Use of Predictive Weather Uncertainties in an Irrigation Scheduling Tool Part I: A Review of Metrics and Adjoint Methods

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Research Impact Statement: Quantitative precipitation forecast data, verification metrics, and adjoint sensitivities are reviewed to advance the quality of irrigation scheduling tools.

ABSTRACT: Irrigation management consists of many components. In this work we review and recommend rainfall forecast performance metrics and adjoint methodologies for the use of predictive weather data within the Colorado State University Water Irrigation Scheduler for Efficient Application (WISE). WISE estimates crop water uses to optimize irrigation scheduling. WISE and its components, input requirements, and related software design issues are discussed. The use of predictive weather allows WISE to consider economic opportunity-costs of decisions to defer water application if rainfall is forecast. These capabilities require an assessment of the system uncertainties and use of weather prediction performance probabilities. Rainfall forecasts and verification performance metrics are reviewed. In addition, model data assimilation methods and adjoint sensitivity concepts are introduced. These assimilation methods make use of observational uncertainties and can link performance metrics to space and time considerations. We conclude with implementation guidance, summaries of available data sources, and recommend a novel adjoint method to address the complex physical linkages and model sensitivities between space and time within the irrigation scheduling physics as a function of soil depth. Such tool improvements can then be used to improve water management decision

performance to better conserve and utilize limited water resources for productive use. ***Editor's note****: This paper is part of the featured series on Optimizing Ogallala Aquifer Water Use to Sustain Food Systems. See the February 2019 issue for the introduction and background to the series.*

(**KEYWORDS:** data assimilation; irrigation; precipitation; soil moisture; statistics.)

INTRODUCTION

Irrigation management is a key enabler of improved yields in semi-arid lands. However, water resources in some regions are not sustainable, and management optimizations require active and timely decision-making to balance water resources, water quality concerns, and economic decisions. For example, the Ogallala Aquifer in the western Great Plains is being depleted by large-scale agricultural irrigation in many areas. More than 30% of all irrigated US agricultural output comes from the lands sustained by the Ogallala Aquifer (USDA NASS, 2009). The constraints of water scarcity and the importance of water for Ogallala regional agricultural production highlights the need to actively manage Ogallala Aquifer groundwater in the context of natural rainfall and drought-related issues, as the deep paleo-era water is depleted (Buchanan et al., 2009; Thelin and Heimes, 1987; Hornbeck and Keskin, 2014; Peterson et al., 2014).

Tested methods at the field-scale are needed to optimize irrigation water use and crop production as the Ogallala water resources undergo change (Cano et al., 2018). Active management of the water resources is important for ensuring community environmental health, soil health, and related air quality issues from wind erosion/dust events (Stewart et al., 2010). For instance, Kansas State University developed the irrigation scheduling tool KanSched (Rogers and Alam, 2007); which is based on agricultural weather data and tabulated crop coefficients. Like KanSched, several other similar tools have been developed in the United States and Worldwide. However, none of the existing tools offer a reliable predictive capability.

We present the Colorado State University (CSU) Water Irrigation Scheduler for Efficient Application (WISE) tool (Andales et al., 2014; Bartlett et al., 2015) and a novel use of aWhere's integrated and scalable cloud-based software framework (aWhere, Inc. system. Accessed August 19, 2019: https://www.aWhere.com). Through this framework, predictive weather information in near real-time is being linked to crop and irrigation scheduling applications such as WISE.

Enhancing decision support tools with predictive weather and other related data (including local weather measurements, hydrologic models, and remotely-sensed data sets) increases their potential to address challenging multi-system problems. Such tools improve water management decision making as the Ogallala Aquifer Region (OAR) transitions to dryland crop management, which in turn has an impact on soil health through soil organic content (SOC) and related carbon climate balances (Cano et al., 2018; Brazil et al., 2017; Kisekka and Aguilar, 2016). Integrated cropland management practices (tillage, irrigation, and e.g., soil health conditioning, among numerous other factors) have wide applicability to many additional agricultural regions. The application importance is more pronounced as water resource demands drive potentially complex sustainability-related impacts, climate-based adaptations, and environmental feedbacks (Segal et al., 1988; Segal et al., 1998; Alter et al., 2015; Asadieh and Karkauer, 2016; Brazil et al., 2017).

The scope of this work is to highlight predictive weather-related effects on WISE output and performance. WISE and its components, input requirements, and related important software design issues are discussed. The discussion is followed by assessing available precipitation observational capabilities, while also identifying several important limitations and constraints of these data. Then the quantitative precipitation forecasts are introduced, including several forecast performance metrics that drive the irrigation tool performance scenarios. The discussion is then advanced from precipitation forecast metrics to the model data assimilation methods that drive the injection of new data within the weather model forecast systems. Lastly, we make recommendations for implementation of these concepts, focusing on the development of using metrics and weather data sets within adjoint sensitivity methods to improve WISE.

WISE Background

Researchers at CSU created WISE (WISE. Accessed August 19, 2019, http://wise.colostate.edu/) in cooperation with growers throughout Colorado. The goal of WISE is to make recommendations for convenient and cost-effective irrigation scheduling to maximize crop yield and minimize water stress or excess irrigation. Currently, there are 329 WISE users and 810 active WISE projects. Most projects consist of center pivot sprinkler irrigated fields (typically 130 acres per field). Some WISE projects involve smaller fields that use other irrigation methods. The CSU Extension Water Resources team has been actively promoting WISE at workshops, field days and producer conferences across Colorado.

The WISE web browser interface combines Geographical Information System (GIS) capabilities with a friendly user interface. After a user draws the boundaries of an irrigated field, the tool automatically collects local soils and daily agricultural weather data from publicly available data sources, such as the Soil Survey Geographic (SSURGO) database (available through USDA's Natural Resources Conservation Service, USDA NRCS, 2018) and the Colorado Agricultural Meteorological Network (Colorado Agricultural Meteorological Network. Accessed August 19, 2019, https://CoAgMet.ColoState.edu). To complete the set-up of a field for irrigation scheduling, the user also inputs the following information: (a) crop information: type, emergence or green-up date, managed root depth; (b) irrigation system information: type and application efficiency; and (c) soil information: initial soil moisture content at emergence or green-up.

