NEW QUALITY ASSURANCE TECHNIQUE FOR METEOROLOGICAL STATIONS BASED ON A PHYSICALLY-BASED HYDROLOGICAL MODEL

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ABSTRACT

Many groups depend on climate data from federal and state supported weather station networks such as the NRCS's SNOTEL, and NOAA's Climate Reference Network. While data from these stations are typically of high quality, there is no statistical parameter available to the public that quantifies the bias and the magnitude of errors in a time series. A time series error analyses could possibly detect subtle data anomalies, and problems with sensors, while providing a general level of confidence in the data for the user. HYDRUS-1D was used to construct a physically-based flow model for water and thermal fluxes for a SNOTEL site in Oregon from June 1, 2008 0:00 to October 31, 2011 23:00. Soil moisture and temperature values were predicted using the model and then compared to soil data measured with Hydra Probe soil sensors placed at 5, 10, 20, 50 and 100 cm. Simulations on hourly data sets typically yield RMSE from about 0.01 to 0.05 and 1 to 3 degrees C for soil moisture and temperature respectively. Model efficiencies decrease and RMSE increase for soil moisture with the presence of the winter snow pack when using degree day based model for snow water equivalent. (KEYWORDS: time series, physically-based model, meteorological station, quality assurance, cloud computing)

INTRODUCTION

State and government sponsored weather station networks such as the NRCS's SNOTEL network and NOAA's Climate Reference Network are playing many important roles and are critical for water supply and draught forecasting as well as a broad number of climate research studies. Many of these network weather stations and weather stations operated by universities take hourly measurements of weather parameters such as precipitation, air temperature, solar radiation wind speed/direction and humidity. In addition to the standard weather parameters, many of these weather stations have Hydra Probe soil sensors at several depths measuring soil moisture and temperature. While the data from most of these weather stations are of high quality with routine station maintenance, few tools have been proposed that address the level of confidence for any particular data set or real time data strings. One such tool capable of identifying data anomalies in precipitation and air temperature data is Parameter–Elevation Regressions on Independent Slopes Model (PRISM). PRISM is a statistical spatial regression model that is capable of accurately predicting precipitation and air temperatures in areas where physical measurements do not exist (Daly, 2008). While PRISM can statically identify data anomalies in air temperature and precipitation in data sets, it does not address the quality assurance of the other critical parameters such as soil moisture, solar radiation, relative humidity, wind speed, and soil temperature.

In this study, a new physically-based model approach was employed to generate time series performance statistics to be used as a quality assurance tool for data sets measured by remote metrological stations. The specific objective of work is to develop a quality assurance method employing a physically-based modeling approach that 1) provides quantitative confidence parameters for meteorological station performance, 2) identify subtle data anomalies, and 3) characterize the magnitude and bias generated from data anomalies.

With this physically-based model, the measured meteorological parameters which include wind speed, %RH, air temperature, precipitation, and solar radiation are used to predict the soil water content and soil temperature. The predicted soil data is then compared to the soil data measured with the soil sensors. The statistical level of agreement between the predicted and the measured soil data can then be used as a quality assurance tool for data sets measured at a particular weather station. The motivation for this work is to provide a quality assurance tool for users of meteorological stations that have soil sensors. Future topics will include model refinements and the use of cloud computing to perform the computations automatically in real time from real time data acquisition. The

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work also shows the potential increased value soil sensors and cloud computing can bring to meteorological stations equipped with telemetry.

