly generated non-Gaussian noise was also assigned to 30 % of the observation series innovations with uniform probability to simulate observation errors. All innovations and/or noise were given pre-specified covariance using their covariance Cholesky decomposition (Shumway 2006). These missing value and non-Gaussian generation methods provide time series which qualitatively match soil moisture observation characteristics (See Section 3.5.2).

For each realization, I apply the EM and SS control methods to estimate the system parameters and compare these with the true values. I compare EM-ColKF/S state estimates to the true hidden state and two alternative estimates of the hidden state, which include ColKF/S run with the true parameter values (as an upper performance bound) and a simple average of all the observations for each time (as a lower performance bound). In terms of correlation with the true hidden state, the EM and ColKF/S performance should always match or beat the most skilled observation or the simple average of all observations, whichever is greater.

3.5.3 Colored Noise Filter/Smoother Performance

I find favorable EM-calibrated ColKF/S performance for all 14 site test cases (Figure 3.2). Median correlations across realizations consistently meet performance criteria by matching or beating the most skilled observation or the simple average of all observations, whichever is greater, within median confidence bounds. Non-Gaussian cases have no perceptible impact on smoother skill for either RR{M,G} or FF{M,G} cases. Missing values degrade smoother skill somewhat (0.94 to 0.93) for RRM, but have less impact in FFM cases. EM-ColKF/S correlations remain within 0.1 of the ColKF/S with perfect parameters in all cases but RRM and RR2 (Figure 3.2). The RR2 case represents the least-favorable performance, with correlation falling to 0.76 (vs. 0.8 for perfect ColKF/S) – nevertheless, the value remains on par with the simple average (0.77) and within median 95% confidence bounds (\pm 0.02). These results indicate that the EM-ColKF/S method remains robust to missing values and non-Gaussian innovations, but encounters difficulty when noise and processes share poles (as for RR2).

Characteristics of the simulated datasets, particularly the RRG, RW, and FFM series, resemble real soil moisture data from a Lethbridge, Alberta, Canada pasture site (Figure 3.3). The Lethbridge data were de-trended and cyclic components were removed from each observation. The benchmark "true" process for this dataset is from Time Domain Reflectometry (TDR) probe *in situ* measurements and "observations" are from the Modern Era Retrospective Reanalysis (MERRA; model reanalysis), Advanced Scanning Microwave Radiometer (AMSR-E; satellite), and another model driven with satellite-based precipitation and evapotranspiration estimates (See Chapter 4). An associated example time-series of EM-ColKF/S state error covariance (from the RM case) shows response to missing observations (Figure 3.3 and Figure 3.4, respectively). For longer gaps, error covariances plateau to a steady value at a rate dependent on the overall system time-response, determined by hidden and error process AR memory length. Smoother error covariances are symmetric across each gap because the smoother draw upon both upstream and downstream information for estimates along the gap's edges.

3.5.4 Expectation Maximization Performance for AR Process

EM recovers system scaling (C) and covariance (Q and R, including off-diagonal elements) parameters for AR error test cases (Table 3.4). Realization mean C estimates are typically within ± 0.1 ranging up to ± 0.3 of the true values. Realization mean covariances typically fall within 0.3 of the true values for the RR, RRM, and RRG cases (excluding RR2), but range up to ± 1.6 for many other cases (Figure 3.5). Missing values increase parameter variability by a factor of ≈ 2 (Figure 3.6), whereas non-Gaussian innovations have little impact on parameter variability (Table 3.4). RR2 overestimates c_2 by 0.28±0.02, while under-estimating r_{22} by -1.58 ± 0.07, with similar bias for the associated off-diagonal elements (Table 3.7). FFM and FF2 are also notable exceptions, with all elements of C overestimated by 0.13-0.18 (\pm 0.17) for FFM and c_2 overestimated by 0.28±0.02. For FFM, the diagonal elements of **R** are also underestimated by \approx -1.0 and Q is under-estimated by -0.8 (Table 3.4). Taken together these results indicate (i) non-Gaussian innovations have little impact on C, Q, and R, (ii) missing values increase estimate variability, which is likely related to the decreased sample size, and (iii) biases occur for long-memory systems with missing-values (FFM) and when errors share poles with the hidden process (RR2).

EM generally recovers underlying hidden process and error AR (ϕ) and fractionaldifferencing (*d*) coefficients (Table 3.5 and Figure 5.5-Figure 5.7). The ϕ coefficients are accurately recovered (within ± 0.01-0.02) for most cases, including the RR2 case which had biased **C**, **Q**, and **R** estimates. Biases increased somewhat for FFM (up to ±0.06). Missing values and non-Gaussian innovations have a similar impact on ϕ and *d* variability as for **C**, **Q**, and **R** estimates. Although mean values for the *d* parameter fall relatively close to the true values (except for FFM), the variability of the d^n estimates across realizations is quite high (>0.1) when ARFIMA errors are present (FF, FFM, and FFG), whereas d^d variability remains smaller. These results are comparable to other state-space-based ARFIMA fitting methods tested in Grassi (2014). For FFM, the d^n estimates are indistinguishable amongst the three observations, indicating they are not well identified. Taken together these results suggest (i) ϕ and d can be accurately identified even when scaling and covariance parameters are biased and (ii) that ϕ and especially d lose accuracy when ARFIMA errors and missing values are present, suggesting that increased sampling is needed to obtain accurate parameter estimates.

3.5.5 Expectation Maximization Performance for AR+W Process

The AR+W error cases give similar performance to the AR cases discussed in Section 3.5.4; however, I find that the AR+W configuration results in substantially less accurate estimates of r_{33} relative to the AR-only cases (Table 3.6). This discrepancy relates to the high noise level assigned to white noise variance ($(\sigma_w^{n3})^2$) and associated loss of predictive power for estimating embedded AR error process in white noise. I also find that d^d is substantially underestimated when missing values and non-Gaussian innovations are present (Table 3.7). In preliminary investigations, I found the AR+W configuration requires more careful initial value selection relative to AR-only cases. If the q, ϕ_1^{n3} , and r_{33} initial parameters are set substantially below their true values (compare initial values for Table 3.4 and Table 3.5 with Table 3.6 and Table 3.7), convergence proceeds very slowly. Therefore, initial values should be selected well above anticipated values at convergence.

3.5.6 Comparison of AR+W and ARFIMA Cases with AR-only Configuration

Since the ARFIMA (i.e. FF cases) and AR+W (i.e. RW) modifications increase algorithm complexity, and results indicate associated reduced robustness, I wondered how well the basic AR-only configurations (i.e. RR cases) would perform when misapplied to such situations. To investigate I ran the RR3 and RR4 configurations on realizations generated for respective FF and RW cases. In the RR3 case, estimated π have higher variability at long lags relative to the FF solution (Figure 3.8). In Figure 3.8a, I see that solving for π at all lags (as in RR3) can lead to apparent model over-fitting where noise disproportionately affects individual π coefficients at longer lags. However, Figure 3.8b shows that application of ARFIMA constraints (as in Eqn. (3.64)) effectively dampens the variability at longer lags leading to a more stable solution. Though the ColKF/S state skill improvement observed here were insignificant, Pearson correlation of 0.974 \pm 0.0027 for FF vs. 0.973 \pm 0.0028 for RR3, the difference could become more crucial with more-biased and noisier real datasets.

In the RR4 case, estimated π have lower values, but persist to longer lag relative to the RW solution (Figure 3.9) and RR4 substantially overestimates $r_{33} + (\sigma_w^{n3})^2$ (Table 3.6). Using (3.3), (3.14), and (3.69), I see that application of the RR4 configuration to AR+W noise gives additional moving average noise of the form $\mathbf{q}_t - \overline{\mathbf{A}}_t^n \mathbf{q}_{t-1}$, requiring additional π lags to approximate. Though the ColKF/S state skill improvement is also insignificant, Pearson correlation of 0.924 ± 0.0079 for RW vs. 0.921 ± 0.0082 for RR4, the improvement may be greater for noisier real datasets. The two situations presented here (i.e. RR4 vs. RW and RR3 vs. FF) underscore the importance of model selection in effective application of the EM-ColKF/S with real datasets.

3.6 CONCLUSION

I have presented an EM method to calibrate a ColKF/S, motivated by the application of jointly merging and characterizing error of multiple global soil moisture datasets. In addition to the basic ColKF/S with AR process and errors, I also address the possibility of long-memory and additional white noise error terms. Our methods build upon previous work developing the ColKF/S (Bryson 1967) and EM methods for KF/S maximum likelihood estimation (Shumway 1982; Wu 1996; Gibson 2005). I test the EM-ColKF/S with a set of test case simulations, designed to mimic specific characteristics of soil moisture time-series.

I find the method capable of recovering system parameters in nearly all cases and in particular it remains robust for non-Gaussian innovations. However, estimates underperform when process and noise share poles, when long-memory processes have missing values, and when white noise and AR bias are jointly present. Nevertheless, I show that the long-memory and AR plus white noise modifications add additional value over the basic AR configuration. These results underscore the importance of model selection when applying the EM-ColKF/S methods. In all test cases, the EM-ColKF/S state estimates meet or exceed the skill of the most skilled observation or the observation average series, whichever is greater – and therefore meet our fundamental performance criteria. I direct interested readers to Jones (2015) where I apply the EM-ColKF/S method to real soil moisture observation datasets. Aside from soil moisture, the AR methods presented here apply to a wide range of structure time-series models and I suspect the EM-ColKF/S may be useful for a wide variety of other fields with redundant, observations prone to bias, noise, and missing data.

APPENDIX

Appendix A. Multi-lag Vector AR State Space Representation

From Section 3.2.3 the multi-lag structure for backshifted observations (Section 3.2.2) requires the following $\sum_{j}^{n} k\{j\} \times n$ leading-observation selection matrix, L:

	$\begin{bmatrix} 1 & 0 & \cdots & 0 \end{bmatrix}$	0		0
г ^т _	0	1 0 … 0		0
_	•	•	·	:
	0	0		1 0 … 0

The multi-lag observation model is as follows:

$$\overline{\mathbf{C}}_{t} = \begin{bmatrix} \frac{c_{1}\mathbf{I}_{k\{1\}} & \mathbf{0}_{k\{1\}\times\max(0, p-k\{1\})}}{c_{2}\mathbf{I}_{k\{2\}} & \mathbf{0}_{k\{2\}\times\max(0, p-k\{2\})}}\\ \vdots & \vdots\\ \hline c_{n}\mathbf{I}_{k\{n\}} & \mathbf{0}_{k\{n\}\times\max(0, p-k\{n\})} \end{bmatrix}$$
(A3.2)

Appendix B. Nonlinear Constraint Example

Consider a non-linear constraint arising from (3.48):

$$\mathbf{A}_{S}(\mathbf{A}^{\mathbf{n}})\mathbf{A}_{S}(\mathbf{C}) - \mathbf{A}_{S}(-\mathbf{A}^{\mathbf{n}}\overline{\mathbf{C}}) = \mathbf{0}, \qquad (B3.1)$$

where $\mathbf{A}_{s}(\bullet)$ is the partition of \mathbf{A}_{s} in terms of a specified parameter. The Taylor expansion of (B3.1), using the chain rule is:

$$\frac{\partial \mathbf{A}_{s}}{\partial \mathbf{A}^{n}} \mathbf{A}_{s}(\mathbf{C}) + \mathbf{A}_{s}(\mathbf{A}^{n}) \frac{\partial \mathbf{A}_{s}}{\partial \mathbf{C}} - \mathbf{A}_{s}(-\mathbf{A}^{n}\overline{\mathbf{C}}) = \mathbf{0}.$$
(B3.2)

Which can be written as,

$$\mathbf{F}_i \operatorname{vec}(\mathbf{A}_s) = \mathbf{0}, \tag{B3.3}$$

where $\mathbf{F}i$ is a matrix of partial derivatives as given in (3.60).

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TABLES

Case	Missing y _t ?	Missing \mathbf{y}_{t-1} ?	State Space Eqns.
1	NO	NO	(3.20) & (3.21)
2	YES	NO	(3.41) & (3.42)
3	YES	YES	(3.41) & (3.42)
4	NO	Х	(3.41) & (3.44)

Table 3.1: State space model partitions for all possible missing value cases.

Table 3.2: System matrix modifications for missing values. If one or more observations are missing, the augmented state will have three partitions: the hidden process, the non-missing observations (denoted with subscript "(1)"), and the missing observations (denoted with subscript "(2)") following Shumway (2006). For \mathbf{y}_t , only the leading observations must be missing, but if any lags of $\overline{\mathbf{y}}_{t-1}$ are missing the entire vector is considered missing (Note: $\mathbf{y}_t = \mathbf{L}^T \overline{\mathbf{y}}_t$).

Miss La	sing 1g	Augmented System Matrix Format									
\mathbf{y}_t	$\overline{\mathbf{y}}_{t-1}$	$\mathbf{H}^* = \overline{\mathbf{A}}^{s*} =$		$A^n =$	$\overline{\mathbf{Q}}^* =$	$\overline{\mathbf{S}}^* =$	$\mathbf{R}^{n} =$				
NO	NO	[H 0]	$\begin{bmatrix} \overline{\mathbf{A}}^{\mathrm{s}} & 0 \\ \overline{0} & 0 \end{bmatrix}$	A ⁿ	$\begin{bmatrix} \overline{\mathbf{Q}} & 0 \\ 0 & 0 \end{bmatrix}$	$\left[\frac{\overline{S}}{0}\right]$	R ⁿ				
YES	NO	$\begin{bmatrix} \mathbf{H}_{(1)} & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$	$\begin{bmatrix} \overline{\mathbf{A}^{s}} & 0 & 0 \\ \overline{0} & 0 & 0 \\ \overline{\mathbf{H}}_{(2)} & 0 & \overline{\mathbf{A}}_{(2)}^{n} \end{bmatrix}$	$\begin{bmatrix} \mathbf{A}_{(1)}^{\mathbf{n}} & 0 \\ \hline 0 & 0 \end{bmatrix}$	$\begin{bmatrix} \overline{\mathbf{Q}} & 0 & \overline{\mathbf{S}}_{(2)} \\ \hline 0 & 0 & 0 \\ \overline{\mathbf{S}}_{(2)}^{\mathrm{T}} & 0 & \overline{\mathbf{R}}_{(22)}^{\mathrm{n}} \end{bmatrix}$	$\begin{bmatrix} \overline{S}_{(1)} & 0 \\ \overline{0} & 0 \\ \overline{\mathbf{R}}_{(12)}^n & 0 \end{bmatrix}$	$\begin{bmatrix} \frac{\mathbf{R}^n_{(11)} & 0}{0 & \mathbf{R}^n_{(22)} \end{bmatrix}$				
NO	YES	$\begin{bmatrix} \mathbf{H}_{(1)} & 0 & 0 \\ \mathbf{H}_{(2)} & 0 & \mathbf{A}_{(2)}^{\mathbf{n}} \end{bmatrix}$	$\begin{bmatrix} \overline{\mathbf{A}^{\mathrm{s}}} & 0 & 0 \\ \hline 0 & 0 & 0 \\ \overline{\mathbf{H}}_{(2)} & 0 & \overline{\mathbf{A}}_{(2)}^{\mathrm{n}} \end{bmatrix}$	$\begin{bmatrix} \mathbf{A}_{(1)}^{\mathbf{n}} & 0 \\ \hline 0 & 0 \end{bmatrix}$	$\begin{bmatrix} \overline{\mathbf{Q}} & 0 & \overline{\mathbf{S}}_{(2)} \\ \hline 0 & 0 & 0 \\ \overline{\mathbf{S}}_{(2)}^{\mathrm{T}} & 0 & \overline{\mathbf{R}}_{(22)}^{\mathrm{n}} \end{bmatrix}$	$\begin{bmatrix} \overline{\overline{S}}_{(1)} & \overline{\overline{S}}_{(2)} \\ \hline 0 & 0 \\ \overline{\overline{R}}_{(12)}^{n} & \overline{\overline{R}}_{(22)}^{n} \end{bmatrix}$	R ⁿ				

Table 3.3: Test cases for simulations and estimates. Case code characters describe simulation and estimate model structure for each experiment. Signal models for hidden processes denoted 'R' for AR or 'F' for ARFIMA. Noise models for observation noise can additionally include 'W' for AR plus white noise. Cases with missing values denoted by 'M' and cases with non-Gaussian innovations with 'G'. Appended numbers indicate use of a 'RR' configuration for estimation of simulated data from another case (RR3 and RR4) or for differing parameter set (RR2).

Case Code	Signal	Noise	Missing	Non-Gaussian
RR{1,2,3,4}	AR	AR	-	-
RRM	AR	AR	Х	-
RRG	AR	AR	-	Х
FR	ARFIMA	AR	-	-
FRMG	ARFIMA	AR	Х	Х
FF	ARFIMA	ARFIMA	-	-
FFM	ARFIMA	ARFIMA	Х	-
FFG	ARFIMA	ARFIMA	-	Х
RW	AR	AR+W	-	-
FW	ARFIMA	AR+W	-	-
FWMG	ARFIMA	AR+W	Х	Х

Table 3.4: EM estimation results for scaling and covariance parameters. Shown are mean (standard deviations) for 30 realizations of each test case (RR4, RW, FW, and FWMG shown in Table 3.6). See Table 3.2 for test case summaries. Control results from Figure 3.5-Figure 3.7 omitted for brevity.

Parameter	<i>C</i> 1	С2	C3	q	<i>r</i> 11	<i>r</i> ₂₂	r 33	<i>r</i> ₁₂	r 13	<i>r</i> 23
True Values	1	0.7	1.5	3	4	6	9	2	-1	0
Initial Values	1	1	1	2	5	5	5	0	0	0
RR1	0.98	0.70	1.45	3.11	3.96	5.90	9.21	1.93	-0.94	-0.03
RR2	0.97 (0.01)	0.98 (0.02)	(0.04) 1.40 (0.03)	3.15 (0.06)	4.00 (0.07)	4.42 (0.07)	9.54 (0.22)	(0.17) 1.09 (0.06)	-0.80 (0.05)	(0.25) -1.18 (0.05)
RRM	0.98	0.72	1.46	3.06	3.97	5.83	9.26	1.92	-1.02	-0.27
	(0.07)	(0.07)	(0.09)	(0.23)	(0.44)	(0.46)	(1.14)	(0.40)	(0.40)	(0.52)
RRG	0.98	0.69	1.47	3.14	3.95	5.91	9.02	1.94	-1.04	-0.07
	(0.04)	(0.05)	(0.04)	(0.20)	(0.23)	(0.25)	(0.67)	(0.22)	(0.23)	(0.28)
FR	0.98	0.68	1.46	3.36	3.68	5.79	8.79	1.80	-1.23	-0.12
	(0.02)	(0.01)	(0.02)	(0.13)	(0.15)	(0.15)	(0.28)	(0.09)	(0.10)	(0.17)
FRMG	0.97	0.69	1.42	3.22	3.75	5.26	8.30	1.69	-1.00	-0.39
	(0.04)	(0.03)	(0.05)	(0.54)	(1.16)	(1.56)	(2.68)	(0.66)	(0.75)	(0.44)
FF	1.10	0.78	1.61	2.73	3.33	5.35	8.14	1.54	-1.35	-0.35
	(0.04)	(0.04)	(0.07)	(0.15)	(0.17)	(0.20)	(0.46)	(0.16)	(0.09)	(0.21)
RR3	1.00	0.75	1.48	2.99	3.46	5.23	7.96	1.53	-1.22	-0.45
	(0.03)	(0.04)	(0.06)	(0.11)	(0.15)	(0.23)	(0.39)	(0.17)	(0.15)	(0.26)
FFM	1.18	0.83	1.65	2.20	2.94	4.72	7.65	1.34	-1.04	-0.19
	(0.14)	(0.11)	(0.17)	(0.41)	(0.40)	(0.36)	(0.83)	(0.34)	(0.33)	(0.49)
FFG	1.09	0.77	1.60	2.74	3.42	5.38	8.07	1.60	-1.33	-0.33
	(0.05)	(0.04)	(0.08)	(0.19)	(0.32)	(0.37)	(0.59)	(0.19)	(0.15)	(0.20)

Table 3.5: EM estimation results for autoregressive and long-memory parameters. Shown are mean (standard deviations) for 30 realizations of each test case (RR4, RW, FW, and FWMG shown in Table 3.7). True values for RR2 test case shown in brackets. RR3 omitted because $\phi_1 \neq \pi_1$ and *a* not estimated. See Table 3.2 for test case summaries.