Once a crop type is selected, default values of crop coefficients are identified (within the tool) to incorporate the effects of crop development on water use. Thus, crop water use or evapotranspiration (ETc) is calculated as a product of crop coefficients and reference evapotranspiration (ETref). ETref uses agricultural weather data. Advanced users can modify the default values to better represent the crop variety they have planted. The tool will then estimate the daily soil water deficit (net irrigation requirement) of the root zone using the estimation of crop evapotranspiration, effective rainfall, and user-entered values of actual applied irrigation (for example, inches of water entered into the pivot control panel). Using the estimate for the daily soil water deficit the tool will recommend a depth of water to apply. Figure 1 contains a flow chart of steps involved in the operation of WISE. Figure 2 contains a graphical example of output for a daily soil water deficit estimate. Further technical details of the modeling approach used within WISE (e.g., for a detailed description of the management techniques and ETc methods used) can be found in Andales et al. (2014) and Andales et al. (2015).

The WISE ETc functions and initial soil moisture state are critical elements of the predictive abilities of the irrigation scheduler. In WISE the ETc is estimated using a linear relationship between ETref, a crop coefficient that varies with crop development, and a water stress coefficient (Allen, et al. 1998). Multiple crop types are supported within WISE. Weather data are the primary source of the reference ETc estimates. When not using predictive weather data, reference ETc is derived from the CoAgMet observational weather data. In limited water conditions, WISE follows the methodology described in Allen et al. (1998) to scale the difference between the total available water in the soil root zone and the soil water deficit by the management allowed depletion (a fractional value) of the total available water. In turn, the fractional value of management allowed depletion is used to estimate an "actual" water-stressed ETc value that is used in a water balance approach to schedule irrigation applications (Andales et al., 2014; Andales et al. 2015). During the growing season the natural precipitation events and irrigation application decisions become more important for mostly semi-arid irrigated conditions (such as the management conditions found in the OAR).

While this work will emphasize the predictive weather uncertainties, model simulations of ETc are also important elements of the water balance, especially for periods in between rain events. Several systems have been created to estimate actual ETc (Eta) at fine spatial scales for a variety of crops. One interesting example is of the Backward-averaged iterative two-source surface temperature and energy balance solution (BAITSSS) algorithm using the Mapping evapotranspiration at high resolution with internalized calibration (METRIC) model (Dhungel et al., 2016). The Dhungel et al. (2016) system leverages satellite-derived LandSat ETc estimates from METRIC and combines errors using a bilinear-in-time triangular error distribution method (Dhungel et al., 2016) between the fine-scale observational estimate and model estimates in between satellite observation times. They found that land surface temperatures could be calibrated within 1 K with ETa mean average errors (MAE) of ~ 0.1 mm h^{-1} and root-mean-squared-differences (RMSD) of ~ 0.2 mm h^{-1}. ETa correlation coefficient values ranged from 0.60-0.68 for their southern Idaho test sites with mixed crop use conditions. Sensible heat flux MAEs ranged from 16 to 90 W m^{-2} and had correlation coefficient values ranging from 0.5 to 0.57.

Likewise, fine-scaled (~30 m) ETc estimates for drip-irrigated vineyard conditions using a widely-used 2-layer Shuttleworth and Wallace ETc model (Shuttleworth and Wallace, 1985; Ortega-Farias et al., 2010) showed improved ETc estimate capabilities as well. The aforementioned Ortega-Farias et al. (2010) system was tested in a vineyard in the Talca Valley, Chile. In those tests the ETc MAE was 0.54 mm d^{-1} with root-mean-squared-errors (RMSE) of 0.51 mm d^{-1} using an eddy correlation measurement system. The Ortega-Farias et al. (2010) algorithm made use of meteorological station measurements in combination with soil moisture observations and improved Leaf Area Index (LAI) vegetation assessments suitable to the vineyard conditions.

The Dhungel et al. (2016) and Ortega-Farias et al. (2010) systems demonstrate the ability of more complex systems to estimate accurate ETc estimates using advanced calibration procedures in data rich environments. In this work we defer improvements to the WISE ETc estimates, but rather use the existing ETc approach.

It is interesting to note that commercial irrigation schedulers are testing value-added weather data approaches as well (e.g., see the Irrigation Innovation Consortium (IIC) web site for additional details, and the IIC commercial partners for an updated list of their current market offerings, IIC. Accessed August 19, 2019, https://irrigationinnovation.org/tools-weather-et-networks/schedulers-calculators-assessment-tools). Thus, this work is timely due to the potential for substantial water savings and optimization of irrigation scheduling using more advanced weather prediction information systems. WISE is therefore unique in its early research use of accurate predictive weather data. Precipitation and irrigation events are a major input driver of the WISE water balance estimate. Since the timing of precipitation events can be forecast several days in advance by weather models with some skill, this provides an opportunity to further optimize the performance of the WISE system. Therefore, for this work, we focus on the WISE precipitation data inputs, predictive probability metrics, and soil moisture initial starting state (through use of adjoint sensitivities). In the conclusions we make recommendations for implementation of these concepts. The concepts introduced within this work are general and can be used by many irrigation scheduling systems that use weather station data for environmental state estimates, regardless of their specific ETc and water balance formulations.

WISE Smartphone Apps

WISE for iPhone® or Android® smartphones can synchronize with the cloud server to display soil water status information for each individual field (Bartlett et al., 2015). The process selects a field and allows views of the soil water deficit or net irrigation requirement for that field relative to the management allowed depletion. Application of irrigation water or precipitation on a specific date can also be entered and calculations performed to estimate the upcoming irrigation requirements given the crop conditions. Currently, the verification of predictive weather data inputs occurs outside of the WISE Smartphone App. However, the WISE system is in the process of adding predictive weather data access via the WISE App linkages to the near real-time aWhere cloud-based data platform (aWhere, Inc. system. Accessed August 19, 2019: https://www.aWhere.com).