PHYSICALLY-BASED MODEL

Vadose Zone Hydrology

Water movement in unsaturated soil can best be described by the one dimensional Richard's equation *(Richards 1931)*,

$$\frac{\partial \theta(h)}{\partial t} = \frac{\partial}{\partial z}\left(K(h)\frac{\partial h}{\partial z}\right) + \frac{\partial K(h)}{\partial z} - S(h) \qquad [1]$$

where θ is soil moisture ($cm^3 cm^{-3}$), t is time, h is unsaturated water potential head, z is depth and $S(h)$ is a loss term that includes evapotranspiration (ET). In this model, the potential ET is calculated using the Penman-Montheith combination equation from the atmospheric flux boundary conditions (FAO, 1990). The $K(h)$ is the head dependent unsaturated hydraulic conductivity which can be determined by the van Genuchten-Mualem Model described by equations [2a], [2b], [3] and [4] (van Genuchten, 1980). The van Genuchten-Mualem Model for determining the numerical values of $K(h)$ is based on a soil's moisture to head relationship which is commonly referred to as the soil water retention curve. A soil water retention curve is the plot of a soil's water potential head verses soil moisture. The fitting parameters of the mathematical function of the retention curve shown in equation [2a] along with the effective saturation value, $S_e(h)$ can be used to estimate the $K(h)$ using equation [4] for soil with variable water contents (Warrick, 2003). In equations [2a], [2b], [3] and [4], θ_r is the residual water content, θ_s is the water content at saturation, $\theta(h)$ is head dependent soil moisture, and n and α are empirical fitting parameter where $m=1-1/n$, and K_s is the saturated hydraulic conductivity. An h value greater than or equal to zero indicates a soil moisture value over its field capacity described by equation [2a] and [2b].

$$\theta(h) = \frac{\theta_s - \theta_r}{[1 + |\alpha h|^n]^m} \qquad \text{when} \quad h < 0 \qquad [2a]$$

$$\theta(h) = \theta_s \qquad \text{when} \quad h \geq 0 \qquad [2b]$$

$$S_e(h) = \frac{\theta(h) - \theta_r}{\theta_s - \theta_r} \qquad [3]$$

$$K(h) = K_s S_e^{\ell}\left[1 - \left(1 - S_e^{1/m}\right)^m\right]^2 \qquad [4]$$

The ℓ term in equation [4] is tortuosity which is assumed to be 0.5 (Šimůnek, 2005). In this work, the modeling software HYDRUS-1D which uses van Genuchten-Mualem Model and finite difference numerical solution to the Richard's Equation was used to calculate soil moisture values from atmospheric boundary flux conditions and soil water retention parameters (Radcliffe, 2010).

Thermal Fluxes

Soil thermal fluxes are highly influenced by water content and include both thermal conduction and convection which can be described by equations [5], where T is temperature, t is time, and z is depth. C_p and C_w are volumetric heat capacities for the porous media and water respectively (Radcliffe, 2010).

$$C_p(\theta)\frac{\partial T}{\partial t} = \frac{\partial}{\partial z}\left((\lambda(\theta).\frac{\partial T}{\partial z}\right) - C_w J_w \frac{\partial T}{\partial z} \qquad [5]$$

The first term in equation [5] represents heat flow by conduction, and the second term takes into account the water contribution of the heat flow, and the heat flux associated with root water uptake where;

$$\frac{\partial \theta}{\partial t} = \frac{\partial J_w}{\partial z} - S \qquad [6]$$

S in equation [6] is the evapotranspiration/water loss term from equation [1]. The heat capacity of the soil/water/air matrix is described by equation [7];

$$C_p(\theta) = C_s(1-\varphi) + C_o\theta_o + C_w\theta + C_a a \qquad [7]$$

where C_s, C_o, C_w, and C_a are the heat capacities of individual solid, organic, water and air phases respectively and θ_o, a, and φ are the water content of the organic portion, air fraction, and porosity. The water dependent soil thermal conductivity $\lambda(\theta)$ can be approximated by equation [8] (Chung, 1987).

$$\lambda(\theta) = b_1 + b_2\theta + b_3\sqrt{\theta} \qquad [8]$$

Where b_1, b_2 and b_3 are empirical coefficients' that are based on soil texture. For heat fluxes, HYDRUS-1D uses a finite element iterative approach to numerically solve equation [5].