Parameter	ϕ_1^d	ϕ_{l}^{n1}	ϕ_1^{n2}	ϕ_{1}^{n3}	d^d	d^{n1}	d^{n2}	d^{n3}
True Values	0.9	0.8 [0.9]	0.6 [0.9]	0.4 [0.9]	0.3	0.1	0.2	0.3
Initial Values	0.8	0	0	0	0.05	0.01	0.01	0.01
RR1	0.90	0.80	0.60	0.41	-	-	-	-
	(0.01)	(0.02)	(0.02)	(0.04)	-	-	-	-
RR2	0.90	0.89	0.90	0.89	-	-	-	-
	(0.02)	(0.01)	(0.01)	(0.02)	-	-	-	-
RRM	0.90	0.79	0.58	0.40	-	-	-	-
	(0.02)	(0.03)	(0.04)	(0.09)	-	-	-	-
DDC	0.90	0.80	0.60	0.42	-	-	-	-
KKU	(0.02)	(0.02)	(0.02)	(0.05)	-	-	-	-
ED	0.91	0.79	0.60	0.42	0.26	-	-	-
ГК	(0.03)	(0.02)	(0.02)	(0.04)	(0.06)	-	-	-
EDMC	0.88	0.80	0.59	0.43	0.30	-	-	-
FRMG	(0.08)	(0.03)	(0.04)	(0.12)	(0.13)	-	-	-
EE	0.90	0.77	0.61	0.46	0.28	0.12	0.17	0.26
ГГ	(0.03)	(0.10)	(0.09)	(0.15)	(0.05)	(0.10)	(0.10)	(0.13)
	0.89	0.64	0.56	0.44	0.32	0.25	0.21	0.26
FFM	(0.05)	(0.24)	(0.13)	(0.22)	(0.09)	(0.21)	(0.12)	(0.20)
FEC	0.88	0.77	0.62	0.40	0.30	0.12	0.17	0.30
FFG	(0.06)	(0.10)	(0.09)	(0.13)	(0.10)	(0.10)	(0.10)	(0.12)

Table 3.6: Same as Table 3.4, except shows cases with AR + W error for \mathbf{y}_t^3 . Note that r_{33} for RR4 should be compared to $r_{33} + (\sigma_w^{n3})^2 = 9 + 70 = 79$ rather than $r_{33} = 9$.

Parameter	<i>C</i> 1	<i>C</i> ₂	C3	q	<i>r</i> 11	<i>r</i> ₂₂	<i>r</i> 33	<i>r</i> ₁₂	<i>r</i> ₁₃	<i>r</i> ₂₃
True Values	1	0.7	1.5	3	4	6	9	2	-1	0
Initial Values	1	1	1	5	5	5	15	0	0	0
DW	0.93	0.68	1.33	3.67	3.77	5.73	12.94	1.75	-0.79	-0.23
KW	(0.03)	(0.04)	(0.11)	(0.27)	(0.32)	(0.30)	(1.22)	(0.26)	(0.75)	(0.63)
DD/	0.97	0.72	1.41	4.21	3.11	5.24	86.49	1.20	-1.95	-1.05
KK4	(0.03)	(0.05)	(0.14)	(0.27)	(0.34)	(0.36)	(3.75)	(0.28)	(0.86)	(0.79)
EW	0.99	0.69	1.47	3.18	4.11	5.94	11.79	2.04	-0.50	-0.26
FW	(0.04)	(0.03)	(0.06)	(0.31)	(0.29)	(0.17)	(1.10)	(0.19)	(0.56)	(0.59)
FWMG	1.07	0.75	1.58	3.66	2.92	5.29	11.64	1.21	-1.38	-0.93
	(0.03)	(0.02)	(0.07)	(0.35)	(0.44)	(1.04)	(1.36)	(0.27)	(1.18)	(1.13)

Table 3.7: Same as Table 3.5, except shows cases with AR + W error for \mathbf{y}_t^3 , with $(\sigma_w^{n^3})^2 = E\{\mathbf{v}_t^{(3)}\mathbf{v}_t^{(3)T}\}$. Initial values for RR4 given in Table 3.5. RR4 does not estimate the $(\sigma_w^{n^3})^2$ parameter.

Case	ϕ_{l}^{d}	ϕ_{l}^{n1}	ϕ_{1}^{n2}	ϕ_1^{n3}	d^{s}	$(\sigma_w^{n3})^2$
True Values	0.9	0.4	0.6	0.8	0.3	70
Initial Values	0.8	0.7	0.7	0.7	0.05	100
DW	0.89	0.38	0.60	0.76	-	66.87
KW	(0.02)	(0.06)	(0.02)	(0.04)	-	(2.95)
	0.81	0.39	0.60	0.17	-	_
KK4	(0.05)	(0.07)	(0.02)	(0.02)	-	-
EW	0.91	0.42	0.60	0.76	0.26	66.85
ΓW	(0.04)	(0.06)	(0.02)	(0.03)	(0.10)	(3.62)
EWMC	0.94	0.40	0.60	0.75	0.12	64.77
F W MU	(0.03)	(0.09)	(0.03)	(0.06)	(0.07)	(5.76)

FIGURES



Figure 3.1: Soil moisture anomaly datasets (i.e. with trend and annual cycle removed), (a) and (b), and relative observation anomaly errors, (c) and (d), from a pasture in Lethbridge, Alberta. Colored (blue, dark green, and red) lines represent a set of three model and remotely-sensed observations and heavy black line indicates *in situ* soil moisture (5 cm depth) from soil probes (here considered a benchmark for the 'hidden process'). Left panels, (a) and (c), show full-length time-series (four years, 2003-2006), whereas right panels, (b) and (d), show associated zoomed detail with extent indicated by left panel inset boxes.



Figure 3.2: Comparison of Pearson correlation between simulated "hidden" process vs. smoother estimates with EM parameters (\Box), smoother with perfect parameters (\blacksquare), observations (O), and mean of observations (Δ) for selected test cases. Symbols and error bars (where visible) respectively represent median correlation and confidence intervals for 30 realizations.



Figure 3.3: Time-series of "hidden" process (heavy black line), smoother estimates (heavy light green line), and observations (thin blue, dark green, and red lines) for selected site test cases. Left panels show full-length time-series, whereas right panels show associated expanded detail with extent indicated by left panel inset boxes (as in Figure 3.1).



Figure 3.4: "Hidden" state (heavy black line) and missing \mathbf{y}_t^3 state (grey line) smoother error covariance time-series for RRM test case. These time-series correspond with the RRM state shown in the uppermost panels of Figure 3.3. Panels and inset box as in Figure 3.3.



Figure 3.5: Parameter estimates for 30 realizations of RR. Estimates are for: (a) observation calibration coefficients (**C**); (b) signal AR(1), ϕ^d , and observation noise AR(1), ϕ^n , coefficients; (c) signal innovation variance, **Q**, and observation noise innovation covariance (**R**). True values shown with bold +, and dashed line denotes a 1:1 relation. Signal-related parameters shown with (\bigstar), whereas observation-related parameters shown with (\bigstar), whereas observation-related parameters shown with (\bigstar), respectively, and × for all off-diagonal elements of **R**. Mean values and standard deviations for EM given in Table 3.4.



Figure 3.6: Same as Figure 3.5, except observations contain missing values (i.e. test case RRM).



Figure 3.7: Same as Figure 3.5, except signal and observation noise AR processes share poles (i.e. test case RR2) and therefore symbols for ϕ^d cover those for ϕ^n in (b).



Figure 3.8: AR coefficients (π) for approximation of ARFIMA(0.9, 0.3, 0) "hidden" process (\mathbf{x}_t) with ARFIMA observation noise using the (a) RR3 (AR with 30 lags) configuration and (b) FF (truncated ARFIMA with 30 lags) configuration. Control realizations in (a) are the same as in (b), but not visible because they are effectively covered by EM realizations.



Figure 3.9: AR coefficients (π) for approximation of \mathbf{y}_t^3 single lag AR+W noise (RW) with 10-lag AR-only noise (RR4). Error-bars show the range (max - min) of RW realizations.

CHAPTER 4: EVALUATING MERGED SOIL MOISTURE FOR IMPROVING ESTIMATES OF ECOSYSTEM RESPIRATION

4.1 INTRODUCTION

I live in a data-rich era. The environmental research community is currently awash in potentially relevant global observational or model-derived datasets, while new datasets of the same or similar parameters are often announced proclaiming improved or accuracy. However, most user applications require a single, consistent view of the world with a well-defined uncertainty range, while reality more often involves multiple, often conflicting and disparate sources of noisy information with subjective and imprecisely known uncertainty. Most users may also want to know when a new dataset is really better for a certain application than what was previously available – in other words, the value of its marginal information. Ensemble estimates, taking the equally-weighted mean of several similar component datasets, usually outperforms an individual dataset on average over a large number of cases, because each individual dataset, however poor its accuracy relative to the other data, brings some useful independent information (Bohn 2010). However, a more optimal strategy would be to compute a weighted average of each dataset based on their individual trustworthiness, or more precisely their error covariance (Crow 2016; Kalman 1961; Kailath 2000). Data assimilation seeks to provide such an estimate, but obviously the outcome depends on how well the weights are specified. Standard maximum-likelihood methods (Crow 2008; Gupta 1974; Dempster 1977), and other closely-related methods such as triple collocation (TC; Gruber 2016a; Scipal 2008), are available to compute the error covariance but come with limiting assumptions that the errors are time-uncorrelated (i.e. white noise) with zero error cross-

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correlation (i.e. diagonal error covariance matrix). Extensions to TC have been recently proposed to account for these factors, but these methods still suffer from the inability to deal quantitatively with error cross-correlation (Pan 2015; Gruber 2016b).

Soil moisture datasets contain auto-correlated and unknown, possibly crosscorrelated error structure, which arise partly from difficultly modeling soil moisture processes and mismatch between model and remote-sensing spatial support, both of which have been exacerbated by previous lack of satellite derived global soil moisture observations to constrain soil moisture models (Qiu 2014; Crow 2012). The methods developed in Chapter 3 were shown to account for these error characteristics in idealized datasets, but questions remain about how well the method performs for real soil moisture datasets both in terms of error covariance estimation and merged state accuracy.

In the case of soil moisture as a key input for ecological process modeling, the ultimate test of the value of a soil moisture dataset hinges on its marginal value for improving the ecological model application relative to other available sources of soil moisture information. This incremental increase in value depends on the accuracy of the soil moisture dataset, its relevant independence from other competing information sources, and crucially, how sensitive the ecological application is to the soil moisture input within its typical range of variability (Entekhabi 2010). One application of specific interest is modeling how ecosystem respiration CO₂ release, an important component of the global terrestrial carbon cycle, responds to soil moisture variability. The sensitivity of ecosystem respiration to soil moisture is defined as the mathematical derivative of the model's effective soil moisture response function; therefore, determining this response

function is a critical step in evaluating the impact of soil moisture information on the model.

In this chapter, I examine a case study whereby soil moisture datasets from different sources were merged to improve application as input into an ecosystem CO₂ respiration model. I employed a simplified version of the joint merging and uncertainty estimation method described in Chapter 3 to merge three different soil moisture datasets, including a global atmospheric weather model driven soil moisture process model; a remotely-sensed rainfall-, snow-, and evapotranspiration-driven simple soil moisture model; and a satellite remote sensing derived soil moisture dataset. I evaluated the merged soil moisture data and compared estimated uncertainties relative to *in situ* soil moisture observations from eddy covariance flux tower locations. I then used the merged soil moisture dataset along with the eddy covariance CO₂ flux tower observations to determine an empirical ecosystem respiration model fit relative to the flux tower observations was evaluated for various alternative soil moisture datasets representing incrementally increasing accuracy and information content.

4.2 Methods

4.2.1 Global Soil Moisture Datasets

This study uses soil moisture data from global Modern Era Retrospective Reanalysis (MERRA; Rienecker 2011); two satellite microwave remote sensing based soil moisture datasets from the Advanced Microwave Scanning Radiometer for the Earth Observing System (AMSR-E) Vrjie Amsterdam (VU) dataset (Owe 2001), and the University of Montana (UMT) AMSR-E land parameter dataset (Jones 2010, described in Chapter 2); and an observed precipitation, evapotranspiration (ET), and snowmelt model (PETS). The MERRA surface soil moisture (0-5 cm depth) dataset was averaged from 3hourly to daily time step and resampled from $1/2^{\circ} \times 2/3^{\circ}$ geographic grid to a global 25km Equal Area Scalable Earth Grid version 1 format (EGv1; Armstrong & Brodzik) using nearest-neighbor resampling to match the baseline format of the AMSR-E datasets (Jones 2010). Further information on MERRA is provided in Chapter 5. The two AMSR-E datasets represent daily soil moisture data obtained from satellite descending orbital overpass brightness temperature retrievals, while further information on the AMSR-E soil moisture datasets is given in in Chapter 2.

The PETS model was developed to incorporate satellite-based precipitation and evapotranspiration (ET) information for estimating soil moisture. The model uses input precipitation from the NOAA Center for Climate Prediction Morphing Technique (CMORPH; Joyce 2004), an observation-based ET dataset developed at the University of Montana (Zhang 2010), and daily snow depth analysis from the Canadian Meteorological Center (CMC; Brown & Brasnett 2010). The CMORPH dataset merges microwave and infrared (IR) satellite rain rate estimates. It is important to note that these data represent rain rate, not rain accumulation, because such satellite observations only provide a "snapshot" in time. Also, the physics of satellite microwave rain rate estimation is different from satellite microwave soil moisture observations; the mathematics of merging rain rate estimates is different from merging soil moisture observations because rain rates are non-Gaussian, positively-constrained, and contain much less temporal auto-

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correlation than soil moisture time series. The CMORPH dataset was aggregated from 3hourly rainfall rates (mm hr⁻¹) to daily rates from $1/4^{\circ} \times 1/4^{\circ}$ geographic grid to EGv1 using nearest neighbor resampling. The ET dataset uses MODIS and NCEP reanalysis meteorological fields to estimate global ET for the period 2002-2008 and was available in daily 25-km EGv1 format (Zhang 2010). The CMC snow reanalysis provides daily snow depth and monthly snow water equivalent information. The PETS model separately integrates daily and monthly differences in water balance estimates (precipitation + snowmelt – ET) as input to a simple finite-impulse response (FIR; closely related to AR models) model. The PETS model FIR parameters were fitted using *in situ* soil moisture measurements and the PETS water deficit data was rescaled to match the variability of MERRA soil moisture for every global grid cell to ensure realistic soil moisture ranges. Details of the PETS model logic are given in Appendix A.

4.2.2 Flux tower Data

The flux tower soil moisture and ecosystem respiration (RECO) data were obtained from a subset of the FLUXNET La Thuile synthesis dataset (Baldocchi 2008). The requirement that the flux tower site data have both surface layer soil moisture and RECO measurements restricted suitable flux towers to 39 locations for the soil moisture analysis (Continental U.S., Europe, and China) and 28 locations for the RECO analysis (Contintental U.S. only). I further required that flux towers have at least two years of available observations and restricted the RECO spatial domain to continental North America from 30° N - 50° N latitude (Continental US, extreme southern Canada, and northern Mexico). Soil moisture values reported as volumetric percent were converted to percent saturation by dividing by the soil porosity (assumed 50 % unless otherwise noted). Here, RECO is defined as the daily sum of autotrophic and heterotrophic respiration within a tower footprint (\approx 1-km²). It should be emphasized that flux tower RECO is an estimate partitioned from tower eddy covariance based net ecosystem CO₂ exchange observations and are therefore not a direct observation. Nevertheless, these partitioned RECO estimates offer the best available benchmark in the absence of more direct observations. Further information on the La Thuile flux tower network and flux partitioning is given in Chapter 5.

4.2.3 Merging and Error Estimation Methods

The merging and error estimation methods employed in this chapter include the Expectation Maximization (EM) Colored Noise Kalman Filter/Smoother (ColKF), Neutral Regression, and Triple Collocation (TC). A simplified version of EM ColKF was used for this chapter - details of the full EM ColKF method are given in Chapter 3. Here the EM ColKF considers only AR(1) signal and noise processes rather than the generalized multi-lag system shown in Chapter 3. Also, the EM ColKF omits missing values in the AMSR-E time-series by eliminating MERRA and PETS data from any lags from which AMSR-E data is missing, whereas missing values are properly handled using conditional estimation in Chapter 3. This procedure distorts the effective auto-correlation parameters of the time-series by shortening time-step positions following missing time-steps. These simplifications were necessary because the analysis presented here was conducted prior to the full derivation considering multiple lags and missing values shown in Chapter 3.

The Neutral Regression method was used for evaluating spatial patterns of merging weights. The Neutral Regression method is based on Mardsen (1999) and described in further detail in Appendix B. The method uses a truncated singular value decomposition to determine the merging weights for each dataset and requires that each dataset is initially rescaled to match the mean and variance of a reference dataset, chosen to be MERRA in this case. The method relies on a common assertion that the noise process of the datasets are confined to smaller eigenvalues, therefore the eigenvectors associated with the two smallest eigenvalues were omitted and the merging weights are taken as the square of the largest eigenvector. The method is *ad hoc* and sub-optimal because it does not directly decompose the individual datasets into error, scaling, and signal components based on tractable statistical principles for the merging problem (i.e. requires *a priori* rescaling and error process assumed independent and identically distributed – a typical assumption for the singular value decomposition used in principle components analysis (Golub & Van Loan 1980)), and also squaring the largest eigenvector is not rigorously mathematically justified. The Neutral Regression method was initially considered prior to development of the EM ColKF method and presented here for regional results because the EM ColKF has not yet been developed for largescale deployment, which requires further refinement and testing.

Triple Collocation (TC) is a method for estimating the root mean square error (RMSE) of individual datasets given a triplet of three datasets (Scipal 2008). TC employs pairwise differences to cancel the underlying signal leaving only the relative error processes, the variance of which is then computed as the RMSE estimate (Appendix C). Scaling factors can also be computed using an iterative procedure (Scipal 2008). The

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central premise of TC is that the errors of each dataset are independent of the errors of the other datasets, and independent of the underlying signal. These independence assumptions imply that the errors are white noise processes although the errors may be pre-whitened using recent modifications of the TC method (Zwiebeck 2012).

4.2.4 Control Benchmark Merging Methods

Two control merging methods were considered to test the merging methods previously described. In the first control method, the equally-weighted average of the three observation datasets was taken after rescaling to MERRA mean and variance (this was termed the "pre-filtered average," because it was computed without further filtering of the data). An optimal method should be capable of always improving upon, or at least matching, the pre-filtered average, or the best of the individual component datasets, whichever is more skillful. The larger of these two quantities then represents the lower bound for an optimally-performing EM ColKF. For the second control method, the ColKF parameters were calibrated using *in situ* soil moisture data records. This method represents ColKF with "perfect" knowledge of merging parameters, which represents the upper bound of possible EM performance because it is achievable only if EM accurately determines the underlying system parameters.

4.2.5 Ecosystem Respiration Model

This chapter uses a simplified ecosystem respiration model based on the model presented in Chapter 5. Ecosystem respiration is computed as:

$$RECO = f_{aut}GPP + f_{EC}(TSOIL)f_{EC}(SMSF)C, \qquad (4.1)$$

where *GPP* represents ecosystem gross primary production derived from partitioned tower eddy covariance measurement based net ecosystem exchange observations; *TSOIL* is from flux tower surface soil temperature (5 cm depth); *SMSF* is surface soil moisture (5 cm depth) from either the flux tower, merged soil moisture, or MERRA. The use of tower-partitioned GPP is an attempt to isolate the effective impact of soil moisture on heterotrophic respiration which is expected to differ from the effective impact of soil moisture on GPP. The \overline{C} term is a normalizing factor which accounts for effective soil organic carbon storage across flux tower sites (as detailed in Eqn. (5.11)). The *f_{EC}(TSOIL)* term is an Arrhenius exponential function of TSOIL from Lloyd & Taylor (1994) and *f_{EC}(SMSF)* is to be determined by inverting (4.1) with respect to flux tower RECO. The f_{aut} term determines partitioning of GPP into autotrophic respiration and was fitted, along with \overline{C} , such that inverted *f_{EC}(SMSF)* 95th percentiles were bounded on the unit interval.

4.3 **Results**

4.3.1 Soil Moisture RMSE Estimates Relative to In Situ Observations

The EM method significantly outperforms TC for estimating the MERRA and PETS model soil moisture errors ($R^2 = 0.91$ and $R^2 = 0.95$ for EM vs. $R^2 = 0.38$ and $R^2 = 0.35$ for TC, respectively), whereas EM performs somewhat less well than TC for estimating AMSR-E VU soil moisture errors ($R^2 = 0.90$ vs. $R^2 = 0.96$; Table 4.1; Figure 4.1a,b). The EM RMSE estimates for MERRA and PETS had little bias, whereas TC tended to underestimate soil moisture RMSE. In contrast, for AMSR-E EM tends to underestimate soil moisture RMSE at the highest end of the range, whereas TC had slight overall underestimation across AMSR-E's RMSE range. The EM method accurately estimated ϕ_1 coefficients for PETS, and estimates ϕ_1 for MERRA were also skillful, although with some outlier sites (Figure 4.1c). In contrast, the EM method consistently under-estimated the ϕ_1 coefficients for AMSR-E and the precision of these estimates was considerably worse than estimates for PETS and MERRA. Notably, some ϕ_1 EM estimates were confined to zero, whereas the benchmark indicated non-zero ϕ_1 . This occurred in locations with high vegetation biomass (usually deciduous broadleaf and evergreen needleleaf forest sites) where AMSR-E observations have high RMSE and little sensitivity to soil moisture.