Predictive Weather Data

In this section we introduce available predictive weather metrics data sources and make recommendations regarding their use with tools such as WISE. In addition to remote sensing geospatial information, predictive numerical weather forecasts can be used to forecast conditions into the future (normally out to 7-10 day forecast periods), thus providing temporal “windows” of decision-making opportunities. Predictive numerical weather forecasts are made using complex computer programs run on supercomputers. They can provide predictions on many atmospheric variables including temperature, pressure, wind, and rainfall. The National Oceanic and Atmospheric Administration (NOAA) National Weather Service (NWS) and the National Centers for Environmental Prediction (NCEP, Accessed August 19, 2019, http://www.ncep.noaa.gov) both provide predictive numerical weather forecasts. Use of these data is underway at CSU as part of the United States Department of Agriculture-National Institute of Food and Agriculture (USDA-NIFA)-funded Ogallala Water Coordinated Agriculture Project (OWCAP, Accessed, August 19, 2019, https://www.ogallalawater.org). The OWCAP work includes efforts to account for the dynamic state of the crop within WISE, which is conditional upon the weather rainfall forecast in near-real time and identifying the kind of error range that is required for successful recommendations. In addition, NOAA releases numerous observational remote sensing data sets that can be used for a variety of calibration and validation purposes. For those seeking additional background, a review of precipitation observational capabilities is available in the online supporting information.

In addition to NOAA observational estimates, numerical weather prediction (NWP) precipitation forecast data are available through a CSU collaboration with aWhere, Inc. aWhere also provides near real-time cloud-based weather data sets for a nominal service fee (Accessed August 19, 2019, https://www.aWhere.com) and distributes CSU precipitation data and NOAA NWP prognostic information via their globally-scalable information platform (Figure 3) (see also Garg and Aggarwal, 2016). The particular NOAA model distributed by aWhere is a spatially-improved and cloud-distributed Global Forecast System (GFS) model output database (EMC, 2003). The aWhere data access is an important step for enabling greater fine-scale data usability. Such information is well suited to WISE.

Probabilistic evaluation of forward-looking decision scenarios is possible if these new data sets are applied in a predictive sense. For example, as rainfall is forecast with a particular assigned error probability, then the error estimates can be accounted for within the decision-making tool to enhance the probability that a decision to irrigate can be successfully delayed without harm to the particular growth-stage of the crop. By comparison, use of high error estimates or more error-prone long-term forecasts for the same scenario may result in a decision tool recommendation to apply water immediately.

We intend to share this predictive capability framework with other irrigation scheduling tools developed for the OAR including KanSched (Rogers and Alam, 2007; Kisekka and Aguilar, 2016), and the Dashboard for Irrigation Efficiency Management (DIEM) irrigation water management and water-limited crop production tools; within the OWCAP team and potentially more widely. For Kansas State University water tools, visit: (KanSched3. Accessed August 19, 2019, https://kansched3.engg.ksu.edu/background); for Texas A&M AgriLife Research and Extension's DIEM tool, visit: (DIEM, Accessed August 19, 2019, https://diem.tamu.edu/dashboard/content/static/landing/LandingPage.html).

Integration Software and the Need for Assessments of Precipitation Forecast Data Sources

At CSU a new effort was started to integrate near real-time predictive weather data with the irrigation decision-tool framework. The integration of the software and data makes use of the CSU Cloud Services Integration Platform (CSIP) framework, environmental Risk Assessment and Management System (eRAMS), and a computer programming language called "Python" (Muller and Guido, 2016; McKinney, 2017). The new prognostic decision-making irrigation scheduler project aims to build on the foundation of WISE using a Python package called Pandas (https://pandas.pydata.org/. Accessed August 19, 2019). The goal is to provide a fast, modular application programming interface (API) for agricultural weather data analysis and crop evapotranspiration modeling. Currently in initial stages of development, this modification of an existing irrigation scheduling tool will make it easy to interface with weather station networks and model databases to calculate parameters of agricultural interest using widely accepted algorithms. By using Pandas, incorporation and testing of incremental improvements should be easier and will facilitate use of products by other compatible integrated software systems.

While built on a solid foundation, the performance of WISE is tied to many additional factors as predictive weather data inputs are used (Andales et al., 2015). Therefore, in this work the predictive precipitation data inputs and forecasts are examined in detail, issues related to the different data sources reviewed, and an introduction to the relevant model-based verification methods and metrics presented. The knowledge of the data input behaviors, model precipitation performance metrics, and adjoint sensitivity methods support the integration of the aWhere predictive weather data for use in WISE. In turn, these metrics and adjoints can be used in sensitivity analyses for improved decision making.

In the following sections, we review: 1) the available GFS model performance verification metrics as applied to the GFS precipitation forecast data sets, and 2) an adjoint sensitivity analysis methodology that is suitable for use with a land model and can be used to guide the input data verification, assessments, and use of WISE as a function of space and time. These capabilities enhance the use of predictive weather data within irrigation tools, which are applied to a set of example case studies in our Part II companion paper (Jones et al., 2019).

PRECIPITION FORECAST VERIFICATION AND METRICS

Since observational precipitation and soil moisture data are available only *after* the events are observed, precipitation forecasts are required for predictive irrigation management decision aid tools. However, it helps to understand the limitations and constraints of the observational precipitation data sets, as the forecast model data outputs are verified against those measurements, and much of the model developments have been achieved through knowledge gained from such observationally-based data intercomparisons. For general information regarding operational precipitation forecast ensembles, please see the review article of Cuo et al. (2011) regarding precipitation forecast use in short- to medium-range streamflow forecasting. Their work highlights the precipitation forecast system status at many of the global weather prediction centers. Cuo et al. (2011) also examines the global centers' contributions to various ensemble model data sets and discuss how ensembles of precipitation forecast models are generated. Here we focus on the irrigation management data uses, key methods and definitions (notably precipitation probability performance information and precipitation forecast verification metrics as a function of forecast verification time), and public sources of available precipitation forecast performance data within the continental United States.