MATERIALS AND METHODS

Study Area

This model was applied to a Billy Creek Divide SNOTEL Site #344. Billy Creek Divide is located in Southern Oregon in the Cascade Range about 5.5 kilometers southeast from Mount McLaughlin approximately 1609 meters in elevation. The site represents a typical SNOTEL location which is situated in an alpine environment that maintains a snow pack for most of the winter and spring. The site receives about 125 cm of precipitation per year most in the form of snow. Snow pack at Billy Creek Divide begins in late November or early December and disappears in early June. The site is forested with conifer trees ranging from 10 to 20 meters in height with sparse small shrubs on the forest floor. The soil has a very thin O horizon with 3 distinct A horizons going down to 23 cm and B horizons going down another 200 cm. The soils in these horizons are about 70% sand and 30% silt. More site information can be found at; (http://www.wcc.nrcs.usda.gov/snotel/Oregon/oregon.html).

The site contains the standard SNOTEL instrumentation with real-time Meteor Burst telemetry. There are analog Stevens Hydra Probe Soil Sensors at 5 depths connected to a Campbell data logger. Wind speed and direction are measured with a RM Young 1503 wind sensor. Solar Radiation is measured with a Li-Corr pyrometer, total precipitation is measured with Sensotec pressure transducer in a "rocket" style collection gage, SWE is measured with a snow pillow and the air temperature is measured with a YSI X-Range sensor.

Statistical Parameters

The calculated, and measured, data can be compared by the commonly recognized root mean square error (*RMSE*) and the mean error (*ME*). The *RMSE* is defined by equation [9] (Loague, 1991) and the *ME* is described by equation [10] (Hall, 2001) where C_i is the calculated values generated by the models and M_i is the measured soil data.

$$RMSE = \left[\frac{\sum_{i=1}^{n}[C_i - M_i]^2}{n}\right]^{0.5} \qquad [9]$$

$$ME = \frac{1}{n}\sum_{n=1}^{n}(C_i - M_i) \qquad [10]$$

The *RMSE* is indicative of the magnitude of the error between calculated and measured data while the *ME* represents the bias. If the *ME* is a negative number, then the model is under predicting the measured data or the soil sensors are over estimating the data. The closer the *RMSE* and the *ME* get to zero, the better the agreement between the model and the measurements. If the *RMSE* and *ME* become large (or *ME* more negative), it may be difficult to determine if the error is associated with the sensors or the model itself; therefore a third statistical parameter is necessary, the model efficiency E_f (Loague, 1991).

$$E_f = \left(\sum_{i=1}^{n}(M_i - \bar{M})^2 - \sum_{i=1}^{n}(C_i - M_i)^2\right) \Big/ \sum_{i=1}^{n}(M_i - \bar{M})^2 \qquad [11]$$

The model efficiency is the skill term used where the closer to one, the better the model performance (Krause, 2005). Unlike r^2, E_f can be negative which indicates that model predicted values are worse than the mean of the measured values (Refsgaard ,2003).

Model Setup

The hydrological model HYDRUS-1D was used to predict soil moisture and temperature at the depths where the soil sensors are placed (at 5, 10, 20, 50 and 100 cm) from hourly atmospheric boundary flux conditions with the soil thermal and water retention parameters. Simulations were run starting from June 1, 2008 0:00 (hour 1) to October 31, 2011 23:00 (hour 29,952) with hourly outputs. The minimum and maximum time steps were specified at 2.4×10^{-6} and 12 hours with a maximum of 30 iterations insured model convergence.

Table 1. Soil water retention curve parameter for the van Genuchten-Mualem Model for each horizon.

Horizon/ Depth	θ_r	θ_s	α	n	K_s	%Sand	%Silt
A1, 2-8 cm	0.001	0.393	0.0413	1.4693	2.88833	71.3	24.6
A2, 8-13 cm	0.001	0.391	0.0405	1.4692	2.71458	71.6	23.4
A3, 13-23 cm	0.001	0.3931	0.0413	1.4693	2.88833	28.1	67.8
B1, 13-52 cm	0.001	0.3938	0.0475	1.7009	4.50375	18.9	79.1
B2, >52 cm	0.001	0.3938	0.0475	1.7009	4.50375	16.8	81.3

Table 2. Thermal parameter of the soil corresponding to equation [7] and [8].