4.3.2 Merged Soil Moisture Estimates Relative to In Situ

An example soil moisture anomaly time-series for the Lethbridge, Alberta, Canada (CA-Lth) site shows EM merged state results alongside the MERRA, PETS, and AMSR-E VU estimates (Figure 4.2) and corresponds with example time-series shown in Figure 3.1b. In this example, the merged estimate (x^s) shows substantial correlation improvement relative to *in situ* soil moisture observations (x) when compared with the three original time-series (MERRA, PETS, and AMSR-E VU). While all of the soil moisture datasets show dry-down rate bias relative to the *in situ* observations, the AMSR-E results also show additional high-frequency variability. The merged soil moisture estimate effectively smooths the high frequency variability while accounting for bias of the various datasets. Notably, the *in situ* soil moisture data-series are not contained

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within the 2-standard deviation merged prediction interval as consistently as might be expected. This discrepancy is possibly related to the soil moisture point-to-pixel or possibly vertical depth spatial support mismatch, or could possibly result from other processes not fully represented by the fitted system.

The soil moisture merging method shows an overall average, although nonsignificant (P>0.05) improvement across sites relative to MERRA (Table 4.2). The improvement is approximately equal for the VU and UMT AMSR-E datasets, but only showing about half of the significant improvement (p<0.05) of the results derived using "perfect" (i.e. fitted to *in situ*) merging parameters. The overall average improvement was degraded for the highest-biomass sites (as indicated by VOD bin average of 0.92; Figure 4.3a). In these locations, the merging method performed significantly worse than the simple (pre-filtered) average, which impacted the overall average improvements. The merging method matched both the site-fit ColKF and the pre-filtered average for all but the highest vegetation optical depth (VOD) bin. Somewhat surprisingly, the pre-filtered average performed better than VOD for the highest VOD bin, despite the much lower skill of the VU and UMT results. The merging method performed significantly (p<0.05) better than MERRA for VOD < 0.72 and on-par with MERRA for areas with VOD levels between 0.72 and 0.81.

As expected, both the VU and UMT datasets showed substantial decrease in correlation with increasing VOD; however, the VU dataset has consistently higher correlation than the UMT results across the entire VOD range. Additionally, the UMT dataset appears to have a much weaker seasonal cycle than VU as evidenced by lower correlations for the full (non-anomaly) data series (Figure 4.3b). Despite lower

correlations, the merged VU and merged UMT soil moisture data series do not significantly differ, indicating that the VU and UMT datasets supply roughly the same amount of independent information to the merged soil moisture data series. The MERRA and PETS derived soil moisture anomalies show somewhat higher correlations for the two lowest VOD bins, and somewhat higher full dataset correlations for the three largest VOD bins. This pattern is likely the result of differing soil moisture variances depending on climate regime. Lower VOD locations tend to be arid, precipitation-driven regimes with little soil moisture seasonal cycle (and hence higher anomaly variance) whereas higher VOD locations tend to have a more pronounced soil moisture seasonal cycle that is less impacted by individual precipitation events (and hence have higher seasonal variance).

4.3.3 Regional RMSE and Merging Weight Maps

The regional soil moisture results show differing RMSE spatial patterns and weight tradeoffs between the MERRA, PETS, and AMSR-E VU datasets (Figure 4.4). All three soil moisture datasets have higher errors in mountainous regions, although the PETS dataset receives most of the weight over mountain areas, which likely results from its observation-based snowfall information provided by CMC (Figure 4.4f). The AMSR-E VU dataset has the lowest error and carries the highest weight for the desert, grassland and cropland portions of the western and mid-western states, whereas it carries the lowest weight for forested regions in eastern, southern, upper mid-western and northwestern forests. The MERRA and PETS datasets share approximately equal weights in these forested regions, compensating for the down-weighting of the AMSR-E VU dataset. The PETS dataset has somewhat larger error and lower weight in the southwest relative to the MERRA and AMSR-E soil moisture datasets.

4.3.4 Ecosystem Respiration Soil Moisture Response Function

The tower carbon flux observations indicate a clear soil moisture constraint on RECO for drier soil moisture conditions (i.e. < 50 % of saturation; Figure 4.5). No evidence was found for decreased RECO at higher soil moisture values as might be associated with anaerobic conditions. Therefore a sigmoidal RECO soil moisture response curve fits the data much better than does the parabolic curve originally hypothesized. A sigmoidal curve fits the data regardless of whether *in situ* soil moisture measurements or MERRA soil moisture is used; however, a stronger constraint would improve the MERRA soil moisture fit under moderately dry (15-40 % saturation) conditions. This differing fit for MERRA indicates that the MERRA reanalysis contains overall dry bias in this soil moisture range relative to the *in situ* soil moisture observations.

4.3.5 Impact of Soil Moisture on Ecosystem Respiration Estimates

Inclusion of soil moisture substantially improves the model RECO estimates as shown for the US-ARc (Oklahoma) grassland site (Figure 4.7). Summer soil moisture dynamics in this location are non-seasonal, mainly driven by periodic intense precipitation from thunderstorms, followed by rapid dry-down periods. The model soil moisture constraint substantially improves RECO estimates during the dry-down periods between thunderstorms. Averages across sites show the overall impact of soil moisture on the model RECO estimates, which show consistently improved correlation against in situ tower RECO observations when more skillful soil moisture datasets are used (Figure 4.7a). The use of *in situ* soil moisture observations gives the most skillful model RECO results, followed by the use of merged soil moisture estimates, which improves upon model RECO estimates derived using MERRA soil moisture, and provides substantially better results than using no soil moisture in the RECO model. Likewise, estimated RECO vs. *in situ* RECO RMSEs follow a corresponding gradient of lower RMSE as the quality of soil moisture input improves (Figure 4.7b).

The RECO correlation improvement with the inclusion of soil moisture as a model input corresponds with the US east-west aridity gradient (Figure 4.8). Inclusion of soil moisture and merged soil moisture show the largest RECO correlation improvement for southwestern, midwestern, and western locations relative to model estimates derived with no soil moisture and MERRA soil moisture, respectively. Correlation decreases were observed for five locations with inclusion of site soil moisture and five locations with inclusion of merged soil moisture (Figure 4.8b). Correlation decreased for both site and merged soil moisture for an evergreen needleleaf forested site in New Hampshire and a broadleaf cropland site in Nebraska. Correlation also decreased for site soil moisture for sites in Missouri (deciduous broadleaf forest), Oregon (evergreen needleleaf forest) and Texas (grassland), whereas correlation decreased for merged soil moisture for sites in Wisconsin (deciduous broadleaf forest), Indiana (broadleaf cropland), and a relatively arid site in Arizona (shrubland). The RECO model sensitivity analysis indicates that the largest improvement from using soil moisture as a model constraint should occur for drier southwestern locations as was observed (Figure 4.9b). By contrast, comparing the merging analysis standard deviation to MERRA estimated RMSE indicates that the
largest improvement in MERRA soil moisture anomalies occurs over the central US (Figure 4.9a). This pattern was largely the result of higher soil moisture anomaly variance relative to seasonal variance in the central US as previously discussed.

4.4 **DISCUSSION**

4.4.1 Soil Moisture Error and State Estimation Performance

The model results indicate that EM capably accounts for AR errors characteristic of modeled soil moisture time series and this translates to improved RMSE performance relative to TC (Table 4.1; Figure 4.1). TC is well known to give model RMSE results that are much lower relative to remotely-sensed datasets (Scipal 2008). TC is typically conducted using two remotely-sensed datasets and one model (Gruber 2016; Scipal 2008), rather than two models and one remotely-sensed dataset as presented here. This two model configuration likely resulted in somewhat degraded TC results than reported in the literature (Miralles 2010) because, as I have shown, models generally do not conform to the independence assumptions underpinning the TC approach. The lessaccurate EM estimates for AMSR-E RMSE relative to TC were unexpected, but correspond with low-biased ϕ_1 estimates. Evidently, EM has some difficulty for forested sites where AMSR-E contains little soil moisture information and is dominated by noise; however, the ϕ_1 low-bias was not confined to this situation. This observation suggests that the AR(1) error model might not be appropriate for AMSR-E, which inspired the investigations of the alternative multi-lag and AR plus white noise (AR+W) model presented in Chapter 3 (See Figure 3.9). Additionally AMSR-E contains missing values, a feature not shared by MERRA and PETS, which likely impacted these results and was also inspiration for the detailed handling of missing values in Chapter 3.

The EM ColKF merged soil moisture estimate substantially improves upon MERRA relative to the *in situ* soil moisture observations (Table 4.2). The level of merged soil moisture skill improvement depends on the level of vegetation biomass as indicated by the VOD biomass proxy. This is expected because AMSR-E derived soil moisture information content decreases with increasing VOD (Figure 4.3). Interestingly, the merged soil moisture performance was indistinguishable regardless of whether the VU AMSR-E or UMT AMSR-E dataset was used. This is an important result because it indicates that the information contents of the two datasets are similar, despite consistently lower skill of the UMT product when considered separately.

Surprisingly, the EM ColKF merged dataset was not substantially more skillful than the simple pre-filtered average of the three datasets (Figure 4.3). This was despite evident skill in estimating RMSE of the individual datasets, which should translate into merging weights which should be more optimal than the equal weighting used in a simple average. I expected that the pre-filtered average would be substantially worse for the highest VOD bin, due to expected degradation of the AMSR-E soil moisture datasets. This unexpected result was likely caused by rescaling of the mean and variance of PETS and AMSR-E data to match MERRA prior to averaging (Section 4.2.4), which had the unintended effect of dampening the AMSR-E error variance, which is proportional to the overall AMSR-E soil moisture variance (Draper 2013). The EM should be able to account for variance changes due to error vs. signal by adjusting the scaling parameter (*C*; See Chapter 3); however, the results indicated that the EM has difficulty correctly

estimating RMSE for the highest VOD bin and therefore also has difficulty correctly estimating *C* because the two parameters have compensating errors. Nevertheless, the EM ColKF has several features lacking from simple averages, including its ability to consider temporal adjacency correlations, enforcing smoothness on the solution and detailed estimation of individual dataset error processes.

The soil moisture neutral regression merging errors and weights show expected patterns (Figure 4.4), which lend some confidence to the idea of determining merging weights. Other studies have found that satellite-based precipitation and soil moisture observations provide similar amounts of complementary information in a model data assimilation system (Qing 2011). Despite reasonable results, the neutral regression approach is an *ad hoc* method with no guarantee of mathematical optimality. I expect that the EM-determined ColKF weights will resemble Figure 4.4, when computed for similar regions; however, because the EM can estimate off-diagonal error covariance elements there is no guarantee that the weights will be positive, potentially complicating interpretation (See Chapter 3).

4.4.2 Improving Ecosystem Respiration Estimates with Soil Moisture Information

Soil moisture had a positive overall impact on the model RECO estimates, with increasing accuracy obtained using more skillful soil moisture datasets as model inputs (Figure 4.7). This impact was closely related to wet and dry events indicated from individual flux tower time series (Figure 4.6). The impact was not positive for all locations (Figure 4.8), but such variability is expected with pixel-to-point comparisons using noisy soil moisture and tower flux observations. Locations with high positive

impact on model RECO accuracy were explained by the model sensitivity analysis (Figure 4.9b), lending confidence to the ability of the model to explain spatial patterns of expected model RECO improvement from using soil moisture information. Predicted model RECO sensitivity patterns are dependent on the fitted empirical soil moisture response curve (Figure 4.5) and dependent on how well the tower locations sample the underlying spatial process of RECO soil moisture constraints and biases between the different MERRA, merged, and *in situ* soil moisture datasets used as model inputs. In practical application such as the TCF model (Chapter 5), the response function should be fitted to the particular model input soil moisture dataset to provide best possible carbon flux estimates, but here I fit the response using *in situ* soil moisture observations to more clearly differentiate the impact of soil moisture skill on improving model results. This expectation relies on the assumption that the *in situ* observations are the most accurate and representative available soil moisture metric, which may not be true in all cases, especially considering large characteristic soil moisture spatial heterogeneity and potential mismatches between *in situ* soil moisture measurement probes (point measurement) and the typical eddy covariance flux footprint (\approx 1-km²). Violations of this assumption, and the fitting of only one response function for all locations may account for RECO degradation at the subset of locations seen in Figure 4.8.

Differing patterns for soil moisture merging improvement versus RECO improvement when employing merged soil moisture as input rather than MERRA (Figure 4.9a,b) underscores the importance of multiple factors in determining the incremental value of soil moisture for improving an application. These results, taken together, indicate that the incremental value of a soil moisture dataset depends on the independent

information in the dataset relative to other competing datasets (Figure 4.4), the independent dataset's signal-to-noise ratio, the merged dataset error-variance reduction (shown in Figure 4.9a), and the sensitivity of the model to the soil moisture input (as shown in Figure 4.9b).

4.5 CONCLUSION AND SIGNIFICANCE

This exploratory case study demonstrates the incremental value of improved soil moisture information for improving model RECO estimates relative to a regional network of tower eddy covariance CO₂ flux observations. First, the ColKF merging methodology was evaluated using *in situ* soil moisture datasets and I found that ColKF merging improves soil moisture skill. Spatial patterns of estimated errors and associated merging weights showed an expected AMSR-E derived increasing soil moisture error gradient with increasing vegetation biomass. The fitted model RECO soil moisture response function indicated that drier soil conditions constrain RECO, but no evidence was found for an anaerobic constraint for wet or saturated soil conditions. The fitted soil moisture response function was used to evaluate the relative improvement in model RECO estimates and I found that the model improvement followed the range of soil moisture information quality. The RECO model sensitivity analysis indicated that patterns of flux improvement across sites were predictable based on an analysis of model dynamics. These results underscore the ability of improving soil moisture information to produce incremental improvement in model CO₂ flux estimates.

The case study presented here was important for tying together and directing more detailed work in Chapters 3 and 5, which was conducted after the work presented here. The EM ColKF merging methodology presented in this Chapter does not account for missing values and only considers single lag AR(1) signal and noise models. These features were addressed in Chapter 3. Additionally, the EM ColKF method is computationally intensive, representing large-scale software implementation challenges, which is why the alternative and less complex neutral regression methodology was used for the regional application presented here. I opted to postpone large-scale implementation of the EM ColKF methodology pending further refinement and evaluation. The RECO results presented here represent a much simplified respiration model relative to the terrestrial carbon flux (TCF) model presented in Chapter 5. In contrast, the TCF model considers all components of the net ecosystem CO_2 flux, including vegetation gross primary productivity, soil organic carbon dynamics and underlying environmental controls. Furthermore, the operational nature of the work in Chapter 5 precludes some of the work presented here, adding additional complexity with regards to required use of the L4SM soil moisture dataset and pre-launch and post-launch availability of SMAP remotely-sensed information. The work presented here shows the impact of AMSR-E soil moisture information. The lower-frequency (1.41 GHz) SMAP instrument is expected to show improved soil moisture sensitivity relative to AMSR-E (6.9 GHz) and this implies that SMAP should provide improved TCF results. However, the additional complexities of the TCF model and L4C product have thus far precluded a clear improvement using SMAP observations (Chapter 5).

APPENDIX

Appendix A. The Precipitation, Evapotranspiration, and Snowmelt (PETS) Model

Surface soil moisture is modeled using a pseudo-diffusivity model for water flux between a surface layer (W_s) and a deeper soil reservoir (W_d):

$$L\frac{\Delta W}{\Delta t} = D(W_s - W_d), \qquad (A4.1)$$

where Δt is a discrete time-step (1 day or 1 month) and T = L/D is the characteristic timescale parameter. The discrete-time numerical integration of (A4.1) for soil moisture θ gives the following propagation equation (Wagner 1999):

$$\theta(t) = \alpha \theta(t-1) + \gamma W_s, \qquad \alpha = \frac{1}{1+T\Delta t}, \qquad \gamma = \frac{T\Delta t}{1+T\Delta t},$$
 (A4.2)

with,

$$W_s = P + S - ET , \tag{A4.3}$$

where *P* is precipitation, *S* is snowmelt and *ET* is evapotranspiration, all in units mm per Δt . The Antecedent Precipitation Index (API) is a special case where W_s is precipitation, $\alpha = 1$, and $\gamma = 1$. Snowmelt is computed from CMC by computing daily backward differences in snow-water equivalent and zeroing negative differences.

The model (A4.2-A4.3) is run using daily inputs, and this result is subtracted from its 30day moving average to produce a daily anomaly series. The model is then run using monthly values, the result is interpolated using cubic splines, and then added to the daily anomaly series to give an estimate of surface soil moisture deficit, which is then rescaled to the mean and variance of MERRA to produce soil moisture in percent saturation units.

Appendix B. Neutral Regression

Neutral regression uses the following data model where each *k*th zero-mean observation time vector, \mathbf{y}_k , is related to unknown time vector, \mathbf{x} , with error process, $\boldsymbol{\varepsilon}_k$, and scaling parameter $\boldsymbol{\beta}_k$:

$$\mathbf{y}_k = \beta_k \mathbf{x} + \mathbf{\varepsilon}_k \,. \tag{B4.1}$$

The observations, errors, and scaling parameters are collected into column matrices as $\mathbf{Y} = \{\mathbf{y}_1, \mathbf{y}_2, \mathbf{y}_3\}, \mathbf{E} = \{\mathbf{\varepsilon}_1, \mathbf{\varepsilon}_2, \mathbf{\varepsilon}_3\}, \text{ and } \mathbf{\beta} = \{\beta_1, \beta_2, \beta_3\}, \text{ respectively.}$ The least squares fit is then minimized with respect $\mathbf{\beta}$ subject to the constraint $\mathbf{\beta}^T \mathbf{\beta}$,

$$L = \mathbf{E}^{\mathrm{T}} \mathbf{E} - \lambda (\mathbf{\beta}^{\mathrm{T}} \mathbf{\beta} - 1), \qquad (B4.2)$$

where λ is a Lagrange multiplier (Marsden 1999). The solution to B2 is the characteristic equation,

$$\mathbf{Y}^{\mathrm{T}}\mathbf{Y}\boldsymbol{\beta} = \lambda\boldsymbol{\beta}\,,\tag{B4.3}$$

where β is identified as an eigenvector associated with each eigenvalue λ . The minimizing solution is the eigenvector corresponding to the smallest eigenvalue, readily obtained from a Singular Value Decomposition. An estimate of the unknown signal is given by,

$$\hat{\mathbf{x}} = \mathbf{K}\mathbf{Y}^{\mathrm{T}},\tag{B4.4}$$

with weights collected in the row vector $\mathbf{K} = \{ \beta_1^2, \beta_2^2, \beta_3^2 \}.$

Appendix C. Triple Collocation

Triple Collocation uses the same underlying data equation (B4.1) as Neutral Regression. However, the error variance estimates \mathbf{r}_{kk} are computed from the following pairwise expectations:

$$\hat{r}_{11} = \left\langle \left(\mathbf{y}_{1} - \mathbf{y}_{2} \right)^{\mathrm{T}} \left(\mathbf{y}_{1} - \mathbf{y}_{2} \right) \right\rangle,$$

$$\hat{r}_{22} = \left\langle \left(\mathbf{y}_{2} - \mathbf{y}_{1} \right)^{\mathrm{T}} \left(\mathbf{y}_{2} - \mathbf{y}_{3} \right) \right\rangle,$$

$$\hat{r}_{33} = \left\langle \left(\mathbf{y}_{3} - \mathbf{y}_{1} \right)^{\mathrm{T}} \left(\mathbf{y}_{3} - \mathbf{y}_{2} \right) \right\rangle,$$
(B4.5)

where $\langle \bullet \rangle$ is the expected value operator and the root mean square estimate (RMSE) is $\sqrt{\hat{r}_{kk}}$. The \mathbf{y}_k can be normalized for $\beta_k \neq 1$ using an iterative approach outlined in Scipal (2008).

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TABLES

Table 4.1 : Skill metrics for RMSE estimates from TC and EM methods relative to RMSE computed in relation to *in situ* soil moisture observations for the MERRA, PETS, and AMSR-E VU soil moisture datasets. These results correspond to scatter plots in Figure 4.1a,b.

Dataset	TC RMSE R ²	EM RMSE R ²
MERRA	0.38	0.91
PETS	0.35	0.95
AMSR-E VU	0.96	0.90

Table 4.2: Change in ColKF merged soil moisture correlation relative to MERRA correlation computed versus in situ soil moisture (ΔR) for three merging filter configurations. Positive ΔR indicates correlation improvement. The Site Fit configuration uses a ColKF calibrated using assumed "perfect" parameters fit to in situ data to merge the MERRA, PETS and AMSR-E VU soil moisture datasets. The EM ColKF VU uses EM to determine system parameters and ColKF to merge MERRA, PETS and AMSR-E VU datasets. The EM ColKF UMT uses EM to determine system parameters and ColKF to merge MERRA, PETS and AMSR-E UMT datasets. These results correspond to overall average of data shown in Figure 4.1a.

Filter Run	ΔR ColKF - MERRA
Site Fit ColKF VU	0.141
EM ColKF VU	0.073
EM ColKF UMT	0.072

FIGURES



Figure 4.1: Soil moisture RMSE estimated by (a) Triple Collocation (TC) and (b) Expectation Maximization (EM) relative to RMSE computed using *in situ* soil moisture observations for MERRA, PETS, and AMSR-E VU soil moisture time-series. (c) Lag-1 AR parameters (ϕ_1) estimated using EM relative to ϕ_1 estimated using *in situ* soil moisture.