Precipitation Forecast Verification Metrics

Metrics are fundamental to all ground-satellite and ground-model gridded data spatial verification studies. In particular, these metrics tend to occur in four categories: 1) neighborhood methods (e.g., Clark et al., 2010), 2) scale separation, 3) field deformation, and 4) object-based methods (Gilleland et al., 2009). The verification metric behavior as a function of spatial resolution is a key concern when using different models at multiple grid resolutions and satellite/radar data resolutions. Traditional verification methods such as the Threat Score (TS), Equitable Threat Score (ETS; or also Gilbert Skill Score), Probability of Detection (PoD), Forecast Bias (FBIAS), False Alarm Rate (FAR), Critical Success Index (CSI) are all grid-point based methods. Therefore, spatial displacement errors are critical to their performance, as a displacement as small as one grid element could mean a "missed" forecast result. Other methods that are less sensitive to displacement errors have been devised to emulate forecaster qualitative assessment of forecasts and instead evaluate model precipitation performance using spatial groupings including object-pattern matching.

Threat Scores

Threat Scores (TS) use simple ratios of correct forecasts (hits) to the sum of predicted forecasted events and actual observed events adjusted for correct forecasts. Forecasted events are hits and false alarms, while observed events are hits and misses. Therefore, the TS is defined as (Wilks, 1995):

$$\mathrm{TS} = \frac{\mathrm{a}}{(\mathrm{a}+\mathrm{b})+(\mathrm{a}+\mathrm{c})-\mathrm{a}}, \qquad (1)$$

or equivalently,

$$\mathrm{TS} = \frac{\mathrm{a}}{\mathrm{a}+\mathrm{b}+\mathrm{c}} \qquad (2)$$

where *a* is the number of "hits", *b* is the number of "false alarms", and *c* is the number of "misses". The TS is also known as the critical success index (CSI) (Wilks, 1995). For the best possible forecast, TS is one, while for the worst forecast, TS is zero. The TS method does not account for random chance but is used widely within the operational weather verification community, especially in older work.

Equitable Threat Scores

Equitable Threat Scores (ETS) traditionally use 2×2 contingency tables of possible forecast outcomes. The table consists of hits, misses, false alarms, and correct negatives (i.e., correct forecasts, observed but not forecasted events, forecasted but not observed, and correct nonevent forecasts). Using this information, the ETS is defined as (Wilks, 1995):

$$\mathrm{ETS} = \frac{\mathrm{a} - \mathrm{chance}}{\mathrm{a} - \mathrm{chance} + \mathrm{b} + \mathrm{c}} \tag{3}$$

where

$$\mathrm{chance} = \frac{(\mathrm{a}+\mathrm{b})(\mathrm{a}+\mathrm{c})}{\mathrm{a}+\mathrm{b}+\mathrm{c}+\mathrm{d}} \tag{4}$$

where *d* is the number of "correct negatives". ETS is also known as the Gilbert Skill Score (GSS) (Wilks, 1995) or the "bias-removed" Threat Score (Novak, 2014). In practice, ETS represents the fraction of correctly predicted observational events, adjusted for the associated random chance of being correct (Clark et al., 2010; Tobin and Bennett, 2012). A perfect ETS is 1.0, no skill is 0, and -1/3 is the lower bound (a perfectly bad model that has the opposite forecast condition all the time). Using various spatial radii distance-of-influence thresholds, verifications can be adjusted for distance for what is considered a successful forecast, or "a hit". Likewise, intensity bins can stratify results into light, moderate, and heavy intensity events, depending on the particular verification objectives.

Other Direct Verification Metrics

Several additional direct verification metrics are available (Wilks, 1995). The Probability of Detection (PoD) or "hit rate" is a measure of the fraction of events that were correctly detected with no regard for renormalization with respect to chance. It is defined as:

$$\mathrm{PoD} = \frac{\mathrm{a}}{\mathrm{a}+\mathrm{c}} \tag{5}$$

Likewise, the False Alarm Rate (FAR) is simply:

$$\mathrm{FAR} = \frac{\mathrm{b}}{\mathrm{a}+\mathrm{b}} \ , \tag{6}$$

where a perfect FAR score is 0. The Frequency Bias (known as FBIAS or just BIAS by some) is defined as:

$$\mathrm{FBIAS} = \frac{\mathrm{a + b}}{\mathrm{a + c}} \ , \tag{7}$$

and represents the comparison of total forecasts to the total number of observations. A perfect score for FBIAS would be 1. The PoD, FAR, and FBIAS metrics are in common use by the weather verification community (Novak, 2014).

An Example of Neighborhood Verification Metrics

A Fraction Skill Score (FSS) is a neighborhood method (Roberts and Lean, 2008) defined as:

$$\mathrm{FSS} = 1 - \frac{\frac{1}{N}\Sigma_N (P_O - P_F)^2}{\frac{1}{N}\left[\Sigma_N {P_O}^2 + \Sigma_N {P_F}^2\right]} \ , \tag{8}$$

where P_O and P_F are the fractions (i.e., normalized counts) of binary observed and forecast fields in each model neighborhood square center (as spatial observational grid coordinates: *i*, and *j* are indexed around each center validation grid point; thus processing over the spatial neighborhood), and FSS is evaluated at all neighborhood scales, L, where N is the number of valid neighborhoods at that particular length scale. Thus, a set of FSS scores as a function of neighborhood scale is created. The FSS metric can also provide insight into distance correlation issues and other spatial resolution behavior (Mittermaier and Roberts, 2010). It should be noted that several additional neighborhood methods are also available (Kochasic et al., 2017).