	Solid Fraction	b1	b2	b3	C_s	C_o	C_w
All Depths	6.069E-01	-9.191E+11	-4.488E+12	1.176E+13	2.49E+11	3.253E+11	5.42E+11

Table 1 and 2 contain the soil water retention parameters and the thermal properties. The longitudinal thermal dispersivity is assumed to be 5 cm and the organic matter is assumed to be negligible.

The data measured with the Hydra Probe Soil Sensors was recalibrated from the direct probe measurement of the real dielectric permittivity using the general soil calibration described by Seyfried (2006). The atmospheric boundary flux conditions are air temperature, relative humidity, total precipitation, wind speed, and solar radiation. There are several data gaps in the data. The largest data gap was the soil sensor at 101 cm was not reporting from the beginning of the simulation until 7/14/2008. The model simulations took the data gap into account.

Model output for the five depths was collected for ten output data sets per month (one approximately every three days). Each output data set is a model output for ten randomly selected hours for a given month containing each of the five depths. The *ME*, *RMSE* and the E_f were calculated two different ways. First the *ME*, *RMSE* and E_f are calculated for each horizon separately for the output data sets on a monthly basis. Second, the *ME*, *RMSE* and E_f are calculated for each output data containing each horizon on a daily basis. This approach will capture both the conditions in the individual horizons on a monthly basis and also capture daily time series conditions for the system as a whole. Tables 3 and 4 illustrate this approach.

RESULTS AND DISCUSSION

Data Anomaly and Time Series Data

Data tables 3 and 4 show the results for the ten output data sets for soil moisture for September 2008. Table 3 is representative of how the model behaves at different depths. The prediction at the 50 cm depth is typically less consistent with the measured values than the other depths. For the 50 cm depth, the *ME* is consistently negative and the *RMSE* is typically 3 to 4 times bigger than the other depths throughout the entire 3 year simulation period. The typical *ME* and *RMSE* for the 50 cm depth when compared to the other depths suggests that there is a problem with the Hydra Probe placement at this depth, a problem with the model setup or incorrect soils data leading to an incorrect *Ks*. Table 4 shows the time series data for the output data sets for the same September 2008 time period.

Table 3, E_f, *ME* and *RMSE* for the September 2008 soil moisture output data sets.

Depth (cm)	E_f	***ME***	***RMSE***
5	0.93	0.00	0.00
10	0.36	0.01	0.01
20	0.71	-0.01	0.01
50	0.68	-0.04	0.04
101	0.71	0.03	0.03

Table 4. Soil moisture output data sets for soil profile in a time series both containing the 50 cm data and without the 50 cm data.

			Containing data at 50 cm			**Data at 50 cm removed**		
Date	Time	Hour	*ME*	*RMSE*	E_f	*ME*	*RMSE*	E_f
9/3/2008	6:00	2263	0.00	0.02	0.45	0.01	0.01	0.71
9/3/2008	12:00	2269	0.00	0.02	0.34	0.01	0.02	0.52
9/4/2008	12:00	2293	0.00	0.02	0.37	0.01	0.02	0.38
9/7/2008	18:00	2371	0.00	0.02	0.45	0.01	0.01	0.63
9/9/2008	18:00	2419	-0.01	0.03	0.04	0.00	0.02	0.42
9/13/2008	6:00	2503	0.00	0.03	0.32	0.01	0.02	0.41
9/17/2008	0:00	2593	-0.01	0.02	0.34	0.00	0.02	0.62
9/19/2008	12:00	2653	0.00	0.02	0.48	0.01	0.01	0.69
9/25/2008	0:00	2785	0.00	0.02	0.51	0.01	0.01	0.69
9/29/2008	0:00	2881	-0.01	0.02	0.39	0.00	0.01	0.67

On the left hand side of table 4, all of the horizons are included in the calculation for *RMSE*, *ME* and E_f. The right hand side of table 4 shows the *RMSE*, *ME* and E_f on the same data set only with the 50 cm removed. After removing the 50 cm data, the overall time series *ME* goes from negative to positive, the *RMSE* improves by about a factor of two at most times.