Figure 4.2: Soil moisture anomaly (i.e. with mean seasonal cycle removed; in % saturation units) time-series for a grassland site near Lethbridge, Alberta, Canada (CA-Lth). Time-series inlcude *in situ* soil moisture (**x**), EM ColKF smoother merged estimate

 $(\mathbf{x}^s) \pm$ smoother prediction error standard deviations ($\sqrt{\mathbf{P}^s}$), MERRA, PETS, and AMSR-E VU soil moisture datasets. Time-series Pearson correlations are given in parentheses for each dataset relative to the *in situ* observations. Plot corresponds with Figure 3.1.



Figure 4.3: Bin averaged (\pm 95 % confidence interval) correlation for soil moisture timeseries estimates relative to *in situ* soil moisture observations for tower flux sites binned by vegetation optical depth. Results are shown for (a) soil moisture anomalies (with seasonal cycle removed) and (b) full soil moisture time-series (sum of anomaly and mean seasonal cycle). Control benchmark merging estimates shown in black and white squares, merged estimates in colored squares, and original model and remotely-sensed time-series estimates in colored circles.



Figure 4.4: Individual soil moisture time-series RMSE patterns and corresponding merging weights estimated using Neutral Regression over the continental US domain. Estimated RMSEs are shown for (a) MERRA, (c) AMSR-E VU, and (e) PETS. Estimated cooresponding merging weights are shown for (b) MERRA, (d) AMSR-E VU, and (f) PETS. Individual merging weights sum to unity for each grid cell.



Figure 4.5: Effective RECO model soil moisture response multiplier ($f_{EC}(SMSF)$) computed by inverting (4.1) using flux tower RECO observations, TSOIL, and \overline{C} . Symbols represent 90th percentile of effective multiplier for bins of 1 % soil moisture saturation using *in situ* (black squares) and MERRA (green circles) soil moisture. Grey field and error bars represent the range 81^{rst} -99th percentile for *in situ* and MERRA soil moisture, respectively. Blue line represents sigmoidal curve fitted result using *in situ* soil moisture and red line represents the originally hypothesized parabolic curve.



Figure 4.6: RECO time-series at a selected Oklahoma grassland flux tower site (US-ARc), including *in situ* tower RECO observations (black line), model (eqn. (4.1)) predictions derived with no input soil moisture (red line), and model (eqn. (4.1)) results derived using *in situ* soil moisture inputs.



Figure 4.7: Overall average RECO model (a) Pearson correlation and (b) RMSE relative to *in situ* flux tower RECO observations for 28 tower sites in the continental US domain. Shown are results for model using site soil moisture as input (Site SM), Expectation Maximization (EM) merged soil moisture as input (Merged SM), MERRA soil moisture as input (MERRA) and no input soil moisture (No SM). Error bars represent \pm one standard deviation across sites. Black squares are correlations for RECO estimates and white squares are correlations for merged and MERRA soil moistures relative to *in situ* soil moisture to show relative skill differences between the two datasets.



Figure 4.8: RECO model Pearson correlation improvement (ΔR) relative to *in situ* tower RECO observations for (a) RECO model using input *in situ* soil moisture minus RECO model without soil moisture input and (b) for RECO model using merged soil moisture minus RECO model without soil moisture input. Results shown here correspond to North American flux tower subset of overall results given in Figure 4.7.



Figure 4.9: Estimated percent improvement for soil moisture and RECO estimates. (a) Estimated soil moisture RMSE percent improvement [%] between the merged and MERRA soil moisture, computed using merging method RMSE estimates. (b) Percent [%] improvement in RECO model by using merged SM inputs relative to standard MERRA SM inputs computed using error propagation.

CHAPTER 5: OPERATIONAL MONITORING OF LAND-ATMOSPHERE CO₂ EXCHANGE USING SATELLITE SOIL MOISTURE: THE SOIL MOISTURE ACTIVE PASSIVE (SMAP) MISSION LEVEL 4 CARBON (L4C) PRODUCT

5.1 INTRODUCTION

Soil moisture is a fundamental requirement of life on land. Plants and microorganisms alike require moisture for growth and turgor; accordingly, soil moisture availability plays a major role in explaining the spatial and temporal variability of the global land CO₂ sink. The land and ocean CO₂ sinks provide a roughly 50 % offset of anthropogenic atmospheric emissions, with seasonal and interannual variability mainly driven by the land sink. Attributing land sink variability to its controlling factors is therefore key to understanding year-to-year changes in the atmospheric CO₂ growth rate (Canadell 2007). Several previous studies have indicated the dominant role played by water-limited ecosystems in determining global land sink inter-annual variability (Ahlstrom 2015;Cleverly 2016; Poulter 2014; Zhao & Running 2010). However, the influence of soil moisture on the global carbon cycle has been obscured by a lack of continuous, high-quality soil moisture observations with global coverage at appropriate spatial and temporal resolution.

Understanding linkages between the global water and carbon cycles is a major objective of the NASA Soil Moisture Active Passive (SMAP) mission (Entekhabi 2010). Using soil moisture observations to improve global estimates of land CO₂ flux and evapotranspiration are a major means to this end. Beginning March 31, 2015, the SMAP satellite began providing L-band microwave brightness temperature (1.41 GHz) observations with global land surface coverage every three days. SMAP brightness

temperature (TB) observations, which typically represent conditions in the top 5 cm of the soil, are assimilated into the NASA Goddard Earth Observing System, Version 5 (GEOS-5) Catchment land surface model to produce daily surface and root zone soil moisture and temperature estimates as part of the SMAP Level 4 Soil Moisture (L4SM) data product (Reichle 2016a; Reichle 2016b). Using L4SM and other input data from MODIS and GEOS-5, the SMAP Level 4 Carbon (L4C) data product provides daily global estimates of terrestrial carbon (CO₂) fluxes and underlying environmental controls (Kimball 2016a; Kimball 2016b; Glassy 2016).

Soil moisture availability controls key biological processes including plant photosynthetic activity, soil litter decomposition and heterotrophic respiration. Photosynthesis and gross primary production (GPP) are the primary pathways of ecosystem CO₂ uptake, whereas ecosystem respiration (RE), the sum of plant autotrophic and soil heterotrophic respiration (RA and RH, respectively), releases CO₂. Photosynthesis supplies the raw carbohydrate building blocks for biomass production, which eventually falls as litter and is converted into soil organic carbon (SOC). Litter is metabolized by soil microorganisms at a rate roughly inversely proportional to the litter carbon to nitrogen (C:N) ratio, or more directly the ratio of lignin to nitrogen (lignin:N), and modulated by soil moisture and temperature conditions as primary environmental control factors (Chapin 2002; Potter 1993; Parton 1987). Whereas GPP is sensitive to plant-available soil moisture within the rooting depth profile, soil litter decomposition and RH are primarily influenced by soil moisture and temperature within the surface (0-5 cm) soil layer where labile litter substrate (low C:N) and abundant oxygen are available (Davidson 2006; Chapin 2002). The physiological details of these processes are closely

tied to the dominant vegetation land cover or plant functional type (PFT).

Previous satellite data driven ecosystem modeling approaches have relied on various proxies to represent moisture constraints to ecosystem productivity and respiration, including vapor pressure deficit (VPD) to represent atmospheric moisture stress or precipitation driven bucket models to represent plant-available soil moisture. The MODIS MOD17 operational GPP product uses VPD as the sole moisture constraint to vegetation productivity without accounting for its interaction with root zone soil moisture (Running 2004). The NASA CASA (Carnegie Ames Stanford Approach) model estimates NEE and SOC dynamics at a monthly time step and relatively coarse (0.5°) spatial resolution using a precipitation driven bucket model to define soil moisture dynamics and environmental controls (Potter 1993). The L4C product extends these previous satellite-based ecosystem models by incorporating SMAP L4SM surface and root zone soil moisture and soil temperature information as primary environmental controls for estimating daily carbon fluxes and SOC dynamics. L4C model processing is conducted globally at 1-km resolution consistent with MODIS land cover and vegetation inputs (Kimball 2014); model outputs are posted to a coarser 9-km global grid, while preserving sub-grid (1-km resolution) PFT heterogeneity within each grid cell.

Although soil moisture retrievals from microwave remote sensing have been available for more than a decade, relatively coarse resolution (≥ 25 km), intermittent data coverage, large uncertainty and variable data quality generally precluded their use within ecosystem models. Additionally microwave measurements reflect conditions in only the top 5 cm of the soil. The L4SM product addresses these problems by providing timely (latency < 3 days), global and temporally continuous estimates of surface to root zone

soil moisture and temperature over a 9-km resolution grid, propagating surface soil information from SMAP over the entire soil profile (0-100cm depth) using the GEOS-5 catchment model (Reichle 2016a; Reichle 2016b). The L4C product integrates L4SM information within a calibrated, data-driven Terrestrial Carbon Flux (TCF) model using GEOS-5 daily surface meteorology, MODIS (Moderate Resolution Imaging Spectroradiometer) land cover and 8-day FPAR (canopy intercepted fraction of photosynthetically active radiation) observations as primary inputs. Resulting L4C product variables include NEE, GPP, RH and surface SOC content. Additional L4C diagnostic variables include primary environmental control factors underpinning the daily carbon flux estimates and detailed quality assurance metrics describing estimated model NEE performance for every grid cell – with random error quantified as unbiased root mean square error (ubRMSE). Thus the L4C product provides a new tool linking ecosystem-atmosphere CO₂ exchange to underlying vegetation, soil moisture and climate variability.

The objectives of this work are: *i*) to link SMAP informed soil moisture observations to ecosystem CO₂ exchange and underlying environmental controls on vegetation growth, soil litter decomposition and respiration processes; *ii*) to determine NEE and component carbon flux sensitivity to soil moisture variability; and *iii*) to determine whether SMAP observations provide added value over other sources of information for estimating NEE and component carbon fluxes, including GPP and RH. These objectives are addressed by investigating output from the L4C model after calibration to historic (pre-launch) tower flux measurements, by performing model sensitivity analyses, and by evaluating the accuracy of the operational L4C data product

against contemporaneous tower carbon flux measurements and other independent, global observational benchmarks.

5.2 Methods

5.2.1 The L4C Data Product

The L4C product fields are summarized in Table 5.1. Each daily L4C hierarchical data format version-5 (HDF5) daily granule contains estimates of global land-atmosphere CO₂ flux (g C m⁻² d⁻¹), including NEE, GPP, and RH. Other L4C product fields include SOC, diagnostic environmental constraint multipliers (EC), quality control flags (QC), and NEE ubRMSE estimates for quality assessment (QA ubRMSE; Kimball 2016a; Glassy 2016). The TCF model and associated L4C product uses a 1-km resolution EASE Grid v2 (EGv2) projection format as its native computational resolution and L4C results are posted to a coarser 9-km grid while preserving sub-grid variability from major PFT categories within each grid cell determined from the nested 1-km processing (Brodzik 2012). The L4C processing runs operationally within the SMAP Level 4 Science Data System of the NASA Global Modeling and Assimilation Office (GMAO). The L4C system provides consistent global daily outputs with an 8-10 day latency suitable for global monitoring and associated applications. For this study, I use data from the Version 2.0, "Validated Release" L4C data product (Science Version ID Vv2040; Kimball 2016b; "mdl" http://dx.doi.org/10.5067/UBK05ZUI7I5V). Three L4C data sets were used in this study – one operational data set (publically available as cited above) and two scientific datasets (available upon request) – including: 1) post-launch

operations (L4C Ops) spanning March 31, 2015 to present (Kimball 2016a); 2) prelaunch calibration, initialization and climatological reference simulations (L4C Calib) representing the period from Jan. 1, 2001 to Dec. 31, 2012; and 3) an "open-loop" simulation (L4C Open Loop) used to evaluate the impact of SMAP observations on postlaunch operations spanning March 31, 2015 to present (Kimball 2016b).

5.2.2 L4C Input Datasets

L4C inputs required for model processing are summarized in Table 5.2. The L4C TCF model requires 1-km EGv2 static PFT and 8-day canopy absorbed fraction of photosynthetically active radiation (FPAR) maps. The L4C TCF model also requires daily 9-km EGv2 inputs include surface soil moisture (SMSF; 0-5 cm depth), root zone soil moisture (SMRZ; 0-100 cm depth), soil temperature (TSOIL; 0-5 cm depth), mean daily incoming photosynthetically active radiation (PAR), minimum daily air temperature (TMIN, 2 m height), and mean daily VPD. The L4C Ops, L4C Calib, and L4C Open Loop datasets derive their 9-km inputs from several native sources, including: L4SM; an L4SM-emulation dataset termed Nature Run version 4 (NRv4) that is not informed by SMAP observations (Reichle 2016b); the Goddard Earth Observing System, Version 5 forward processing system (GEOS-5 FP); and the Modern Era Retrospective Reanalysis (MERRA), which uses the same GEOS-5 land model (Rienecker 2011).

The native source formats of the L4C inputs are given in Table 5.3. The L4C Ops simulations uses soil temperature and soil moisture (surface and root zone) inputs from L4SM, and PAR, TMIN, and VPD from the GEOS-5 FP. The L4C Calib simulations use soil temperature and soil moisture (surface and root zone) inputs from NRv4, and PAR, TMIN, and VPD from MERRA because L4SM and GEOS-5 FP data were not available

for the SMAP pre-launch period. The L4C Open Loop simulations use soil temperature and soil moisture (surface and root zone) inputs from NRv4, and PAR, TMIN, and VPD from GEOS-5 FP to isolate the impact of SMAP observations on L4C Ops. MODIS provides static PFT and 8-day FPAR inputs for each L4C simulation.

The L4SM data assimilation system provides 3-hourly soil temperature and soil moisture (surface and root zone) in EGv2 9-km format (Reichle 2016b). The 3-hourly L4SM data are aggregated to daily averages as an L4C preprocessing step. Root zone soil moisture (SMRZ) in percent saturation units is rescaled to SMRZ_{rsc} using the following normalized log-transform,

$$SMRZ_{norm} = \ln\left(\frac{SMRZ_{max} - SMRZ_{wp}}{100 - SMRZ_{wp}}\right) * 100 + 1, \qquad (5.1)$$

$$SMRZ_{rsc} = \ln(SMRZ_{norm} - 101)*95 + 5),$$
 (5.2)

where $SMRZ_{max and} SMRZ_{wp}$ are the grid cell record soil moisture levels for respective maximum soil moisture and plant wilting point conditions. The above rescaling increases the SMRZ dynamic range across time and space, especially in arid regions where sparse rainfall may not fully saturate soil, but soil water is still accessible to arid-adapted plants. The rescaling adjustment represents a compromise between using soil water matric potential and using soil moisture with linear GPP response (Figure 5.1).

The SMAP L4 processing system uses an Ensemble Kalman Filter (EnKF) assimilation to combine SMAP Level 1C orbital swath TB retrievals (~36 km resolution) with the Catchment Model simulations coupled with an L-band emission model and GEOS-5 FP meteorological forcing fields (Reichle 2014). The L4SM algorithm rescales 163

SMAP TB observations into the L-band emission model climatology to minimize bias in the assimilation system (Reichle 2004). The L-band emission model and rescaling parameters were calibrated prior to the SMAP launch using similar satellite L-band TB observations from the ESA Soil Moisture Ocean Salinity (SMOS) mission (De Lannoy 2013). Because SMAP and SMOS TB observations are not cross-calibrated, some minor bias is unavoidable in the current L4SM version (Reichle 2016c). Eventually this bias is expected to further decrease as more SMAP data becomes available for model recalibration. In this study I used input data from the Version 2 "Validated Release" L4SM data product (Science Version Vv2030; "gph" http://dx.doi.org/10.5067/YK70EPDHNF0L; "aup" http://dx.doi.org/10.5067/JJY2V0GJNFRZ, and "Imc"

http://dx.doi.org/10.5067/VBRUC1AFRQ22 series).

The NRv4 dataset was created to support scientific development and evaluation of SMAP Level 4 products (Reichle 2016b). The NRv4 record is derived using an identical land model to L4SM (i.e. Catchment Model), but is not informed by SMAP TB observations, including data assimilation adjustments to model soil moisture and temperature fields - hence the "Open Loop" designation. The NRv4 record is available from 2000-present to support SMAP science team investigations. The SMAP Level 4 soil moisture and carbon models require pre-launch calibration and initialization, and post-launch evaluation. Specifically, the L4C system required pre-launch calibration of model parameters, initialization of soil carbon pools, and a baseline for evaluating post-launch L4C results which are potentially impacted by changes in SMAP instrument calibration, changes in the L4SM data assimilation system in addition to natural soil moisture and

temperature anomalies. The NRv4 record provides a temporally consistent dataset meeting L4 requirements for pre-launch model calibration and initialization, and post-launch evaluations of SMAP observation impacts.

The GEOS-5 FP (Luchessi 2013; https://gmao.gsfc.nasa.gov/GMAO products) provides 3-hourly surface meteorological fields in $1/4^{\circ} \times 3/8^{\circ}$ geographic grid format, including net incoming short wave radiation (SWGDN), air temperature (2 meter height; T2M), surface skin temperature (TSURF), surface air pressure (PS), and water vapor mixing ratio (2 meter height; QV2M). The L4C preprocessor aggregates the GEOS-5 FP meteorology to a daily time step consistent with model processing. Daily photosynthetically active radiation (PAR) was estimated as a proportion (45%) of SWRAD and used with MODIS 8-day FPAR inputs to estimate canopy-absorbed PAR (APAR) on a daily basis. Minimum daily air temperature (TMIN) was computed as the minimum 1-hourly temperature. Daily landscape freeze-thaw (FT) status was computed from TSURF using a simple pure water freezing-point threshold (273.15 K). The original plan to use SMAP radar based FT observations was abandoned due to the radar sensor failure on July 7, 2015. However, alternative FT observations derived from the SMAP TB observations will be used in future L4C versions. Daily average vapor pressure deficit (VPD) was computed using the remaining GEOS-5 FP fields. Similar to GEOS-5 FP, MERRA input fields are available in a coarser $(1/2^{\circ} \times 2/3^{\circ})$ geographic grid for the 1980-2015 record (Rienecker 2011). All MERRA and GEOS-5 FP fields are converted to the same 9-km EGv2 projection prior to L4C processing using nearestneighbor re-sampling.

MODIS provides the fine-resolution (1-km) data used within L4C, including

global land cover (MOD12Q1) and 8-day FPAR (MOD15A2) information on 500-m and 1-km sinusoidal grids, respectively. The MOD12Q1 Plant Functional Type (PFT; Type 5) classification (Friedl 2010) is resampled to 1-km EGv2 format and used in L4C model processing; the temporally static MOD12Q1 land cover classification currently used for L4C operational processing distinguishes up to eight different global PFT classes. The PFT classes were used to stratify L4C model parameters and environmental response characteristics for different biomes. The L4C simulation was also summarized by the 1km PFT classifications, allowing differential environmental responses within each 9-km grid cell posting. The MOD15A2 (Collection 5) product (Knyazikhin 1999) is resampled to 1-km EGv2 and used to define dynamic (8-day) canopy FPAR variability for L4C processing. Missing or low quality (QC) FPAR data for a given 1-km pixel were filled prior to L4C processing using an ancillary average 8-day best QC climatology established from the MODIS historical (2001-2012) record. L4C simulations were performed only for vegetated pixels (PFT classes 1-8) having an available FPAR climatology. If MODIS 1-km FPAR observations were not available for a given 8-day period, then the ancillary 1-km FPAR climatology was substituted. Climatological FPAR substitution rates are flagged within the QA bit fields of each L4C granule if substitution rates exceed >50% for a given 9-km grid cell.

5.2.3 L4C Model Logic

NEE is defined as total ecosystem respiration (RE; autotrophic (RA) plus heterotrophic respiration (RH)) less GPP, i.e. NEE = RE – GPP, where a negative sign convention denotes net ecosystem uptake of atmospheric CO₂. The L4C product uses a light-use-efficiency (LUE) model within a Jarvis-Stewart constraint framework for estimating GPP (Whitley 2009; Monteith 1977; Prince & Goward 1995; Kimball 2009),

$$GPP = APAR * \varepsilon_{\max} * Emult, \qquad (5.3)$$

$$Emult = f_{EC}(VPD)f_{EC}(TMIN)f_{EC}(SMRZ)f_{EC}(FT), \qquad (5.4)$$

where canopy-absorbed PAR (APAR) is defined as the product of PAR and FPAR; ε_{max} is a maximum light use efficiency parameter defined for individual PFT classes under optimal (non-limiting) environmental conditions; and *Emult* is the relative reduction in estimated photosynthetic light use efficiency from potential (ε_{max}) due to sub-optimal environmental conditions. Such conditions include excessive VPD, cold TMIN or frozen (FT) conditions, and dry SMRZ. *Emult* is defined as the product of equally weighted dimensionless (0-1) scalar multipliers representing PFT-specific responses to each environmental variable. The *f*_{EC}(*x*) terms in (4) are described using linear ramp functions ranging from optimal (1) to fully constrained (0) conditions (Running 2004) for each environmental variable:

$$f_{EC}(x) = (x - x_{\min}) / (x_{\max} - x_{\min}),$$
(5.5)

where x_{min} and x_{max} are model parameters specified for each PFT class (Kimball 2014). An exception to (5) is f_{EC} (FT), which is flagged as zero if frozen and unity under nonfrozen conditions. RA is then computed as the PFT prescribed fraction (f_{aut}) of estimated GPP (i.e. RA = f_{aut} GPP; Waring 1998). Many previous LUE formulations are available as reviewed in Xiao (2014); however, the L4C model combines LUE and soil decomposition models to determine a more comprehensive daily carbon budget, using daily SMRZ inputs as an additional moisture constraint to GPP and RH, and employs model calibration using historical daily CO₂ flux observations from the global tower (FLUXNET) observation network.