Regional Verification Metrics

Regional precipitation forecast verification metrics are also available at (NOAA/NCEP. Accessed August 19, 2019: https://www.wpc.ncep.noaa.gov/rgnscr/verify.html) and allow further customization and stratification of the model error results by geographical region. These verification metrics are important to users of the model precipitation forecasts, as the models produce unique biases and have predictive seasonal behavior. Therefore, users should attempt to understand regional behavior in their local area of interest. The OAR region is covered by the Northern Plains (NPL) and the Southern Plains (SPL) regions of the WPC verification analysis.

Object-based Verification Metrics

An object-based spatial verification method, the Method for Object-based Diagnostic Evaluation (MODE), is developed and distributed by the Developmental Testbed Center (DTC) (DTC, Accessed August 19, 2019, http://www/dtcenter.org/). MODE is available within the Model Evaluation Tools (MET) and has been used in numerous model verification studies (Davis et al., 2006; Cai and Dumais, 2015; Mittermaier et al., 2016; Griffin et al., 2017; Abayomi et al., 2018). Essentially the MODE technique matches features and tracks changes through time grouping the results for statistical analysis. Various controls are available to modify how the object-based grouping is performed. Typically, an Intensity Sum (IS) or total rain volume (mm) is tracked and normalized over the whole domain, resulting in a normalized IS, or IS-Domain (ISD). An excellent example of using MODE object-oriented techniques in combination with other more traditional precipitation forecast verification metrics as applied to the GFS model output is available in Yan and Gallus (2016), including an analysis of diurnal forecast accuracy variations. Displacement errors, areal coverage, and other spatial orientation artifacts can easily be examined in more detail by using the MODE system.

Radar Data Assimilation

Weather radar data assimilation would seem like an obvious solution to weather model improvements; however it is difficult to achieve in practice because a host of supportive environmental variables are required to properly initialize the weather model (e.g., moist air, clouds, thermodynamic vertical profiles, vertical wind shear, and pre-convective horizontal wind flows). These contextual environmental variables are necessary to carry the rainfall event forward in time in a realistic manner. For example, if a rain event was placed into an artificially high vertical wind shear or dry water vapor environment, the storm formation might be “torn apart” or prematurely evaporated. The physical interactions related to convective cloud growth and decay are numerous. So, in practice, advanced radar data assimilation systems tend to improve just the early convective on-set within the first 0-12 hrs period of the precipitation forecast (Yan and Gallus, 2016; Xiao et al., 2007; Moser et al., 2015). Multiday forecasts tend to benefit less from the advanced radar data assimilation methods. However, with higher-resolution model runs using radar data assimilation, the rainfall performance can be improved up to 9h (Sun et al., 2012).

Verification Performance Method Summary

Using the above verification methods, some general conclusions are possible about the GFS model verification performance: 1) the obvious and expected conclusion that future forecasts at greater prediction times are less accurate due to increasing model error (i.e., model skill typically monotonically declines as a function of increased time) and 2) that the lowest skill is also a function of the time of day, and tends to occur in the late morning through the afternoon, due to the physical non-linearities of convective events being more difficult to forecast accurately. The temporal effects are related to the nature of afternoon convection, including their specific geographical position, and storm cell intensities and various atmospheric environment feedbacks (Yan and Gallus, 2016).

TIME-SCALE IMPACTS

Data assimilation is used to reinitialize prognostic models so that model errors are minimized using the available input data and knowledge of the various physical dynamics and observational errors (Fletcher, 2017). Data assimilation frameworks can be a multi-stage complex process, including data cycling, data quality control, and numerous other aspects to properly precondition data inputs into the data assimilation system (Jones and Fletcher, 2013). In this case, we use data assimilation adjoint methods to offer model system insights into complex model interactions with their input data sets as a function of time, which in turn can shape irrigation tool design requirements (Errico and Vukicevic, 1992; You et al., 2017). A Richards equation-based land surface model (Ross, 1990; Rathfelder and Abriola, 1994) will be used to examine the time-scale impacts within the vertical profile of the soil (Jones et al., 2019). As a numerical sensitivity study, it helps to provide insight into the types of issues and concerns that irrigation tool users of precipitation forecast data should be looking for to maximize impact to the irrigation schedule performance, beyond the surface-flux-centric precipitation forecast metrics. The study is directed toward inciting further analysis, and to encourage users of precipitation forecast data to more fully understand their potentially complex data input needs as part of a more complete solution for their intended applications.

The Microwave Land Surface Model (MWLSM)

In the Microwave Land Surface Model (MWLSM) (Jones et al., 2004) a temporal variational data assimilation methodology is used to derive deep soil moisture profile sensitivities and tendencies for use in understanding the soil profile interactions as a function of precipitation amount and rainfall event timing, as well as interaction behavior as a function of soil depth. In this work the adjoint sensitivity methodologies are applied to a 2D land surface model (vertical profile and time), and then used to demonstrate likely temporal requirements for irrigation tool development using precipitation forecast performance estimates. The MWLSM operator is connected to the Land Ecosystem-Atmosphere Feedback (LEAF2) model (Walko et al., 2000) which is the land surface subcomponent of the CSU Regional Atmospheric Modeling System (RAMS) mesoscale weather model (Pielke et al., 1992), additional details of the MWLSM are discussed in Jones et al. (2004). It is a fully functional soil model with vegetation fluxes, thermal, and moisture energy balances using atmospheric boundary layer exchanges.