Snow Melt on Time Series Data

In this alpine environment, the soil will remain wet at or slightly below field capacity starting in the fall when the season precipitation starts until the snow pack disappears in June. The soil stays moist during the winter because there are occasional melting events in the winter months while ET is at a minimum. After the snow pack disappears in early June, precipitation seasonally decreases and ET becomes large drying out the soil. Figure 2A, 2B, and 2C shows the calculated and measured soil moistures for the 2008 season spring melt and soil dry out period. In the simulations that generated Figure 2A, 2B and 2C, the *RMSE*, *ME* and E_f were calculated for the whole data set for the time period from June 2008 to October 2008.

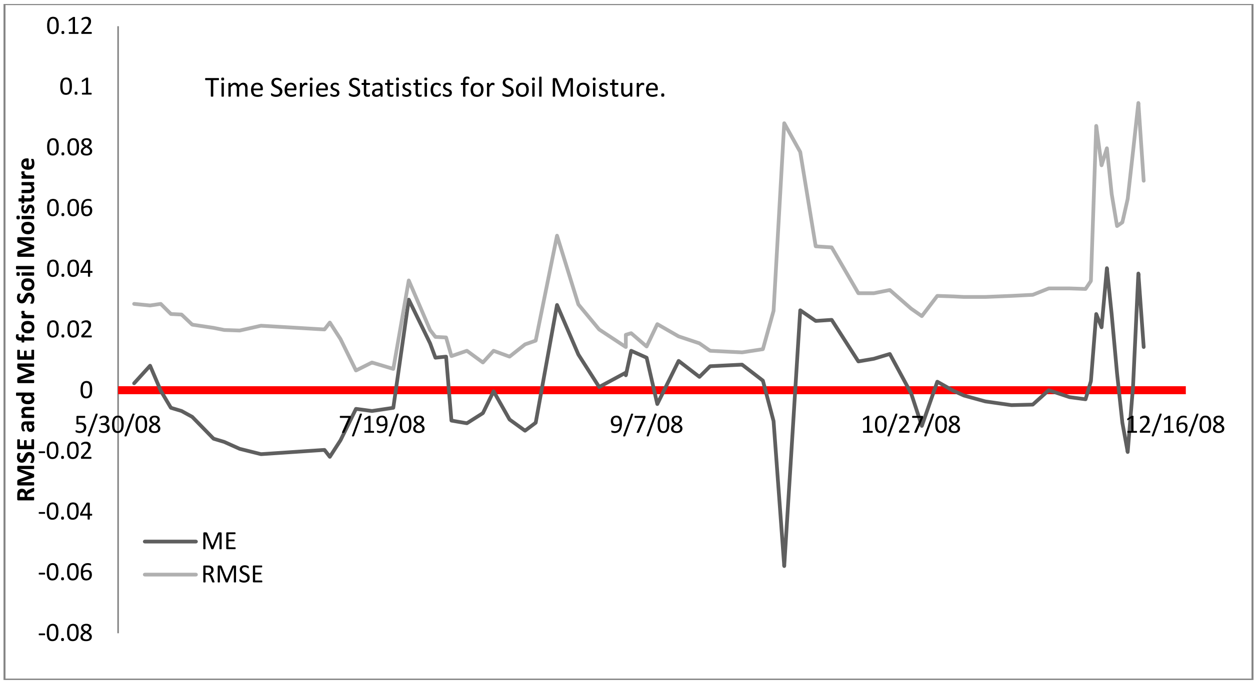

Figure 1. RMSE and ME for 2008, comparing modeled vs measured soil moisture.

<u>Snow Hydrology and Snow Pack Errors</u>

Most of the precipitation at the Billy Creek Meadows site is in the form of snow and thus the soil water content is mostly attributed to snowmelt. Snowmelt processes in an alpine setting can be complex and can be driven by many factors other than temperature such as dust particles in and on the snow surface, sublimation, and the thermal properties of the vegetation (Ewing, 2007).