A three pool soil decomposition model with cascading SOC quality and associated decomposition rates is used to estimate RH. Carbon fixed by GPP enters the SOC pools as litterfall (L_{fall}) specified as a constant daily fraction of estimated mean annual net primary productivity (NPP = GPP – RA). Daily SOC change for each of the three SOC pools is specified as (Kimball 2009; Kimball 2014; Ise & Moorcroft 2006),

$$\frac{dC(t)_{fast}}{dt} = L_{fall} \mathbf{f}_{fast} - RH(t)_{fast}, \qquad (5.6)$$

$$\frac{dC(t)_{med}}{dt} = L_{fall} (1 - \mathbf{f}_{fast}) - RH(t)_{med}, \qquad (5.7)$$

$$\frac{dC(t)_{slow}}{dt} = \mathbf{f}_{med} RH(t)_{med} - RH(t)_{slow},$$
(5.8)

where subscripts denote typical SOC decay rates relating to labile leaves and fine roots (low C:N), structural coarse woody roots (moderate C:N, high lignin content), and recalcitrant SOC (high C:N, tannins, phenols, SOC bound in clay and permafrost), respectively. RH is computed for the *i*-th SOC pool in (5.6)-(5.8) using surface soil moisture and soil temperature as primary controls on SOC decomposition (Kimball 2009),

$$RH_i(t) = f_{EC}(TSOIL)f_{EC}(SMSF)k_iC_i(t), \qquad (5.9)$$

where $f_{EC}(TSOIL)$ is an Arrhenius exponential function of TSOIL (Lloyd & Taylor 1994); $f_{EC}(SMSF)$ is a ramp function of surface (0-5 cm) soil moisture (SMSF) and k_i is the optimal decay rate for the *i*-th SOC pool. Total RH is derived as the sum of RH_i, including the adjustment RH₂ = (1-f_{med})RH_{med} to account for material transferred into the slow pool during humification (Potter 1993).

Random error uncertainty estimates for NEE, as indicated by the ubRMSE metric, are produced using analytical error propagation. I define the ubRMSE of two random variables as the variance of the residuals of their least-squares regression. I then compute the Jacobian (**J**) by taking derivatives of NEE of the above model with respect to each input dataset. I then assign a diagonal input error covariance matrix (\mathbf{E}_{input}) as part of the L4C calibration process (Section 5.2.4). The estimated NEE error is computed as:

$$E_{NEE}(t) = \mathbf{J}(t)\mathbf{E}_{input}\mathbf{J}^{\mathrm{T}}(t), \qquad (5.10)$$

for each 1-km pixel and daily time step. The now scalar quantity E_{NEE} term is spatially averaged using the sum of squares within each 9-km grid cell and the NEE ubRMSE QA metric is computed as the square-root of this average.

5.2.4 Model Calibration and Initialization

The L4C model was calibrated during the mission pre-launch phase using a global network of *in situ* tower eddy covariance CO₂ flux measurement records (2001-2008) from the FLUXNET La Thuile Collection (Baldocchi 2001). This dataset consists of 238

flux tower locations representing the major global biomes and PFT classes, although spatial coverage heavily favors temperate forest and cropland ecosystems in the United States and Europe (Baldocchi 2008). I use only tower sites having at least two years of observations, leaving 228 remaining sites (Figure 5.2). I used daily NEE, GPP, and RE computed from half-hourly NEE as reported by the La Thuile site investigators. Daily GPP and RE estimates were partitioned from half-hourly NEE measurements based on the short-term temperature response of respiration to night-time NEE (Reichstein 2005; Desai 2008). Since gap-filling of flux data requires pre-assigned meteorological responses, I use only daily data values reported as non-gap-filled. Tower flux data from multiple locations were pooled according to the dominant (highest coverage) PFT of the 9-km model grid cell overlying each tower location and model parameters were calibrated separately for each PFT class. The towers used for model calibration were also screened to ensure consistency between the dominant PFT represented within the tower footprint and the overlying 9-km model grid cell.

Model calibration proceeded in three steps using daily eddy covariance CO₂ flux observations from the 228 tower calibration sites: 1) the L4C GPP model outputs were fitted to the tower GPP observations; 2) the RE model outputs were then fitted to the tower RE observations using the new estimates from the calibrated GPP model; 3) the NEE ubRMSE estimates were then fitted to NEE RMSE computed using the newly calibrated model NEE vs the tower NEE observations. Calibrated parameter values are given in Table 5.4. The L4C model fitted parameters for GPP included ε_{max} , VPD_{min} , VPD_{max} , $TMIN_{min}$, $TMIN_{max}$, $SMRZ_{min}$, and FT_{mult} ; the model RE fitted parameters included F_{aut} , and $SMSF_{min}$ (Table 5.5). The model parameters were confined to pre-
defined realistic bounds, and were fixed at default values if constraints were not well represented by the tower calibration sites (e.g. VPD for tropical EBF rarely exceeds 3 kPa). All optimizations were fitted using least-squares non-linear regression.

After fitting the L4C TCF model, I performed a GPP model input sensitivity analysis to determine the relative explanatory value of each input variable relative to tower GPP. The model was run for six different combinations of input variables including: full model with all inputs, without FT, without TMIN, without SMRZ, without VPD, and finally without EMULT (i.e., with APAR only). Model skill was evaluated using Pearson correlation relative to tower GPP for sites dominated by each plant functional type. Correlations were computed using data pooled from across each site, indicating across-site explanatory skill, and were computed as averages across sites, indicating within-site explanatory skill.

Soil moisture and temperature inputs to the L4C TCF model for the calibration period (2001-2012) were provided by the SMAP L4_SM NRv4 dataset. Remaining daily surface meteorological inputs were provided by the MERRA reanalysis, which uses the same GEOS-5 land model as the NRv4 dataset (Section 5.2.2). MODIS land cover and 8-day FPAR inputs to the L4C TCF model were available for the calibration period. A mean daily climatology of all model inputs was derived from the longer (2001-2012) data records and used for L4C TCF model calibration and initialization.

The L4C TCF model SOC values were initialized to steady-state conditions during the SMAP pre-launch phase using the daily input climatology. The resulting L4C NEE source/sink strength thus depends on the effective differences of current conditions versus those from the recent (2001-2012) period used to define the SOC pool available

for decomposition and RH. Because most ecosystems are not in steady-state (Baldocchi 2008; Carvalhais 2010), the L4C model tends to underestimate the effective carbon sink strength indicated from tower observations. This results in L4C RE and NEE as high-biased and low-biased, respectively, relative to most tower observations in undisturbed ecosystems (Carvalhais 2010). To mitigate these site-to-site biases when calibrating RE against tower data, I determine the 95th percentile of RE from each tower site and substitute this quantity as a constant effective SOC factor (\overline{C}) during L4C model calibration:

$$\overline{C} \cong \sum k_i C_i, \tag{5.11}$$

This procedure is imperfect because C_{fast} is seasonally dynamic (i.e. has sub-annual turnover time), but for practical purposes it reduces the effective model bias during calibration.

After calibration, L4C SOC levels were initialized to steady-state conditions using two steps. In the first step, I analytically solved Eqns. 6-8 using the L4C Calib inputs. This solution provided steady-state annual mean SOC values. In the second step, these values were used to initialize a numerical solution (i.e. "spin-up"), which cycles the input MERRA, NRv4, and FPAR climatologies until the annual NEE is within ± 1 g C m⁻² y⁻¹. Since the analytical values were quite close to the numerical steady state (e.g. closer for C_{slow} than C_{fast} , because C_{fast} has a larger seasonal cycle), this procedure usually required only a few (≤ 10) annual cycles. This resulted in a global 1-km SOC map for each day of a climatological year, which was then used to initialize L4C Ops for the March 31, 2015 beginning of the SMAP operational record.

5.2.5 Multi-tier Validation Strategy

The targeted performance metric for the L4C product is to estimate NEE at the level of uncertainty commensurate with *in situ* tower measurement based observations (ubRMSE ≤ 1.6 g C m⁻² d⁻¹ or 30 g C m⁻² y⁻¹). The L4C product accuracy was primarily assessed against independent CO₂ flux measurement based observations from a global network of 26 tower core validation sites (CVS) having concurrent overlapping observations with the L4C operational record for the March 31, 2015 to Dec. 31, 2015 period (Table 5.6; Figure 5.2).

The L4C operational product was also verified against other similar global observational benchmarks, including MOD17 GPP (Running 2004), Max Plank Institute Model Tree Ensemble (MPI-MTE) ecosystem fluxes (Jung 2010), NOAA CarbonTracker biological flux (Peters 2007), and Solar Induced canopy Fluorescence (SIF) from the ESA GOME-2 sensor on the MetOp-A satellite, which was used as a proxy for global GPP (Guanter 2013). GOME-2 provides Level 3 global monthly 734 nm – 758 nm (Channel 4) SIF retrievals on a $0.5^{\circ} \times 0.5^{\circ}$ grid extending from 2007-present (Joiner 2013). The GOME-2 record was selected for this study over other SIF observations, including the NASA Orbiting Carbon Observatory (OCO2; Frankenberg 2014), because of the longer record and consistent global gridding available from GOME-2.

I compared L4C effective NEE source/sink patterns against alternative NEE estimates derived from NOAA CarbonTracker atmospheric transport model inversions of global CO₂ flask measurements (Peters 2007). CarbonTracker adjusts continental-scale land and ocean carbon flux magnitudes using EnKF data assimilation combining TM-5 wind transport simulations with atmospheric CO₂ flask measurements, and adjusted using

estimated CO₂ contributions from anthropogenic and fire emissions. CarbonTracker's sub-continental spatial biospheric flux patterns are based on the GFED-CASA land model, which provides both NEE prior conditions and estimated fire CO₂ emissions, whereas the ecoregion-scale flux magnitudes are adjusted using CarbonTracker's the CT atmospheric inversion (van der Werf 2006). Comparing L4C NEE with the CarbonTracker biospheric flux provides an atmospheric perspective and a means for evaluating L4C potential to inform future inversion studies.

I compared the alternative MOD17 GPP dataset and the Max Plank Institute Model Tree Ensemble (MPI-MTE) GPP, RECO, and NEE datasets for comparison with L4C. MOD17 uses a LUE model similar to L4C but lacking a soil moisture constraint and, unlike L4C, was not calibrated using daily tower flux data (Running 2004). By contrast, MPI-MTE relies on a machine learning approach rather than a LUE model and was calibrated using the same La Thuile flux tower dataset as L4C (Jung 2010). MPI-MTE provides two estimates of GPP, one derived using RECO estimates based on nighttime fluxes from Reichstein (2005; abbreviated MR), and the other based on the relation between GPP and incoming radiation from the method of Lasslop (2010; abbreviated GL). The MOD17, MPI-MTE, and L4C grids were resampled to monthly $0.5^{\circ} \times 0.5^{\circ}$ and $1^{\circ} \times 1^{\circ}$ grids to compare with the SIF and CarbonTracker grids, respectively.

The L4C SOC outputs were compared with independent SOC estimates derived from global and regional soil inventory records, including IGBP-DIS global and NCSCD northern polar SOC maps (Global Soil Data Task Group 2000; Hugelius 2014). Within the soil column, the largest SOC levels are generally found within surface soil layers, declining exponentially with depth (Jobbagy & Jackson 2000). The IGBP-DIS and

NCSCD SOC values represent the top 1 m soil layer and were systematically decreased by a factor of 1/3 to approximate surface (< 10 cm) soil conditions represented by the L4C SOC outputs.

5.2.6 Model Sensitivity Analyses

I performed two types of model sensitivity analyses to quantify the impact of soil moisture on L4C derived carbon fluxes. First, I ran L4C Calib using the daily climatology inputs and incrementally removed the model soil moisture constraints to investigate their individual impact on the L4C estimated annual GPP and RH fluxes. Since RE is impacted by both GPP and RH, I focused on GPP and RH separately (rather than RE) to decouple their differential responses to soil moisture. Next, to assess the impact of SMAP observations on the carbon model calculations, I compared the L4C Ops record against L4C Open Loop simulations derived using NRv4 inputs without the influence of SMAP. The L4C Ops, L4C Open Loop, and L4C Calib results were then evaluated against the CVS tower daily carbon flux observations. A guiding hypothesis for the model sensitivity analysis was that the SMAP informed L4C Ops simulations should show similar or better accuracy than the L4C Open Loop simulations derived without the benefit of SMAP observations and also should outperform the L4C Calib climatological predictions. A similar approach was employed by the L4SM team to evaluate impacts of the L4SM data assimilation using a different set of soil moisture validation sites (Reichle 2016c).

5.3 **Results**

5.3.1 L4C Calibration

The L4C TCF model optimization tends to fit the constraint function along the outer edge of the relationship between each input field (VPD, SMRZ, and TMIN) and effective EMULT computed by inverting (5.3) using tower GPP (Figure 5.3). The constraining edge is clearly defined for VPD (Figure 5.3a) for the shrubland PFT class. However, the constraint function for TMIN has fitted *TMIN_{min}* much lower than the freezing point (273 K) as expected based on Figure 5.3b (Table 5.4). Unscaled SMRZ displays no distinct constraint and carries no weight in the optimization (i.e. *SMRZ_{max}* fitted below the lower range of SMRZ). Rescaled SMRZ shows a much more distinct constraining boundary and more realistic value for *SMRZ_{max}* (Figure 5.3; Table 5.4). Fitted parameter values for the full L4C model and all PFT classes are given in Table 5.4 alongside a model parameter glossary (Table 5.5).

Comparing L4C GPP performance amongst model runs with alternative input fields indicates the relative explanatory skill of each input field across plant functional type (Figure 5.4). TMIN is a relatively important predictor for all plant functional types, showing a consistent correlation drop when excluded. TMIN was a notable predictor of across-site GPP variability for productive PFTs including cereal and broadleaf crops, deciduous broadleaf forest, and especially for evergreen broadleaf forests. VPD was a stronger predictor for evergreen needleleaf, evergreen broadleaf, and shrublands; a somewhat weak predictor for deciduous broadleaf forests and grasslands; and was not a significant predictor for deciduous needleleaf forest and croplands. SMRZ had a significant impact on grasslands and shrublands, but little impact on other PFTs. FT showed little significant impact for any PFT.

5.3.2 Comparison with Core Flux Sites

The L4C Ops overall mean NEE RMSE was 1.04 g C m⁻² d⁻¹ and NEE ubRMSE was 0.79 g C m⁻² d⁻¹ relative to the CVS tower carbon flux benchmark measurements (Table 5.7). The SMAP L4C targeted accuracy threshold for NEE is $ubRMSE \le 1.6 \text{ g C}$ $m^{-2} d^{-1}$ mean across all sites, so the overall site mean NEE ubRMSE is well within this threshold. The L4C GPP results showed the highest correlation with the tower observations, followed by RE, while NEE showed the lowest correlations relative to the tower observations. The RMSE differences were generally proportional to the size of the carbon flux, with GPP and NEE having the highest and lowest RMSE levels, respectively. In contrast, NEE shows a somewhat larger though non-significant (p > 1)0.05) correlation increase than GPP when the L4C Ops and L4C Calib climatology results are compared, whereas RE is generally consistent between the L4C Ops and L4C Calib results. Likewise, no significant correlation skill differences were observed between L4C Ops and L4C Open Loop. Example L4C Ops time series for two tower locations with widely different climate and moisture conditions (US-Ivo and US-SRM) indicate that L4C Ops reproduces both the seasonal cycle and shorter-term variability of the tower carbon flux observations (Figure 5.5).

Two sites (CA-Oas and US-PFa) exceed the targeted (1.6 g C m⁻² d⁻¹) ubRMSE performance threshold for L4C Ops NEE, with respective ubRMSE differences of 2.06 and 2.13 g C m⁻² d⁻¹. Two other sites (AU-ASM and AU-Stp) show negative correlations between L4C and tower observations for GPP and NEE, respectively (R = -0.23 and -

0.19; Figure 5.6). Both CA-Oas and US-PFa towers are located in productive deciduous broadleaf forests. CA-Oas is located within an aspen grove surrounded by spruce forest, so the L4C model classifies the overlying 9-km tower grid cell as ENF dominant based on the MODIS land cover inputs. The US-PFa site is surrounded by wetlands which are not identified in the MODIS PFT classification, although the L4C model classifies the 9-km tower grid cell as DBF dominant. The small negative correlations for the AU-ASM and AU-Stp sites occur because the primary growing season at these arid sites is between January and March, which falls outside of the April-December study period such that the GPP and NEE observations are near zero with little variability.

The L4C results had higher monthly correlations with tower site GPP and SIF than MOD17, and the correlation of SIF with tower site GPP was substantially lower (R = 0.85 vs. R = 0.63 and R = 0.81, respectively; Table 5.8). L4C maintained a relatively high correlation with SIF and MOD17 (R = 0.73 and R = 0.85, respectively). Example time-series of L4C, SIF, and MOD17 are shown for the Tonzi Ranch California oak savannah (US-Ton; Figure 5.7). The three time-series generally follow the seasonal cycle of tower GPP, although SIF shows substantial variability about the seasonal cycle. The three time-series also show a negative anomaly relative to the interannual mean seasonal cycle in agreement with anomalously low tower GPP responding to severe drought conditions during the spring and summer of 2015 (Figure 5.7b).

5.3.3 L4C Uncertainty Metric Assessment

Comparison of the NEE ubRMSE QA metric against observed model and tower ubRMSE differences for the tower calibration sites show favorable correspondence for ubRMSE ≤ 2 g C m⁻² d⁻¹ (Figure 5.8a). However, the estimated ubRMSE QA metric shows apparent saturation and degraded performance at higher error levels (above ≈ 2 g C m⁻² d⁻¹), especially for relatively productive ENF, DBF, CCR and BCR cover types. Nevertheless, a similar comparison against the independent CVS observations shows favorable model correlation (R² = 0.71; p<0.01), indicating that the NEE ubRMSE QA metric provides a reasonable indicator of the site-to-site variability in L4C TCF model accuracy (Figure 5.8b).

The global L4C NEE QA pattern indicates that model ubRMSE accuracy tends to scale proportionally with overall ecosystem productivity (Figure 5.9). The estimated ubRMSE results indicate that the targeted 1.6 g C m⁻² d⁻¹ accuracy threshold for NEE is met for 66 % of the global domain and 83 % of the northern domain (\geq 45 °N). The highest estimated error occurs in relatively productive croplands, temperate deciduous forests, and tropical evergreen broadleaf forests, where the NEE ubRMSE typically exceeds 1.6 g C m⁻² d⁻¹. However, redefining estimated model uncertainty as a proportion of the estimated total carbon flux indicates that a 30 % relative error (i.e. NEE ubRMSE over the sum of GPP and RE) threshold is met for 82 % of the global model domain; these results indicate that the L4C product provides meaningful accuracy in many productive areas even though the estimated ubRMSE levels may exceed the 1.6 g C m⁻² d⁻¹ threshold.

5.3.4 Comparison with GOME-2 SIF

The L4C Calib GPP and GOME-2 SIF derived seasonal climatology results show generally consistent global patterns (R = 0.83; Table 5.9), although L4C results indicate a somewhat longer growing season in some regions (Figure 5.10). Poleward of 35°N, SIF and GPP show close agreement in apparent growing season onset, peak and duration.

From 20°N - 35°N, the L4C results indicate a longer and more persistent growing season than SIF, with increasing difference toward the tropical southern portion of this region. From 5°S - 15°N, the L4C results indicate peak growing season productivity during August and September, while the GOME-2 SIF results indicate a seasonal productivity minimum during this period. In contrast, poleward of 5°S, the L4C GPP and GOME-2 SIF results show similar peak timing and seasonality, although the L4C results show a somewhat longer growing season in the 35°S - 45°N region.

MPI-MTE and MOD17 GPP seasonal climatologies had somewhat higher and lower respective correlations with SIF (R = 0.85 and R = 0.79, respectively; Table 5.9) relative to L4C Calib. MPI-MTE matches SIF seasonal patterns more closely than L4C in the 20°N - 35°N latitude zone, whereas L4C matches SIF more closely in the 35°N -45°N zone. Tropical (5°S - 15°N) seasonal patterns are more similar amongst the GPP datasets than any individual dataset relative to SIF, with L4C Calib showing intermediate GPP between MOD17 and MPI-MTE.