Adjoint Sensitivity Methodology

Minimal variational data assimilation component requirements are: 1) a physical model, 2) its associated tangent linear model, 3) an adjoint model, and 4) observational data operators (and their associated observational operator adjoints) that represent the transfer functions between model and observation space variables (Jones and Fletcher, 2013). Adjoints are used within variational data assimilation techniques to determine how to best adjust the model initial conditions to accommodate the observational sensor data information. Quantitatively a "cost function", J, is used to measure the distance that the model state is from the observational data. The probability of the model state is maximized with respect to the observational data by using the gradient of the cost function to find the cost function minimum. The adjoints are used to compute the gradient behavior of the cost function by targeting particular model state variables for retrieval. The optimization of the model state initial conditions $\mathbf{x}$ (t_0) at time t_0 is the most typical use of data assimilation systems (Reichle, et al., 2007: Li et al., 2010; Ren et al., 2010; Koster et al., 2014). Cost functions can also be defined using a set of cost function constraints, J_C, thus serving as a penalty function for constrained optimization methods (Fletcher, 2017). In our case, the rainfall performance metrics can also be used as a partial constraint. Additional factors such as economic costs and irrigation scheduling capacities can be also incorporated into the optimization strategy through modification of the cost function.

Components of the data assimilation methodology can be used to provide insight into the links between model physics behavior when adjoints are used as a diagnostic tool. In time-dependent variational techniques such as four-dimensional variational (4DVAR) data assimilation, the cost function can be determined as a function of the temporally-integrated adjoint sensitivities (Fletcher, 2017). In our case, the control variables are the soil moisture at various soil depths. The adjoint sensitivities, $\mathbf{L}\,(t_i, t_0)^{\mathrm{T}}$, are computed with respect to these control variables, where **L** is the tangent linear operator of the forward model, **M**. The adjoint sensitivities and forward model operator are combined with the model background error and observational error covariance fields (**B** and **R**, respectively) and the non-linear observational operator, H, (and **H,** the tangent linear operator of H) to determine the cost function gradient with respect to the model state initial conditions, $\mathbf{x}\,(t_0)$. The model background error covariance is estimated relative to "truth", as are the observational error covariance fields which are estimated instrument noise errors relative to "truth". The non-linear observational operator, H, transforms the model state information into the observational state (e.g., soil moisture and surface temperature model state information are transformed into passive microwave brightness temperatures). The cost function and its gradient are key factors that determine the new initial model state estimate, when used for optimized model reinitialization.

It is interesting to note that the adjoints are integrated backwards in time because interest is in the propagation of data analysis increments, $[\mathbf{H}(\boldsymbol{x}_i) - \boldsymbol{y}_i]$, back to the initial model time, t_0, where $\mathbf{H}(\boldsymbol{x}_i)$ is the tangent linear observational operator as a function of the model state variable, $\boldsymbol{x}_i$, and $\boldsymbol{y}_i$ is the matching data observation (i.e., the model is being used to simulate the value of an observational measurement). If these data analysis increments can be reduced, the cost function values are reduced as well. We now look at a simple Gaussian-based variational data assimilation cost function, J, for clarity (Fletcher, 2017). Additional non-Gaussian terms are added within a mixed lognormal-Gaussian variational data assimilation, but with the adjoints similarly defined. Therefore, the simplified concepts shown here are useful for discussion of the key concepts. In this simplified case the full-field cost-function is:

$$J[\mathbf{x}(t_0)] = \frac{1}{2}[\boldsymbol{x}(t_0) - \boldsymbol{x}^b(t_0)]^T \mathbf{B}_0^{-1}[\boldsymbol{x}(t_0) - \boldsymbol{x}^b(t_0)] + \frac{1}{2}\sum_{i=0}^{n}[\mathbf{y}_i - \mathbf{y}_i^o]^T \mathbf{R}_i^{-1}[\mathbf{y}_i - \mathbf{y}_i^o], \tag{9}$$

where $\boldsymbol{y}_i \equiv H_i[\mathbf{x}(t_i)]$, and $\mathbf{B}_0^{-1}$ is the *a priori* background error covariance matrix. The cost function is minimized with respect to the initial state vector, $\boldsymbol{x}(t_0)$. The transpose of the cost function gradient (used in finding the cost function minima) is given by:

$$\left[\frac{\partial J}{\partial \mathbf{x}(t_0)}\right]^T = \mathbf{B}_0^{-1}[\boldsymbol{x}(t_0) - \boldsymbol{x}^b(t_0)] + \sum_{i=0}^{n}\mathbf{M}(t_{i+1}, t_0)^T \mathbf{H}_i^T \mathbf{R}_i^{-1}(\mathbf{y}_i - \mathbf{y}_i^o), \tag{10}$$

where

$$\mathbf{M}(t_{i+1}, t_0)^T = \prod_{j=0}^{i-1}\mathbf{M}(t_{i+1}, t_0)^T \tag{11}$$

and $\mathbf{M}(t_{i+1}, t_i) \equiv \mathbf{M}_i$. The adjoint model, $\mathbf{M}(t_{i+1}, t_i)^T$, is defined by the linearized model operator (Errico, 1997). The adjoint observation operator, $\mathbf{H}_i^T$, is defined similarly as the transpose of the linearized forward operator, $\mathbf{H}_i$, however the observation operator is typically defined for a single observational event or time. Note that the tangent linear models are *gradients* of the original operators. The adjoint is identical to the transpose for real numbers when using partial derivatives with respect to the discretized equations; however, for complex numbers the adjoint computations need to account for the phase behavior of the complex number partial derivatives (Jones et al., 2004). Adjoints are built upon a linearized forward model, with a series of numerical tests performed to ensure accurate construction of the adjoint (Jones et al., 2004). Adjoint models can be time consuming to create (Errico, 1997), but once built, adjoints can be integrated in time as needed. As apparent from (10) and (11), multiple temporal model states (and their corresponding temporally-integrated adjoint model sensitivities) may need to be stored during the computation of the cost function sensitivities within 4DVAR.

The use of cost function constraints is straightforward in principle (Fletcher, 2017), and involves augmenting the traditional cost function definition (9) with an additional term:

$$J = J[\mathbf{x}(t_0)] + \alpha \; J_C \tag{12}$$

where α is an alpha scaling term (a scalar factor to balance constraint requirements), and J_C is the cost function constraint term. The cost function augmentation approach is similar to that used for balancing constraints of digital filters (Fletcher, 2017, see section 17.1, pp. 714-717). It can also be useful to augment the length of the original control vector, **x**, which normally contains a subset of the model physical state variables, with additional constraints such as "tunable" model parameters or bias adjustment terms. The Augmented Control Vector (ACV) method (Cucuci et al., 2016) is commonly used by weather prediction systems to estimate biases as part of the data assimilation system, and also allows for key model parameters within the system to be optimized. In the case of irrigation schedulers this be could particularly useful for integration of more advanced fine-scale ETc estimates. The J_C term can also include additional functions related to irrigation capacity limitations, economic costs, and other factors. Ideally, such terms would be added into a full multiple equation set with respective adjoints developed for each term, however for expediency, the J_C term approach can be used to augment methods for practical implementation concerns. However, if ad hoc J_C terms are defined and used as constraints, the system will no longer be optimal, but rather "expedient" in its development, and the final selection of functions and recommended scaling terms for verification tests is left as an experiment design choice. Use of additional cost function constraints and augmented control vector methods will be explored in future studies and work. We focus on the rainfall performance metrics and use of that information within the adjoint sensitivity method to address questions related to interactions between root-zone growth stages and crop health during dry-down periods after a rain event as a function of space and time.

CONCLUSIONS

This work has reviewed two key aspects of the use of predictive weather data within irrigation scheduling tools for improved management of water resources: 1) predictive rainfall performance metrics and 2) adjoint sensitivity methods. The performance metrics of the predictive weather data were reviewed for probabilistic consistency, as multiple metrics can be used by the weather data centers over different time scales, and consistency of application of these metrics is important for irrigation tool developers. Also, the on-line automatic generation and archival of these performance metrics by the major weather data centers can allow irrigation tool developers to leverage the considerable development expenses that the NWP community has invested to diagnose NWP precipitation forecast verification metrics for their own regional use. Adjoint sensitivity methods were also reviewed and are used to diagnose complex space-time relationships between predictive rainfall, and water amounts within the vertical column of the soil profile. Use of water as a function of soil depth can have a large impact on effective root-zone water use, and is another area of potential crop management optimization, as water application frequency and irrigation delivery amounts are considered. Balancing these factors could lead toward the development of future methods which optimize conditions based on crop maturity and associated root zone penetration depths versus probabilistic estimates of rainfall and management allowed depletion rates.

The following specific findings are made:

(1) The multiple precipitation thresholds of the NWP precipitation forecast metrics allow for significant customization for irrigation pivot system speeds (affecting the time to complete a full irrigation application cycle, or in some cases the ability to use variable-rate irrigation systems), as multi-day NWP forecasts are available, and some crop management practices (and irrigation management tools) will need to be customized to these field-by-field equipment-dependent time constraints.

(2) Regionalized precipitation forecast verification metrics are available and should be used to isolate spatially-varying climatological biases and skill differences to the particular area of interest.

(3) Adjoint model sensitivity methods can be used to examine complex soil profile issues that are a function of meteorological data, soil conditions, and crop growth stage. The methods are also helpful to diagnose the timing of sensitivities and data forcings that are in complex interdependent physical relationships. In turn, this allows for the optimization of the physical relationships to achieve desired goals.

(4) Two data assimilation method extensions are introduced: the augmented control vector (ACV) method and the cost function constraint. Both allow for adjoint sensitivity development pathways toward pragmatic irrigation scheduler requirements, such as incorporating optimal model parameter tuning capabilities, and applying economic irrigation capacity constraints. Such approaches demonstrate the flexibility and adaptability of the data assimilation methodologies.

The public availability of predictive weather performance metrics and adjoint sensitivity methods are useful when combined to examine the complex interactions between moisture and energy fluxes within the soil and crops as it relates to crop growth stages. We plan to use these methods in additional tests to improve the WISE usage of weather predictive information to account for various uncertainties as they propagate through the land surface model physics. We anticipate in the future that additional economic irrigation cost information and other constraints can be tested in novel combinations to further improve cost-effective irrigation decision making within WISE and other irrigation scheduling systems. A follow-on study is underway on the results of the irrigation tool behavior within a variety of crop management and irrigation-decision situations, as well as subsequent crop yield estimates from these tool-based management decisions.

SUPPORTING INFORMATION

Additional supporting information may be found online under the Supporting Information tab for this article: A review of precipitation observational capabilities and Brier Score metrics.