The L4C Calib results show larger seasonal GPP amplitude and annual mean than MOD17 and MPI-MTE across much of the globe (Figure 5.11). Relative to MOD17, L4C shows larger seasonal amplitude in the central US croplands, arid Asian midlatitudes, India, Australia, and savannah portions of tropical and sub-tropical South America and Africa. Relative to MPI-MTE, L4C also shows larger amplitude in central US croplands, Asian mid-latitudes and Australia, but results are more mixed for South America and Africa. The L4C results generally had a somewhat smaller seasonal cycle across the Eurasian boreal latitudes relative to MOD17 and MPI-MTE, but has a larger seasonal cycle than MPI-MTE and a smaller cycle than MOD17 over the North American boreal latitudes. L4C also had a somewhat smaller seasonal cycle over central Africa relative to MOD17 and MPI-MTE.

The L4C results show the largest interannual monthly variance about the mean seasonal cycle in global arid regions, central US, and portions of the tropics (Figure 5.12a). MPI-MTE shows similar patterns of variability, but with little year-to-year variability in the tropics (Figure 5.12c). In contrast, MOD17 shows its highest variance in the tropics and also shows higher variability in northern high-latitudes than L4C (Figure 5.12b). SIF shows its highest variance in South America, the west coast of Africa, and Southeast Asia, with relatively low and uniform variance throughout the rest of the globe. As such, overall SIF global patterns substantially disagree with the three GPP datasets, although SIF corroborates high MOD17 variance in South America (Figure 5.12d).

5.3.5 Comparison with CarbonTracker Bioflux

The L4C Calib NEE and CarbonTracker biological flux results show coherent mean seasonal cycles (i.e. climatologies) for all latitudes, and similar latitudinal gradients (R = 0.60; Table 5.10). However, the timing, length, and depth of the estimated CO₂ uptake periods are most consistent poleward of 30°S with notable L4C and CarbonTracker differences elsewhere (Figure 5.13). Poleward of 30°N, the CarbonTracker results indicate earlier CO₂ uptake onset, earlier peak uptake, and larger fall CO₂ release relative to L4C NEE. Between 0°-30°N, CarbonTracker shows greater CO₂ release prior to CO₂ uptake onset. Between 0°-30°S, the L4C Calib NEE results show a longer and deeper CO₂ uptake period directly followed by peak CO₂ release from August to September, whereas CarbonTracker indicates a relatively short and shallow uptake period followed by peak CO₂ release from October to November. The L4C Calib NEE seasonal cycle matches CarbonTracker biological flux much more closely than MPI-MTE NEE and NEE computed using MOD17 with MPI-MTE RECO (R = 0.53 and R = 0.36, respectively; Table 5.10). In contrast, the MPI-MTE NEE seasonal cycle closely resembles the MPI-MTE GPP seasonal cycle, indicating only limited area of seasonal CO₂ release relative to CarbonTracker, and an especially strong CO₂ sink in the tropics. Although MOD17 (with MPI-MTE RECO) shows a somewhat weaker global sink than MPI-MTE NEE, the pattern shows little global resemblance to either CarbonTracker or MPI-MTE NEE. Notably, despite high GPP agreement (R =0.99; Table 5.9), the MPI-MTE GL method indicates somewhat different effective global RECO patterns than MPI-MTE MR GPP method, which correlate better with CarbonTracker (R = 0.53 vs. R = 0.49, respectively; Table 5.10).

The L4C, MOD17, and MPI-MTE derived, NEE interannual monthly variance about the seasonal cycle resemble the corresponding patterns shown by their respective GPP datasets (Figure 5.14a-c). In contrast, CarbonTracker indicates the largest-year-toyear differences in the central portion of North America and somewhat lower variance across mid-latitude Eurasia. Notably CarbonTracker shows little variance in Australia and India, in relative disagreement with the other three datasets. CarbonTracker shows moderate variability in southern Africa and South America indicating some agreement with the other three datasets in these regions. In absolute terms, the CarbonTracker seasonal cycle and interannual variance are substantially larger than L4C NEE, MPI-MTE NEE, and MOD17 NEE, implying a larger and more variable land CO₂ sink.

5.3.6 Comparison with Soil Organic Carbon Maps

The L4C Calib results generally reproduce the global SOC patterns indicated from the soil inventory records, including relatively higher SOC stocks in the high northern latitudes relative to the mid-latitudes. However, several discrepancies were observed (Figure 5.15a). In tropical and arctic regions the L4C derived SOC stocks are somewhat less than the IGBP and NCSCD inventory records indicate (Figure 5.15b). In the circumpolar boreal latitudes (50°-60°N), the L4C results show contrasting regions of high- and low-bias but similar overall zonal average SOC stocks relative to the IGBP record. The L4C SOC distribution peaks in the boreal forest zone (50° - 60° N), whereas the SOC distributions from IGBP and NCSCD peak near 65°-70°N. Notably L4C SOC low-bias relative to IGBP in boreal and artic regions (50°-70°N) is associated with the prevalent spatial distribution of extensive wetlands characterized by thick organic sediments (Hugelius 2014). Although the inventory records show similar mean SOC polar latitudinal gradients, considerable differences in SOC spatial patterns also occur between the IGBP and NCSCD records. The NCSCD record may be more accurate since it contains additional ground samples, and estimation focused on high-latitude conditions particularly including wetland soil types (Hugelius 2014); however, a recent comparison with a radar-based estimate has shown considerable over-estimation in many areas (Bartsch 2016).

5.3.7 Soil Moisture Sensitivity Analysis

The L4C Calib climatological model sensitivity analysis indicates that root zone soil moisture (SMRZ) has substantial impact on annual GPP (\geq 30 % annual difference) over approximately 12 % of the global model domain and some impact (\geq 5 % annual

difference) over 38 % of the global domain focused on drier climate areas (Figure 5.16a). The GPP results reflect the direct impact of soil moisture on estimated productivity in addition to other direct and indirect moisture constraints contributed from the model FPAR and VPD inputs. Atmospheric VPD has relatively more widespread impact on estimated GPP than SMRZ, with notable importance for tropical "dry" (seasonal) forests including Africa, and also for boreal forests, particularly in North America (Figure 5.16b). Moisture constraints from SMRZ and VPD show little impact on GPP for broadleaf crops, deciduous needeleaf forests, and tropical forests (with the exception of central Africa), although the L4C flux tower calibration dataset lacked DNF tower site representation.

The impact of surface soil moisture (SMSF) on RH is much more widespread than the root zone soil moisture impact on GPP (Figure 5.16a, Figure 5.16c). These results are consistent with the larger number of environmental controls influencing the L4C GPP (and RA) calculations, whereas only SMSF and soil temperature are used as the primary environmental controls on model estimated SOC decomposition and RH. Surface soil moisture has little impact on RH in equatorial tropical forests which lack a pronounced wet season.

The L4SM soil moisture analysis increment indicates that SMAP observations most impact L4SM in arid and semi-arid regions, which generally align with higher L4C soil moisture sensitivity (Figure 5.16d). However, L4SM SMSF analysis increment variability (i.e. data assimilated SMSF vs. forecast SMSF) is relatively small compared to overall soil moisture variance because the L4SM data assimilation affects only TB anomalies and therefore mostly affects sub-seasonal soil moisture variations. Likewise,

the largest L4C Ops and L4C Open Loop differences occur in arid regions (Figure 5.17). GPP shows relatively larger soil moisture sensitivity than NEE because the GPP and RH responses partially offset each other in the residual NEE term (Figure 5.17a). The L4C NEE response patterns were generally similar to GPP, but with notable exceptions, including Southern Africa, the northern Sahel and circumpolar boreal forest where the RH response dominates the NEE pattern (i.e., showing positive anomalies in GPP and NEE; Figure 5.17b).

5.4 **DISCUSSION**

5.4.1 L4C GPP Calibration and Input Data Evaluation

Root zone soil moisture had a substantial impact on L4C TCF model skill for grassland and shrubland PFT, but only if rescaling is applied (Figure 5.3 and Figure 5.4). These soil moisture patterns and the relatively larger impact of VPD for forested PFT relative to grassland and shrubland are consistent with another recent study examining the drought sensitivity of half-hourly flux data to VPD and soil moisture at Ameriflux sites (Novick 2016). The lack of discernable FT impact might be a result of the step-function assumed for the FT constraint. This constraint is likely too severe and immediate, because plant phenological release from freezing conditions and response to frozen tissue damage may not immediately impact GPP.

TMIN has substantial explanatory skill for GPP amongst-site variability, especially for evergreen broadleaf forests (Figure 5.4). TMIN skill is generally largest for the most productive PFT types (including evergreen broadleaf forest, deciduous

broadleaf forest, cereal crops, and broadleaf crops) and accompanied by a tendency for the model to fit rather shallow-sloped TMIN constraints with TMIN_{min} parameter much less than the freezing point (273 K) and ε_{max} higher than might be expected for each PFT as reported in the literature. This shallow slope puts a larger-than-expected penalty on high GPP points when TMIN is above the freezing point (usually >280 K). Much larger pooled-site correlations relative to site-average correlations, indicate that every even broadleaf forests have much larger across-site GPP variability than among-site variability. Also, the large impact of TMIN indicates that TMIN is a strong predictor of across-site GPP variability for these forests. Evergreen needleleaf forests have higher site-average correlations relative to pooled-site correlations because the seasonal variance of each site is larger than the across-site spatial variance. Taken together, these observations suggest that predictability of across-site variance is an important consideration for fitting the light use efficiency model, and that TMIN generally has more power to explain across-site variability in effective maximum light use efficiency, rather than accounting for seasonal cold conditions within each site as generally expected.

5.4.2 L4C Uncertainty Evaluation

The CVS flux tower comparisons indicate that L4C Ops captures daily-toseasonal variations and regional patterns in tower observed terrestrial carbon fluxes spanning a broad range of global climate and vegetation conditions (Figure 5.5; Figure 5.6). The L4C Ops derived GPP seasonality was generally proportional to RE, resulting in relatively lower NEE seasonality (Figure 5.13). The NEE results showed generally lower RMSE than GPP or RE relative to the tower observations because of smaller characteristic magnitude of the residual NEE flux (Table 5.7). Likewise, higher correlations between the tower observations and L4C results for GPP and RE relative to NEE were largely due to the smaller seasonal cycle of NEE rather than actual model skill differences (Figure 5.13). However, somewhat lower correlations between measured and modelled RE and NEE relative to GPP were partially impacted by model SOC mismatches relative to local site conditions which affect both L4C derived carbon fluxes and estimated error (ubRMSE) variance. Larger-than-expected model carbon flux ubRMSE and negative correlations with tower observations for some CVS locations were attributed to land cover (PFT) differences between the local tower footprint and MODIS 1-km land cover map used to define PFT heterogeneity in the L4C model, or to a limited (Apr-Dec, 2015) study period that missed the primary growing season for some sites (AU-ASM and AU-Stp). More productive tower sites (CA-Oas and US-PFa) also had relatively larger carbon fluxes and associated ubRMSE levels, although relative model error, expressed as a proportion of the total estimated carbon flux magnitude, indicated meaningful model accuracy across a broad range of global vegetation, productivity and climate conditions (Figure 5.8).

The NEE ubRMSE QA results for L4C Ops and L4C Calib indicate a general increase of model error with estimated carbon flux magnitude over the global domain (Figure 5.9). However, the model calibration results indicate that the explanatory power of the NEE QA metric saturates for higher ubRMSE levels beyond $\approx 2 \text{ g C m}^{-2} \text{ d}^{-1}$, which is generally characteristic of productive croplands and forests (Figure 5.8a). Croplands often contain diverse crop types, riparian areas and fallow fields, whereas forestland is often interspersed with cropland and pasture, and might be composed of different age classes and recovery stages from prior land use change, burning or harvesting. The

resulting sub-grid spatial heterogeneity in vegetation and soil conditions will tend to increase both random and bias errors in estimated carbon fluxes, leading to degraded ubRMSE accuracy. Other factors such as sub-grid PFT spatial heterogeneity and disturbance history likely dominated overall model uncertainty for such locations. Despite these limitations, the CVS results indicate that the L4C Ops ubRMSE QA metric provides a relatively robust measure of model NEE uncertainty (Figure 5.8b). Prior studies using similar satellite data driven LUE models (Heinsch, et al., 2006) indicate that model input uncertainty is a major source of model error (up to 30%), whereas the L4C QA metric provides a daily estimate of the aggregate effects of model inputs and assumptions on product accuracy.

5.4.3 L4C Evaluation Relative to SIF, CarbonTracker, and SOC Inventory Global Datasets

The L4C Calib and CarbonTracker derived NEE climatologies were generally consistent over the global domain (Figure 5.13). However, some regions showed different NEE spatial and temporal patterns, which may reflect model differences in seasonal litterfall regimes. Model differences in underlying climatic drivers and control factors affecting GPP and RE also impact these patterns but likely to a lesser extent. The CASA land model has a prescribed litterfall phenology (Randerson 1996) and provides the estimated monthly NEE priors used in the CarbonTracker inversion; CASA model NEE priors are responsible for most of the CarbonTracker sub-continental spatial variability. Unlike CASA, the L4C model has a daily time step and evenly distributes litterfall throughout the year (i.e. L_{fall}) in (5.6) and (5.7) constant for all *t*. Since NEE peak uptake is mainly driven by GPP, the relatively early CarbonTracker uptake onset and seasonal

peak in northern (>40°N) regions are at odds with both GOME-2 SIF and L4C Calib GPP climatologies which suggest that the ecosystem carbon uptake onset and peak should occur later (Figure 5.13). Nevertheless, L4C Calib carbon flux patterns generally align with typical GPP and NEE seasonal trends indicated from the GOME-2 SIF and CarbonTracker NEE benchmark datasets.

Changes in NEE trends over the long-term (several years) will result in changes to SOC stocks. Although comparisons of dynamic models, such as L4C, with inventorybased SOC maps are problematic, understanding their differences potentially gives insight regarding model and sampling uncertainty, and driving processes. The relative L4C under-estimation of SOC in the high latitudes is attributable to a lack of detailed information on wetlands (Figure 5.15). The L4C Calib results show peak SOC accumulation in the boreal latitudes because of the combination of moderate litterfall and cold conditions favoring SOC accumulation. Matching the larger SOC levels indicated from the soil inventory data would therefore require lengthening of L4C effective SOC turnover times for boreal and arctic latitudes. The apparent difference in L4C derived vs. effective turnover times may reflect the prevalence of boreal and tundra wetlands and peatlands, and associated anaerobic soil conditions, or differences in SOC quality (Ise & Moorcroft 2006) that may not be effectively represented by the model inputs and assumptions.

Although SOC may provide some insight for improving L4C RH estimates, the potential for improvement is ultimately limited by several factors. SOC development generally occurs over long periods (i.e. thousands of years or more) subject to changing climate and ecological conditions, so L4C model based SOC estimates derived from

recent satellite and meteorological records are expected to diverge from soil inventory records. Wetlands and peatlands accumulate large SOC stocks, and are common in boreal, arctic, and equatorial (tropical) biomes where relatively large model and inventory discrepancies were found. These areas are not well-represented by the global flux tower network, and there is little available flux information for robust L4C calibration of global wetland dynamics. Furthermore, SOC characteristically shows large spatial heterogeneity in wetland regions influenced by surface and sub-surface soil moisture dynamics that exist beneath the resolution of coarser scale SMAP observations and model derived products (L4C and L4SM). New fine-scale radar-based remote-sensing approaches for estimating soil carbon indicate approximately 25 % lower SOC in some arctic areas than indicated from NSCDC inventory records (Bartsch 2016). Considering such mismatches, inventory based SOC assessments may benefit from the comparison of climate-induced dynamics and spatial covariance metrics provided by the L4C product and other remote-sensing datasets.

5.4.4 L4C Evaluation Relative to MOD17 and MPI-MTE Global Datasets

The L4C GPP and NEE perform reasonably well relative to MOD17, MPI-MTE, CarbonTracker and SIF independent benchmarks, and when each is compared to flux tower observations. With the exception of global SIF where the correlation of MPI-MTE was somewhat higher (Table 5.9), L4C generally had higher correlation than MOD17 and MPI-MTE relative to the benchmarks (Table 5.8, Table 5.9, and Table 5.10). L4C also showed reasonable seasonal variability relative to MOD17, MPI-MTE, and the SIF and CarbonTracker global benchmarks. The L4C results indicated larger seasonal range than MOD17 and MPI-MTE in the seasonally moisture-constrained regions and major cropland regions (Figure 5.11). This result is consistent with improved use of soil moisture information and flux tower calibration in L4C, because underestimated seasonal amplitude can be a symptom of relatively poorer model fit; however, although an indicator, this observation is not by itself sufficiently conclusive of an improved model. L4C also had substantially better agreement with CarbonTracker seasonality than MPI-MTE NEE. This result could be because L4C model logic is related to the underlying CASA model used as a prior in CarbonTracker. Alternatively, a dynamic model such as L4C may inherently have more skill for estimating RECO and NEE relative to regression-type approaches, such as MPI-MTE which do not model SOC dynamics and therefore cannot account for seasonal limitation of substrate limitation for soil heterotrophic organisms.

L4C shows highest interannal GPP and NEE variability in arid regions (Figure 5.12; Figure 5.14). L4C innterannual variability was spatially similar to MPI-MTE, but generally larger than MPI-MTE variability, which indicates potential improvement in explanatory skill. The L4C, MPI-MTE, and MOD17 NEE interannual variability spatial patterns tended to resemble their respective GPP spatial patterns. However, the spatial interannual variability spatial patterns of SIF and CarbonTracker were largely inconsistent with one another and did not generally match the L4C, MPI-MTE, and MOD17 spatial patterns over the globe. Additionally, MOD17 GPP and SIF indicate that ecosystem productivity interannual variability is highest in the tropics, whereas L4C, MPI-MTE and CarbonTracker indicate that interannual variability is largest in arid regions, savannahs, and central US croplands. These mismatches in spatial patterns of productivity interannual variability cast some doubt that these datasets show coherent

global sensitivities to recent interannual climate variations. Nevertheless, MOD17, SIF, and L4C showed a coherent productivity response to the 2015 California drought, although the SIF monthly variability was quite noisy (Figure 5.7). This indicates that despite mismatches in global interannual variability, the datasets do agree on anomalous conditions in certain regions. More research will be required to understand the mismatches in global productivity interannual anomalies from these datasets and gain more confidence in estimated patterns of interannual variability in land-atmosphere CO₂ source-sink activity.

5.4.5 Value of Soil Moisture and SMAP Observations

The L4C Calib model sensitivity analysis indicates a widespread impact of soil moisture on terrestrial carbon fluxes (Figure 5.16). Root zone soil moisture (SMRZ) primarily impacts GPP in arid regions, whereas surface soil moisture (SMSF) has a more widespread impact on RH. SMRZ is used with VPD inputs to represent both soil water supply and atmospheric moisture demand controls on GPP. SMRZ provides an additional impact on GPP extending beyond VPD controls over drier climates of the global domain, where the SMAP observations have generally greater impact on the GEOS-5 land model assimilation used to derive the L4SM soil moisture and temperature inputs. The impact of surface soil moisture (SMSF) on RH was more widespread than for GPP because SMSF provides the sole moisture constraint to the model RH calculations. RH also has an exponential dependence on temperature in the L4C model so that dry conditions have relatively greater impact on respiration when co-occurring with high temperatures. SMSF has generally larger dynamic variability than SMRZ so that RH shows larger daily variability in response to rapid wetting/drying of the surface soil layer.

Other recent studies have highlighted the importance of arid regions for controlling inter-annual variability of the global land carbon flux (Cleverly 2016; Zhao & Running 2010; Poulter 2014; Ahlstrom 2015). This global variability is strongly influenced by periodic wet and dry (drought) cycles, and concomitant effects on vegetation growth and NEE in dryland ecosystems, including grasslands, shrublands, and savannahs (Poulter 2014). In arid and seasonally-arid regions, RECO rapidly responds to rainfall (i.e. the so-called "Birch effect" (Unger 2010)) and in both arid and non-arid ecosystems, root exudates from trees and shrubs can provide "priming" effects increasing RE after soil wetting (Xu 2004). Both effects underscore the importance of daily soil moisture for modeling RE and NEE fluxes. In contrast, carbon flux spatio-temporal variability in humid biomes, especially forests, may be relatively more impacted by the interaction of drought with disturbance (fire, harvesting, etc.) and recovery processes, which are not explicitly modeled in the current L4C Ops product. Saturated soils can inhibit RH by decreasing oxygen availability and causing anaerobic conditions (Ohta 2014); however, inclusion of an inverse-parabolic RH response curve degraded the PFTspecific L4C calibration fit in relation to the global tower calibration sites used in this study (e.g.Figure 4.5). The lack of an apparent anaerobic response may be due one or more factors including a general lack of wetland representation and flooding in the FLUXNET tower site record used for model calibration; the relatively coarse (9km) resolution L4SM information used to define model soil moisture conditions may not effectively capture saturated or ephemerally flooded conditions, while plant rootmediated oxygen transport may partially offset anaerobic conditions (Reddy & DeLaune 2008).