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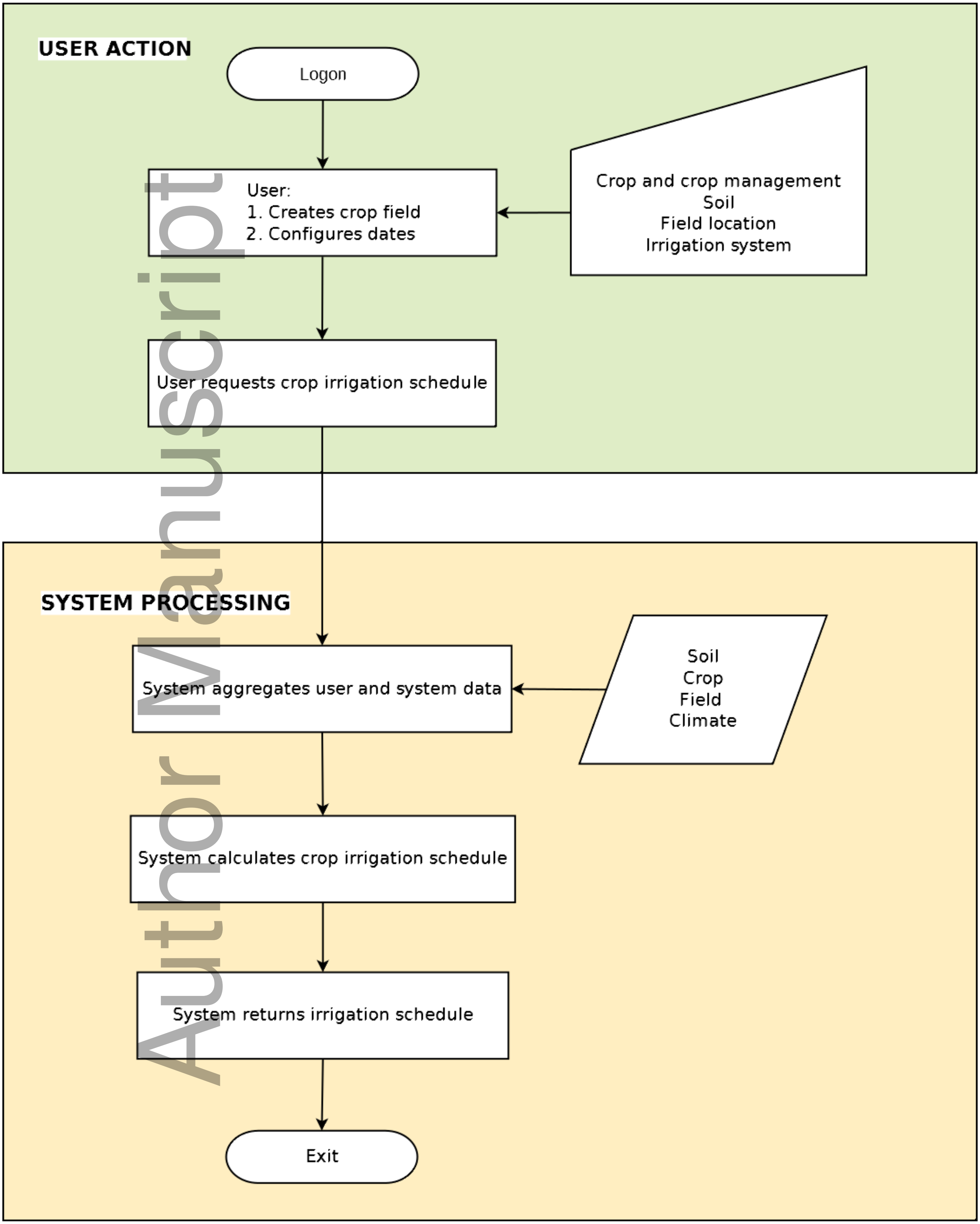
FIGURE CAPTIONS

Figure 1. Flow chart showing steps in the operation of the Water Irrigation Scheduler for Efficient Application (WISE) tool.

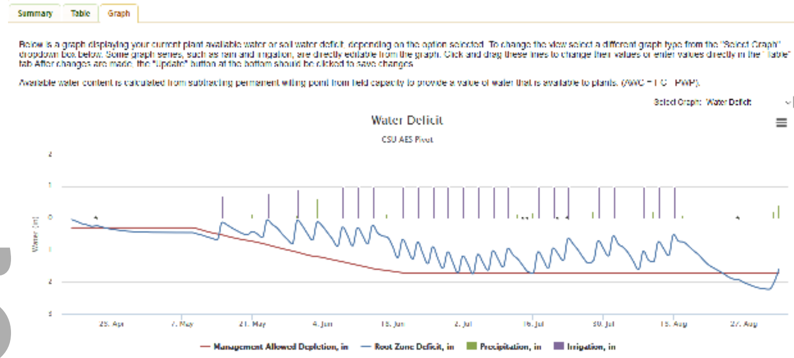
Figure 2. WISE estimated soil water deficit for an example barley crop at Center, Colorado from April 15 to September 3, 2018. Lines depict as a function of time: (blue) soil water deficit (net irrigation requirement, in), and (red) soil water deficit at management allowed depletion (MAD, in). Vertical green bars represent the magnitude and timing of precipitation (in inches), while the purple bars represent the irrigation applied (in inches) as a function of time to maintain the irrigation management objectives given the natural precipitation forcing.

Figure 3. CSU satellite precipitation data (enhanced National Oceanographic and Atmospheric Administration (NOAA) Blended Rainrate (BRR) operational product documentation. Accessed August 19, 2019, https://www.ospo.noaa.gov/Products/bRR/Algo.html), dynamically available in near real-time for global agricultural regions via the aWhere platform (aWhere, Inc.

system. Accessed August 19, 2019, https://www.aWhere.com) and can be readily linked to SmartPhone app databases. In this example, CSU satellite precipitation data are shown over New Delhi, India for May 24, 2014 to Nov. 12, 2014. High resolution global precipitation data are available starting at approximately 2008 to the present.



jawra_12810_f1.tif



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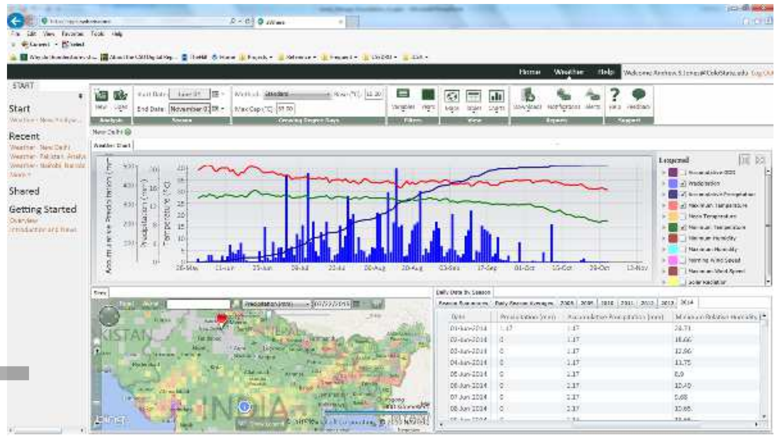

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