The full global range of vegetation and climate conditions, including climate extremes, disturbance, and recovery, are generally under-sampled by the available flux tower network. Since tower data were used to acquire process understanding through model calibration, the above global soil moisture sensitivity analysis is biased to the existing tower network (Schimel 2015; Beer 2010). The relatively short time period used in this study restricts a more comprehensive soil moisture sensitivity assessment because many locations (e.g. tropical evergreen broadleaf forests) may only respond to extreme events that that occur infrequently and may not be represented in the relatively recent (2001-2012) MODIS and NRv4 records used to derive the L4C simulations. These types of sampling biases affect all L4C results in this study, have been noted by other global studies and are largely unavoidable (Beer 2010; Jung 2010). Additionally, methods used to partition GPP and RE components of NEE from tower eddy covariance CO_2 flux measurements are modelled following various assumptions and therefore do not truly represent "observations" (Desai 2008). Each tower's effective spatial footprint changes with wind direction and may be inconsistent with the associated 1-km L4C modeling pixel. Effective SOC storage mismatches between the L4C model steady-state initialization cause further uncertainty. The use of model cross-comparisons and rescaling with alternative observation benchmarks such as GOME-2 SIF and CarbonTracker provide for additional model validation, these somewhat indirect comparisons can also be difficult to interpret.

The accuracy and performance of L4C Ops was on par with the L4C Open Loop and only marginally better than the L4C Calib climatology at the core validation sites (Table 5.7). These results indicate only a relatively small benefit of the SMAP observations on the L4C calculations based on the limited data record examined in this study. The results are also impacted by the inclusion of CVS locations where low soil moisture is not generally limiting to ecosystem carbon fluxes. The relatively early mission phase currently limits capabilities for a more robust assessment of the impact of SMAP observations on the L4C model skill. These limitations include a relatively short SMAP operational record, which represented less than an annual cycle at the time of this study. The microwave emission model used for assimilating SMAP observations and L4SM production was necessarily calibrated using SMOS data during the SMAP mission prelaunch phase, and recent comparisons show significant global biases between SMOS and SMAP which inevitably lead to inefficiencies in the data assimilation system. Similarly, the L4C model was necessarily calibrated using NRv4 inputs (L4C Calib), which may dampen or bias results when confronted with SMAP informed L4SM soil moisture and temperature inputs used in the L4C Ops product. Biases are particularly common for soil moisture datasets from both model and remote-sensing sources (Reichle 2004), and perhaps more pervasive than for other meteorological fields such as air temperature and humidity (Yi 2011). This is partly because global soil moisture fields have been historically poorly observed, and because soil moisture has generally large characteristic heterogeneity. Such biases are problematic for L4C, especially if the magnitude of soil moisture bias exceeds its temporal variability, because these biases can lead to model calibration errors affecting the PFT-specific soil moisture constraint curves. Despite these limitations, the results from this study show clear and unique value of global soil moisture information to estimate terrestrial CO₂ fluxes, with larger impacts in drier climates and areas with less vegetation cover where SMAP observations are

expected to have greater soil moisture sensitivity, and assimilation impact on land model based soil moisture estimates. Planned model calibration refinements and a continuing SMAP operational record are expected to lead to further improvements in L4C global accuracy and performance.

5.5 CONCLUSION

The SMAP L4C product provides consistent, operational global daily estimates of ecosystem-atmosphere (CO₂) fluxes, surface soil organic carbon stocks and their underlying environmental controls. Our initial global assessment using several independent observation benchmarks indicates that the L4C accuracy and performance is consistent with product design specifications and target accuracy requirements, and that the L4C product is suitable for a range of science investigations, including drought-related impacts on vegetation growth and the terrestrial carbon cycle. The L4C product provides a new tool for monitoring global land carbon dynamics informed by model data assimilation of SMAP satellite observations with enhanced L-band microwave sensitivity to soil moisture and thermal conditions.

The L4C product suite includes internally consistent estimates of NEE, component carbon fluxes (GPP and RH) and surface SOC stocks. Additional product variables include underlying environmental control factors influencing GPP and RH, and NEE ubRMSE QA metrics that provide enhanced diagnostic capabilities for analysis and attribution of estimated carbon fluxes and driving processes. The L4C model outputs are derived at a daily time step and 1-km resolution, capturing weather related daily variability at the level of a tower carbon flux measurement footprint.

The results of this study document the L4C accuracy relative to independent tower carbon flux observations. The L4C results were also verified against other available carbon observation benchmarks including satellite based SIF from GOME-2, used as a surrogate for GPP; atmosphere transport model inversion constrained NEE estimates from CarbonTracker; other global GPP products from MOD17 and MPI-MTE; and global soil carbon inventory records. These results indicate that L4C performance is within the targeted accuracy threshold for NEE (ubRMSE ≤ 1.6 g C m⁻² d⁻¹ or 30 g C m⁻² y⁻¹) over approximately 66 % of the global domain, and with larger absolute error but still meaningful accuracy (relative error ≤ 30 %) over 82 % of the global domain. The L4C product performance for estimated carbon fluxes is generally commensurate with the level of uncertainty associated with in situ tower carbon flux observations. Model comparisons with CarbonTracker indicate that the L4C results contain potentially new information for informing global carbon flux inversions, including linking NEE variability and underlying soil moisture and thermal constraints to ecosystem productivity, respiration and terrestrial carbon storage processes. Model sensitivity analyses indicated that soil moisture adds significant new information for improving the estimation of terrestrial carbon fluxes and underlying environmental controls, especially in drier climate regions where SMAP observations are most informative for the L4SM data assimilation and where the land carbon flux shows large year-to-year variability. The L4C record will continue to benefit from continuing SMAP operations and ongoing sensor and model calibration refinements. The L4C product provides the means for addressing mission carbon cycle science objectives to improve understanding of the purported missing carbon sink on land, and link terrestrial water and carbon cycles.

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TABLES

Table 5.1: L4C standard output datasets available in L4C daily HDF5 granules (Kimball 2016a; Glassy 2016). Group and Dataset names correspond to HDF5 dataset paths (See Glassy (2016) for details). Brackets indicate up to eight individual datasets (e.g. $\{1..8\}$) representing each of eight global MODIS PFT classes. Spatial format for all datasets is 9-km EGv2 (1624 × 3856 grid cells; Brodzik (2012) and temporal sampling is daily unless otherwise specified in footnotes. Counts are temporally static as derived by ancillary MODIS (MOD12Q1) PFT inputs (See Table 5.4). Bit flag contains several fields, some which provide static information, and others provide daily information (See Glassy (2016) or HDF5 granule metadata Kimball (2016) for details).

Group	Dataset	Units
NEE	nee_{mean, stdev}	g C m ⁻² d ⁻¹
NEE	nee_pft{18}_mean	g C m ⁻² d ⁻¹
GPP	gpp_{mean, stdev}	g C m ⁻² d ⁻¹
GPP	gpp_pft{18}_mean	$g C m^{-2} d^{-1}$
RH	rh_{mean, stdev}	$g C m^{-2} d^{-1}$
RH	rh_pft{18}_mean	$g C m^{-2} d^{-1}$
SOC	soc_{mean, stdev}	g C m ⁻²
SOC	soc_pft{18}_mean	g C m ⁻²
EC	emult_mean	%
EC	tmult_mean	%
EC	wmult_mean	%
EC	frozen_area	%
QA	nee_rmse_mean	g C m ⁻² d ⁻¹
QA	nee_rmse_pft{18}_mean	$g C m^{-2} d^{-1}$
QA	qa_count	count
QA	qa_count_pft{18}	count
QA	carbon_model_bitflag	bit fields

Table 5.2: L4C input datasets used for the three L4C model runs (L4C Ops, L4C Calib, and L4C Open Loop). Dataset names and units are described in L4C product documentation (Glassy (2016); See text for abbreviations). Derived inputs computed from native sources (listed in Table II) as follows: SMSF and SMRZ in % Sat. units derived by dividing by ancillary porosity data provided by L4SM or NRv4; TMIN derived from daily minimum of 1-hourly T2M; FT for L4C Ops was computed using daily mean of 1-hourly TSURF for this study; VPD derived as the daily mean from 1-hourly PS, QV2M, and T2M; PAR is derived from SWGDN assuming conversion factor of 0.45.

Dataset Name	Units	Spatial Res.	L4C Ops	L4C Calib	L4C Open Loop
Plant functional Type (PFT)	Class	1-km	MOD12Q1	MOD12Q1	MOD12Q1
Fraction of absorbed PAR (FPAR)	Dim.	1-km	MOD15A2	MOD15A2	MOD15A2
Surface soil moisture (SMSF)	% Sat.	9-km	L4SM	NRv4	NRv4
Root zone soil moisture	% Sat.	9-km	L4SM	NRv4	NRv4
(SMRZ) Soil temperature (TSOIL)	K	9-km	L4SM	NRv4	NRv4
Minimum air temperature (TMIN)	K	9-km	GEOS-5 FP	MERRA	GEOS-5 FP
Freeze-thaw state (FT)	logical	9-km	GEOS-5 FP	MERRA	GEOS-5 FP
Vapor pressure deficit (VPD)	Ра	9-km	GEOS-5 FP	MERRA	GEOS-5 FP
Photo-synthetically active radiation (PAR)	$W m^{-2} d^{-1}$	9-km	GEOS-5 FP	MERRA	GEOS-5 FP

Table 5.3: L4C input source data native formats used in L4C Ops, L4C Calib, and L4C Open Loop. Dataset names are specified from original data sources (See text for abbreviations): MOD12Q1 and MOD15A2 are available in sinusoidal projection tiles; NRv4 uses EGv2; MERRA and GEOS-5 FP use the geographic projection.

Source	Variables	Spatial	Temporal
Source		Resolution	Resolution
MOD12Q1	PFT	500-m	Static
MOD15A2	FPAR	1-km	8-day
NRv4	SMSF, SMRZ, TSOIL	9-km	3-hourly
MERRA	SWGDN, QV2M, PS, T2M, TSURF	$1/2^{\circ} \times 2/3^{\circ}$	1-hourly
GEOS-5 FP	SWGDN, QV2M, PS, T2M, TSURF	$1/4^{\circ} \times 3/8^{\circ}$	1-hourly
Table 5.4: L4C parameter biome property lookup table fitted using La Thuile flux tower network (228 sites). Glossary of parameter names and definitions given in Table 5.5. Plant Functional Type abbreviations: ENF = Evergreen Needle-leaf Forest; EBF = Evergreen Broad-leaf Forest; DNF = Deciduous Needle-leaf Forest; DBF = Deciduous Broad-leaf Forest; SHR = Shrubland; GRS = Grassland; CCR = Cereal Crops; BCR = Broad-leaf Crops.

Parameter	Units	ENF	EBF	DNF	DBF	GRS	SRB	CCR	BCR
$\varepsilon_{\rm max}$	[g C MJ ⁻¹]	1.64	1.96	1.20	1.54	1.51	2.03	2.55	2.50
TMIN _{min}	[K]	240	251	245	249	254	240	250	271
TMIN _{max}	[K]	311	320	314	302	294	319	319	301
VPD _{min}	[Pa]	1	13	1500	2	0	3	1	1500
VPD _{max}	[Pa]	3132	6421	7000	4389	4369	7000	6940	7000
SMRZ _{min}	[% Sat.]	0	0	0	0	0	0	0	0
SMRZ _{max}	[% Sat.]	27	7	6	5	90	88	68	22
SMSF _{min}	[% Sat.]	-23	-50	0	-54	-47	-3	-29	-100
SMSF _{max}	[% Sat.]	129	5	63	137	99	66	123	96
$\mathrm{FT}_{\mathrm{frozen}}$	[dim.]	0.85	1	0.75	0.95	1	0.95	0.95	0.85
FT _{thawed}	[dim.]	1	1	1	1	1	1	1	1
TSOIL _{β0}	[K]	308.56	308.56	308.56	308.56	308.56	308.56	308.56	308.56
$\text{TSOIL}_{\beta l}$	[K]	66.02	66.02	66.02	66.02	66.02	66.02	66.02	66.02
$\text{TSOIL}_{\beta 2}$	[K]	227.13	227.13	227.13	227.13	227.13	227.13	227.13	227.13
f _{aut}	[dim.]	0.15	0.3	0.12	0.1	0.26	0.26	0.21	0.3
f _{fast}	[dim.]	0.49	0.71	0.67	0.67	0.62	0.76	0.78	0.78
\mathbf{f}_{med}	[dim.]	0.3	0.3	0.7	0.3	0.35	0.55	0.5	0.8
k _{fast}	[d ⁻¹]	0.0303	0.0301	0.0331	0.0342	0.0222	0.0298	0.0286	0.032
k _{med}	[dim.]	0.4	0.4	0.4	0.4	0.4	0.4	0.4	0.4
Kslow	[dim.]	0.0093	0.0093	0.0093	0.0093	0.0093	0.0093	0.0093	0.0093

Table 5.5: L4C biome property lookup table parameter glossary with units and parameter descriptions. Parameter values given in Table 5.1.

Parameter	Units	Description
\mathcal{E}_{\max}	[g C MJ ⁻¹]	Maximum optimal light use efficiency for Gross Primary Productivity (GPP)
TMIN _{min}	[K]	Air temperature (daily minimum 2 m level) where Gross Primary Productivity (GPP) fully constrained.
TMIN _{max}	[K]	Air temperature (daily minimum 2 m level) where Gross Primary Productivity (GPP) unconstrained.
VPD _{min}	[Pa]	Vapor Pressure Deficit (daily average 2 m level) where Gross Primary Productivity (GPP) unconstrained.
VPD _{max}	[Pa]	Vapor Pressure Deficit (daily average 2 m level) where Gross Primary Productivity (GPP) fully constrained.
SMRZ _{min}	[% Sat.]	Soil Moisture (daily average root zone) where Gross Primary Productivity (GPP) fully constrained.
SMRZ _{max}	[% Sat.]	Soil Moisture (daily average root zone) where Gross Primary Productivity (GPP) unconstrained.
SMSF _{min}	[% Sat.]	Soil Moisture (daily average surface zone) where Heterotrophic Respiration (Rh) fully constrained.
SMSF _{max}	[% Sat.]	Soil Moisture (daily average surface zone) where Heterotrophic Respiration (Rh) unconstrained.
FT_{frozen}	[dim.]	Frozen soil constraint on Gross Primary Productivity (GPP).
FT_{thawed}	[dim.]	Non-Frozen soil constraint on Gross Primary Productivity (GPP).
TSOIL _{β0}	[K]	Soil Temperature Arrhenius response curve parameter for Heterotrophic Respiration (Rh).
TSOIL _{β1}	[K]	Soil Temperature Arrhenius response curve parameter for Heterotrophic Respiration (Rh).
$\text{TSOIL}_{\beta 2}$	[K]	Soil Temperature Arrhenius response curve parameter for Heterotrophic Respiration (Rh).
f _{aut}	[dim.]	Fraction of Gross Primary Productivity (GPP) remaining after autotrophic respiration (i.e. NPP/GPP ratio).
f _{fast}	[dim.]	Fraction of daily litterfall entering metabolic Soil Organic Carbon (SOC) pool.
f _{med}	[dim.]	Structural Soil Organic Carbon (SOC) pool carbon entering recalcitrant SOC pool as a fraction of structural pool Rh.
k _{fast}	[d ⁻¹]	Metabolic Soil Organic Carbon (SOC) optimal rate for Heterotrophic Respiration (Rh).
k _{med}	[dim.]	Structural Soil Organic Carbon (SOC) rate for Heterotrophic Respiration (Rh) as a fraction of metabolic SOC rate.
K _{slow}	[dim.]	Recalcitrant Soil Organic Carbon (SOC) rate for Heterotrophic Respiration (Rh) as a fraction of metabolic SOC rate.

Table 5.6: Eddy covariance flux tower core validation site and principle investigator (PI) list. Investigators from these 26 sites made data available which met requirements for temporal overlap with the SMAP L4C data record from March 31, 2015 to December 31, 2016. Site names and abbreviations as provided by FLUXNET. PFT for each tower location was determined by the overlying MOD12Q1 1-km pixel. Shading indicates adjacent tower site records which share the same L4C 9-km grid cell. RE flux estimates not available for FI-Sod and AU-GWW sites.

Site	Name	PFT	Location	Lat.	Lon.	PI	Affiliation
FI-Sod	Sodankyla	ENF	Finland	67.36 °N	26.64 °E	M. Aurela	Finnish Meteorol.
CA-Oas	SK-Old Aspen	DNF	SK, Canada	53.63 °N	106.20 °W	H. Wheater	U. Saskatchewan
US-ICt	Imnavait Creek Tussock	SHR	AK, USA	68.61 °N	149.30 °W	E. Euskirchen	U. Alaska, Fairbanks
US-ICh	Imnavait Creek Heath	SHR	AK, USA	68.61 °N	149.30 °W	E. Euskirchen	U. Alaska, Fairbanks
US-ICs	Imnavait Creek Sedge	SHR	AK, USA	68.61 °N	149.31 °W	E. Euskirchen	U. Alaska, Fairbanks
US-PFa	Park Falls WLEF Tall Tower	DBF	WI, USA	45.95 °N	90.27 °W	A. Desai	U. Wisconsin
US-BZs	Bonanza Creek Spruce	ENF	AK, USA	64.70 °N	148.32 °W	E. Euskirchen	U. Alaska, Fairbanks
US-BZb	Bonanza Creek Bog	ENF	AK, USA	64.70 °N	148.32 °W	E. Euskirchen	U. Alaska, Fairbanks
US-BZf	Bonanza Creek Fen	ENF	AK, USA	64.70 °N	148.31 °W	E. Euskirchen	U. Alaska, Fairbanks
US-Atq	Atgasuk	GRS	AK, USA	70.47 °N	157.40 °W	W. Oechel	San Diego State U.
US-Ivo	Ivotuk	SHR	AK, USA	68.47 °N	155.73 °W	W. Oechel	San Diego State U.
US-SRM	Santa Rita Mesquite	SHR	AZ, USA	31.82 °N	110.87 °W	R. Scott	USDA Agric. Research Service
US-Wkg	Walnut Gulch Kendall Grassland	GRS	AZ, USA	31.74 °N	109.94 °W	R. Scott	USDA Agric. Research Service
US-Whs	Walnut Gulch Lucky Hills	SHR	AZ, USA	31.74 °N	110.05 °W	R. Scott	USDA Agric. Research Service
US-Ton	Tonzi Ranch	SHR	CA, USA	38.43 °N	120.97 °W	D. Baldocchi	U. California, Berkeley
US-Var	Vaira Ranch	SHR	CA, USA	38.41 °N	120.95 °W	D. Baldocchi	U. California, Berkeley
AU-Whr	Whroo	SHR	Australia	36.67 °S	145.03 °E	J. Beringer	U. Western Australia,
AU-Rig	Riggs Creek	CCR	Australia	36.65 °S	145.58 °E	J. Beringer	U. Western Australia,
AU-Ync	Yanco	CCR	Australia	34.99 °S	146.29 °E	J. Beringer	U. Western Australia,
AU-Stp	Sturt Plains	GRS	Australia	17.15 °S	133.35 °E	J. Beringer L. Hutley	U. Western Australia, Charles Darwin U.
AU-Dry	Dry River	GRS	Australia	15.26 °S	132.37 °E	J. Beringer L. Hutley	U. Western Australia, Charles Darwin U.
AU-DaS	Daly River Uncleared Savannah	GRS	Australia	14.16 °S	131.39 °E	J. Beringer L. Hutley	U. Western Australia, Charles Darwin U.
AU-How	Howard Springs	GRS	Australia	12.50 °S	131.15 °E	J. Beringer L. Hutley	U. Western Australia, Charles Darwin U.
AU- GWW	Great Western Woodlands	SHR	Australia	30.19 °S	120.65 °E	C. Macfarlane	CSIRO
AU-ASM	Alice Springs	SHR	Australia	22.28 °S	133.25 °E	J. Cleverly, D. Eamus	U. Technology, Sydney
AU-TTE	Ti Tree East	SHR	Australia	22.29 °S	133.64 °E	J. Cleverly, D. Eamus	U. Technology, Sydney

Table 5.7: L4C validation summary statistics from CVS comparisons. Each statistic represents means taken across 26 tower sites for locations shown in Table 5.6 and corresponding to individual site statistics given in Figure 5.6. RE unavailable for sites FI-Sod and AU-GWW, therefore RE mean statistics taken across 24 tower sites. L4C model runs abbreviated as follows: Ops indicates L4C with L4SM inputs (L4C Ops); OL indicates L4C with NRv4 inputs (L4C Open Loop); and Calib indicates L4C with NRv4 (L4C Calib) climatology inputs. R = Pearson correlation, RMSE = root mean square error, ubRMSE = un-biased RMSE, N = number of tower sites.

Flux	R			RMSE			ubRMSE		
L4C Run	Ops	OL	Calib	Ops	OL	Calib	Ops	OL	Calib
NEE	0.52	0.52	0.48	1.04	1.05	1.01	0.79	0.79	0.80
GPP	0.72	0.72	0.71	1.27	1.31	1.21	0.85	0.85	0.83
RE	0.65	0.65	0.66	1.16	1.20	1.10	0.62	0.62	0.62

Table 5.8: Pearson correlation of monthly GPP time-series pooled across flux tower CVS locations.

	Site	SIF	L4C
SIF	0.63		
L4C	0.85	0.73	
MOD17	0.81	0.63	0.85

Table 5.9: Pearson correlation of monthly GPP global $(0.5^{\circ} \times 0.5^{\circ} \text{ grid})$ mean seasonal cycle (climatology), representing all grid cells pooled for the globe and twelve-month climatology. All 95% confidence intervals < 0.005.

	SIF	L4C	MOD17	MPI MR
L4C	0.83			
MOD17	0.79	0.94		
MPI MR	0.85	0.93	0.93	
MPI GL	0.85	0.93	0.92	0.99

Table 5.10: Pearson correlation of monthly NEE global ($1^{\circ} \times 1^{\circ}$ grid) mean seasonal cycle (climatology), representing all grid cells pooled for the globe and twelve-month climatology. All 95% confidence intervals < 0.05.

	СТ	L4C	MOD17	MPI MR
L4C	0.60			
MOD17	0.36	0.33		
MPI MR	0.49	0.48	0.47	
MPI GL	0.53	0.47	0.38	0.85

FIGURES



Figure 5.1: Effective GPP soil moisture constraint as given by the log-transform rescaling (Eqns. (5.1) and (5.2)) compared to the originally assumed unscaled linear constraint, and rescaling based on soil matric potential for soil with loam texture.



Figure 5.2: Core validation (CVS) and calibration tower sites used for evaluating operational L4C results and for pre-launch L4C model calibration, respectively. Basemap shows global plant functional types from the MODIS Collection 5 global land cover classification (MOD12Q1 Type 5). Abbreviations: WAT = Water; ENF = Evergreen Needle-leaf Forest; EBF = Evergreen Broad-leaf Forest; DNF = Deciduous Needle-leaf Forest; DBF = Deciduous Broad-leaf Forest; SHR = Shrubland; GRS = Grassland; CCR = Cereal Crops; BCR = Broad-leaf Crops; URB = Urban; ICE = Permanent Snow/Ice; BAR = Barren.



Figure 5.3: Effective bulk GPP environmental constraint (*Emult*) computed by inverting (5.3) using flux tower GPP, L4C input APAR, and fitted ε_{max} to indicate the impact of individual response functions for (a) vapor pressure deficit (VPD), (b) minimum daily air temperature (TMIN), (c) unscaled root zone soil moisture (SMRZ), and (d) rescaled SMRZ. Solid red lines indicate calibrated response functions (Eqn. (5.5)). Dashed red lines indicate maximum *Emult* = 1, but L4C calibration allows loose fit of ε_{max} to largest tower GPP values allowing effective *Emult* > 1. Low APAR (APAR < 0.1) was omitted to avoid large effective *Emult*.



Figure 5.4: Correlation of fitted L4C Calib GPP relative to La Thuile flux tower GPP for alternative L4C configurations grouped by plant functional type. Correlations given for all sites pooled within each plant functional type (solid symbols) to indicate among-site fit and averaged across sites within each plant function type (open symbols) to indicate within-site fit. Error bars represent 95 % confidence intervals, which are much smaller for pooled data because of larger sample size. Alternative L4C configurations include the standard L4C GPP model with all constraints (Full; Eqn. (5.3)), without freeze-thaw constraint (No FT), without minimum daily air temperature constraint (No TMIN), without root zone soil moisture constraint (No SM), without vapor pressure deficit constraint (No VPD), and without any constraints (No *Emult*; i.e. APAR only).



Figure 5.5: Time-series of L4C Ops fields and tower observations (if available) for selected tower locations: US-Ivo (Alaska arctic tundra) and US-SRM (Arizona desert shrubland). Fields include (a-b) NEE, (c-d) GPP, and (e-f) L4C environmental constraints (EC), including GPP light-use-efficiency constraint from Eqn. (1), *Emult*. RE soil temperature and moisture constraints from Eqn. (6), *Tmult* and *Wmult* respectively. Shaded bars represent L4C frozen soil classification.



Figure 5.6: Core validation site (CVS) statistical summaries of tower observation agreement for the daily L4C Ops record including (a) Pearson correlation (R), (b) root mean square error (RMSE), and (c) unbiased-root mean square error (ubRMSE). Negative correlations (not shown) include AU-ASM (NEE) and AU-Stp (GPP). Sites AU-GWW and FI-Sod did not report RE observations. Sites sorted from left to right in order of increasing annual carbon flux magnitude from the L4C NRv4 climatology. Shaded bars indicate spatially adjacent tower sites within the same L4C 9-km grid-cell. Dashed line indicates L4C NEE ubRMSE target accuracy (1.6 g C m-2 d-1).



Figure 5.7: Effect of California drought on (a) GPP and (b) GPP anomaly (i.e. mean seasonal cycle removed) time-series at the Tonzi Ranch flux tower site (US-Ton) during 2015.



Figure 5.8: L4C QA ubRMSE error estimates vs. ubRMSE calculated using L4C NEE and tower site observed NEE. (a) Fitted L4C Calib average daily NEE ubRMSE (g C m-2 d-1) QA metric relative to ubRMSE calculated using calibration site tower NEE. (b) L4C Ops average daily NEE ubRMSE (g C m⁻² d⁻¹) QA metric relative to ubRMSE calculated using independent CVS tower NEE observations. Symbols denote dominant PFT classification of each tower location.



Figure 5.9: Mean daily L4C Calib NEE QA ubRMSE (g C m-2 y-1) computed as the annual mean sum-of-squares of the daily QA ubRMSE estimates. Areas outside of the L4C model domain in are denoted in white.



Figure 5.10: Monthly mean seasonal cycle averaged across latitude for (a) SIF, (b) L4C GPP, (c) MOD17 GPP, and (d) MPI-MTE GPP. Averages represent period 2001-2012 for all datasets, except SIF which was averaged from 2007-2014.



Figure 5.11: Mean annual daily GPP for (a) L4C minus MOD17 and (b) L4C minus MPI-MTE, and mean monthly GPP seasonal range (averaged across years, expressed as average daily rate (g C $m^{-2} d^{-1}$)) for (c) L4C minus MOD17 and (d) L4C minus MPI-MTE.



Figure 5.12: Standard deviation of interannual GPP monthly anomalies (expressed as mean daily rate, (g C m-2 d-1)) for (a) L4C, (b) MOD17, (c) MPI-MTE, and (d) SIF. GPP anomalies computed by subtracting the mean monthly average daily GPP across years from the monthly average daily GPP for a given year. Dataset periods of record same as in Figure 5.10.



Figure 5.13: Monthly mean seasonal cycle averaged across latitude for (a) CarbonTracker NEE, (b) L4C NEE, (c) MOD17 NEE (i.e. MPI-MTE RECO minus MOD17 GPP), and (d) MPI-MTE NEE. Averages represent period 2001-2012 for all datasets. Individual color-bar limits adjusted to show characteristic variability range for each dataset.



Figure 5.14: Standard deviation of interannual NEE monthly anomalies (expressed as mean daily rate, (g C m-2 d-1)) for (a) L4C, (b) MOD17, (c) MPI-MTE, and (d) CarbonTracker. NEE anomalies computed by subtracting the mean monthly average daily NEE across years from the monthly average daily NEE for a given year. Dataset periods of record same as given in Figure 5.13.



Figure 5.15: Comparison of L4C Calib initialized SOC (representing <10 cm depth) to global and high-latitude inventory-based SOC (depth adjusted to <10cm depth) datasets including (a) differences between L4C initialized steady-state SOC and FAO-IGBP (i.e. L4C–IGBP) and (b) zonal mean SOC for L4C, NCSCD (>50 N only), and FAO-IGBP. Non-vegetated areas outside of the L4C model domain in (a) are denoted in white.



Figure 5.16: Global metrics indicating impact of soil moisture sensitivity analysis and operational SMAP observations on L4C Calib flux climatology fields. Percentage decrease in annual (a) GPP computed using SMRZ vs. without SMRZ, (b) GPP computed using VPD vs. without VPD, and (c) RH computed using SMSF vs. without SMSF. (d) L4SM SMSF analysis increment (data assimilation update minus model forecast) standard deviation in percent saturation units. Non-vegetated areas outside of the L4C model domain in (a)-(c) are denoted in white.



Figure 5.17: Root mean square differences (RMSD) between L4C Ops and L4C Open Loop simulations of average daily carbon fluxes (g C m-2 d-1) from March 31, 2015 to December 31, 2015 for (a) GPP and (b) NEE.

CHAPTER 6: CONCLUSIONS AND LOOKING FORWARD

6.1 **OBJECTIVES AND FINDINGS SUMMARY**

6.1.1 Estimates of Ecologically Relevant Information from Satellite Microwave Observations

A global land parameter database was developed to support ecosystem studies using AMSR-E satellite passive microwave remote sensing brightness temperature observations (Chapter 2). The land parameter retrieval algorithm consists of two components. The first component uses the 18.7 and 23.3 GHz brightness temperature observations to solve for daily surface air temperature minima and maxima, total column atmospheric water vapor, and surface fractional open water cover estimates. The second component uses 18.7 GHz and10.7 GHz brightness temperature observations to solve for soil moisture and vegetation optical depth.

Primary validation focused on daily air temperature minima and maxima using *in situ* weather station observations (Jones 2010a). The AMSR-E derived air temperature estimates were found to be generally accurate to within 1-3 K relative to surface weather station observations and other satellite based temperature estimates from AIRS. The highest AMSR-E temperature retrieval accuracies (0.5-2.5 K) occurred over forested regions, particularly boreal forests, whereas desert regions had biases ranging up to 4-6 K. The AMSR-E air temperature estimates represented a slight improvement over AIRS for cloudy regions, suggesting that microwave observations provided some advantage over AIRS cloud-screening methodologies.

Secondary land parameter validation activities focused on evaluating patterns of fractional open water, soil moisture, total column atmospheric water vapor, and vegetation optical depth retrievals (Jones 2009). Fractional open water and soil moisture showed expected responses relative to major precipitation events with flooded area differing in spatial extent and dry-down timing, and corresponding with known flood zones. Unexpected widespread fractional water cover was indicated for some desert regions, suggesting incorrect emissivity parameter specification (Jones 2010b). The AMSR-E vegetation optical depth retrievals showed close correspondence with satellite optical-IR remote sensing derived leaf area index and other vegetation indices (NDVI and EVI), although timing of the VOD canopy phenological peak tends to lag optical-IR index peaks for higher biomass locations (Jones, M. O., 2012). Further validation has shown close correspondence of vegetation optical depth with grassland and shrubland phenology indicated from GPS reflectivity (Jones, M. O., 2014) and also boreal forest disturbance recovery (Jones, M. O., 2013). Watts (2012) evaluated the AMSR-E fractional open water estimates over the circumpolar arctic and found increasing and decreasing fractional open water trends corresponding with continuous and discontinuous permafrost zones, respectively. The AMSR-E derived atmosphere total column water vapor retrievals show expected spatial and seasonal patterns corresponding well with independent measurements; however, diurnal differences were somewhat larger than expected. Further work by Du (2015), Du (2016a), and Du (2016b) has substantially improved the AMSR-E water vapor, vegetation optical depth, and fractional open water retrieval accuracy.

6.1.2 Demonstration of Merging Concept and Impact for Improving Soil Moisture Estimates

A joint merging and error estimation algorithm was developed for multiple time series data with a focus on soil moisture characteristics, including slowly varying error components (i.e. "colored noise") and long-term temporal dependence (Chapter 3; Jones, in prep.). The merging method developed in this study uses the expectation maximization algorithm for estimating time series parameters including time series error structure and the colored noise Kalman filter and smoother to provide merged soil moisture optimal estimates from multiple soil moisture data sources.

A simulation study was conducted to test the merging algorithm accuracy and robustness to missing soil moisture values and violation of assumptions. Simulations of soil-moisture-like time series - including non-Gaussian innovations and random and deterministic missing data gaps- indicate that the method skillfully reproduces the underlying state and accurately recovers system parameters, including uncertainty covariances. The basic methodology remains relatively robust for long-memory and bias plus white noise errors, although the appropriate modifications may be crucial for noisier real-world applications. Regression scaling coefficients were not identifiable if the underlying process and time series observations shared AR poles. In all considered simulated cases, the method out-performed or matched performance of the simple average of the time series, indicating improvement over relatively simple approaches to combining data. Correct selection of AR model order remains important because results substantially improve when the number of parameters correctly reflects the structure of the underlying system. Incorrect model specification can substantially decrease

robustness of the merging method to violations of underlying assumptions. Therefore, improving model identification and robustness should be a major focus of future work.

6.1.3 The Value of Soil Moisture to Improve an Ecosystem Respiration Model

Merged soil moisture state and uncertainty information were evaluated relative to *in situ* observations, and the impact of this soil moisture information for improving model ecosystem respiration fluxes was evaluated relative to *in situ* eddy covariance flux tower observations (Chapter 4). Effective merging parameters and soil moisture dataset information content spatial patterns were evaluated over a continental US domain. This evaluation also involved determining and fitting an effective ecosystem respiration soil moisture constraint curve. The fitted response curve was then used with a model error propagation approach to predict where better soil moisture information could most improve model ecosystem respiration estimation accuracy and RMSE performance.

The merged soil moisture results show significant correlation improvement relative to the individual component soil moisture time series for lower vegetation biomass (VOD) areas. This improvement is nearly as large as that with control methods assuming perfect knowledge of system uncertainty and scaling parameters; the improvement also meets or exceeds the performance of the simple equally-weighted time series mean and the most skillful time series, thus meeting prior criteria for practical optimality. However, the merging method performance degrades with increasing VOD and for the highest VOD areas, primarily forest sites, the merging method fails to match the skill of the equally-weighted time series mean and the most skillful time series, indicating sub-optimal performance and contrary to prior expectations. In high VOD locations the satellite microwave remote-sensing based soil moisture retrievals are

dominated by error and contain little or no information on actual soil moisture conditions. Methods for screening such sites from the analysis would likely improve overall results. It is also important to note that these results apply only to a simplified version of the merging method described in Chapter 3 and therefore do not fully account for missing values and multiple lags. Despite degraded performance for VOD areas, the merging parameters show expected spatial patterns, indicating reduced remote-sensing accuracy for high-biomass vegetation and reduced model accuracy for complex terrain; the algorithm also properly identifies merging weights based on these factors.

The ecosystem respiration estimates were most improved for low-biomass waterlimited locations when using merged soil moisture relative to standard model-derived soil moisture inputs. This improvement results from increased model sensitivity to soil moisture variability in arid locations, which are generally located in sparse vegetation areas where satellite microwave soil moisture retrievals contribute the most benefit to the merged soil moisture estimates. Using *in situ* soil moisture and tower RECO observations, no support was found for an original hypothesis that saturated soils limit ecosystem respiration due to anaerobic conditions, leading to a parabolic constraint curve. Anaerobic conditions are likely localized and sub-grid saturated conditions may be difficult to detect within relatively coarse tower eddy covariance (1-km footprint) and soil moisture (9-km footprint) effective spatial sampling footprints. Saturated soils and localized flooding are likely a considerable source of error in current remote-sensing and model soil moisture products. Further research should investigate the potential of fractional water estimates to inform the ecosystem respiration model by indicating anaerobic conditions resulting from flooding, irrigation, and wetlands.

6.1.4 Implementation of Satellite based Soil Moisture Observations for Operational Monitoring of Land-Atmosphere CO₂ Exchange

The Soil Moisture Active Passive Mission Level 4 Carbon (SMAP L4C) product was developed to exploit SMAP remotely-sensed soil moisture information (Jones, in review; Jones 2016). Rather than use SMAP soil moisture estimates, which contain missing values and measurement noise, the L4C product uses the SMAP Level 4 Soil Moisture (L4SM) product which merges SMAP observations with a data assimilation constrained land surface model forecast. The L4C product was evaluated using concurrent tower eddy covariance CO₂ flux observations as primary validation and comparisons with other global-scale terrestrial carbon observation benchmarks as secondary validation. Various metrics including model sensitivity analysis, data assimilation diagnostics, and model runs using alternative soil moisture inputs, were used to quantify and evaluate the impact of SMAP observations on L4C product accuracy and performance.

Primary and secondary validation comparisons indicate that the SMAP L4C product has skill for estimating Net Ecosystem CO₂ exchange (NEE) and its Gross Primary Productivity (GPP) and Ecosystem Respiration (RECO) components. Primary validation metrics indicate that L4C is within expected NEE average error tolerance (1.6 g C m⁻² d⁻¹) relative to tower eddy covariance observations and that the L4C results capture seasonal and daily ecosystem CO₂ flux variability across a global range of locations as indicated by the global flux tower network. L4C uncertainty was found to vary proportionally with overall annual CO₂ flux magnitude.

Secondary validation indicates that L4C GPP results show global and seasonal productivity patterns consistent with satellite Solar Induced Fluorescence (SIF)

observations used as a proxy for GPP. The L4C results also produced similar global and seasonal patterns in relation to atmospheric transport model inversion based estimates of net biological CO₂ fluxes from NOAA CarbonTracker. Coherent spatial patterns of L4C GPP seasonal variability were observed with SIF, MOD17, and MPI-MTE, but with notable differences for the tropics in seasonal phase (relative to SIF and MOD17) and amplitude (relative to SIF, MOD17, and MPI-MTE). The L4C results generally exceeded MOD17 correlation skill and matched or exceeded MPI-MTE skill relative to SIF, CarbonTracker, and tower GPP and NEE benchmarks. Patterns of L4C interannual variability show that seasonally arid and cropland regions contribute to interannual variability in global GPP and NEE. This pattern was broadly corroborated by MPI-MTE, MOD17, and CarbonTracker. Also L4C also shows some sensitivity to interannual variability in the tropics and southern portions of the boreal forests, which was broadly corroborated by MOD17, and CarbonTracker. Aside from these general patterns, a large degree of inconsistency exists between SIF, CarbonTracker, MOD17, MPI-MTE, and L4C in representing global patterns of interannual variability in CO₂ source-sink activity. Nevertheless, the results of this comparison generally aligns with the expectation that seasonally arid and cropland regions contribute to global interannual NEE variability.

Although the model sensitivity analyses indicate widespread impact and significant relevance of soil moisture information for L4C, the impact of SMAP observations has not as-yet resulted in detectable L4C improvement over the use of alternative soil moisture inputs derived without the benefit of SMAP observations. The L4C sensitivity analysis concurs with conclusions of Chapter 4 that the primary impact of soil moisture on the ecosystem model derived carbon fluxes occurs in arid regions.

Likewise, the L4SM assimilation diagnostics and the RMS differences between "openloop" and operational L4C model runs (i.e. with and without SMAP information, respectively) indicate the largest impact of SMAP observations for arid regions. However, these impacts do not as yet amount to discernable L4C improvement. This result is perhaps unsurprising given the relatively short SMAP record available at the time of this study (< 1 full seasonal cycle) and that the initial L4C and L4SM products necessarily required pre-launch calibration not informed by SMAP observations. Complexities of L4SM data assimilation also limit current impact because SMAP data must be carefully screened and bias-corrected to improve model agreement prior to assimilation. Nevertheless, detectable benefits of SMAP observations for improving L4C CO₂ estimates are expected as more SMAP data become available. Improvements in soil moisture merging methods described in Chapters 3 and 4 could benefit L4SM data assimilation leading to detectable impact on land-atmosphere CO₂ exchange estimates and uncertainty information as seen for ecosystem respiration in Chapter 4.

6.2 CONCLUSION AND FUTURE RESEARCH

In this work, satellite passive microwave remote sensing measurements were synthesized to provide ecologically relevant information, specifically soil moisture, with the goal of improving estimates of land-atmosphere net ecosystem CO₂ exchange. Primary validation was conducted against best-available *in situ* observational benchmarks and compared with both state and uncertainty estimates. Secondary validation consisted of multiple independent global datasets wherever possible. Sensitivity analyses, simulation experiments, and model control runs were used to understand algorithm behavior under idealized circumstances. Using these tools, the value of satellite microwave observations for improving soil moisture estimates was demonstrated, the importance of soil moisture for modeling land-atmosphere CO₂ flux was determined, an operational framework for using soil moisture to estimate land-atmosphere CO₂ flux operationally was established, and early operational results were evaluated. This work resulted in two publically-available datasets including the AMSR-E land parameter database and the SMAP Level 4 Carbon product (Jones 2010b; Kimball 2016).

Opportunities remain to further develop many facets of this research. More research is needed to determine the spatial and temporal variability of effective soil moisture and CO₂ exchange response curves, and underlying processes including how these curves relate to stomatal conductance, nutrient limitation, anaerobic conditions, and the differential response of photosynthesis versus respiration to soil water limitation. Irrigation, temporary flooding, and plant-accessible ground water are additional sources of uncertainty which could be better addressed by remote-sensing and land-surface models. Further work on merging methods can provide insight on these aspects because diverse remote-sensing instruments can provide proxies for many of these biologicallyrelevant components of the water cycle at multiple spatial and temporal scales. This study took a rather limited view of the terrestrial biosphere carbon budget by considering only the immediate impacts of soil moisture on photosynthesis and respiration, and soil carbon storage without explicitly addressing nutrient limitations. A more complete view should include above- and below- ground living biomass, nutrient cycling, and consider how drought-induced damage or mortality and related disturbance, especially fire, impact land-atmosphere CO_2 exchange. Many facets of the terrestrial carbon cycle are not well

constrained by available observations and knowledge as represented by models, and yet much information contained in the recent deluge of available observational data remains under-utilized. Synthesis and inter-comparison of existing datasets, aided by merging algorithms, represent a step forward in better understanding the terrestrial carbon cycle today and where it is headed in the future.

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