Contained within the Hydras code, is a simplified snow hydrology feature based solely on air temperature. The model assumes that if the air temperature is below -2^{o}C, all precipitation will be in the form of snow, and if the temperature is above +2^{o}C, the precipitation will be rain. A linear transition occurs between -2^o and 2^o C. If the temperature is above zero C, the model calculates the rate at which the snow will melt by equation [12] (Šimůnek, 2005, 2008 & 2009).

$$T_a K_s = M_d \qquad [12]$$

Where T_a is the air temperature, K_s is the snow melt constant and M_d is the daily SWE reduction to the snow pack. Typical vales for Ks are 0.02 to 0.6 cm/C and the default value is 0.43 cm/C.

Figure 3 is a plot of the SWE both reported from the SNOTEL site and calculated in HYDRUS using equation [12]. The model over predicts the SWE from 11/8/2013 to about 11/18/2013 where it under predicts the SWE until the end of the season. A more robust snow melt model that takes into account the thermal properties of the canopy and ground litter may be required to achieve an output consistent with the SNOTEL data. The degree day method can generate large errors in SWE; and consequently, introduce large errors in the model's boundary flux conditions which in turn leads to large errors in simulated soil moisture and temperature outputs during times when there is a snow pack (Wöhling, 2009). Table 5 shows the *ME*, E_f and *RMSE* for two different time frames during snow pack conditions. The top part of table 5 is for a time period during which the model is over predicting the SWE and the bottom part of table 5 shows output when the model under predicts the SWE. There are noticeable differences in the output statistics between the two data sets. For soil moisture, the *RMSE*, and *ME* for the times the model is under predicting SWE are half that from the times the model is over predicting SWE. Similarly, the model efficiency improved when the model is under predicting the SWE when compare to when it is over predicting SWE. The behavior of the temperature outputs for the under or over predictions of SWE are less pronounced than what was observed on the soil moisture data.

Induced Error Perturbation and Statistical Parameter Reponses

With no snow pack in the summer months, typically HYDRUS 1D generates outputs that reasonably resemble the measured data from June through September. Table 3 shows values that are typically observed for times with no snow pack. For the June of 2008 soil water data set, the *RMSE* ranged from 0.01 to 0.04, the *ME* from 0 to -0.03 and the E_f remained close to 1. To observe and test the data set quality assurance potential of HYDRUS, simulations were performed that contained a perturbation of known biases in the meteorological boundary condition data set. This was performed by intentionally introducing errors into the meteorological boundary conditions so that the differences between the modeled outputs and the measured sensor data values could be compared. This test would demonstrate the sensitivity of the HYDRUS model's ability to detect data anomalies in a meteorological data set. The data that was chosen for this test was June of 2008 because it had a high skill and a low bias and absolute error. To simulate a rain gage malfunction, 0.1, 0.2 and 0.3 cm of precipitation were manually added to the hourly precipitation input data followed by modeled simulations for each condition. Figures 4A, 4B, and 4C show the results. The differences are noticeable starting at 0.1 cm of rain an hour and only get more pronounced with the 0.2 and 0.3 cm simulations. It's interesting to note that the model simulation had about a 7 day lag time before the anomaly was detected.

Table 5, Depth, time series statistics, and model efficiencies during periods of under and over prediction of SWE. (* indicates no data available)

	11/8/2008 through 11/18/2008 (SWE over predicted)					
	Soil Moisture			**Temperature**		
Depth (cm)	E_f	ME	RMSE	E_f	ME	RMSE
5.0	0.949	0.040	0.052	-12.693	-1.975	8.848
10.0	0.811	0.076	0.084	0.521	0.554	1.785
20.0	0.883	0.050	0.069	0.548	0.813	1.746
50.0	*	*	*	-0.097	3.487	4.408
101.0	-0.028	-0.192	0.211	*	*	*
	11/23/2008 through 12/8/2008 (SWE under predicted)					
	Soil Moisture			**Temperature**		
Depth (cm)	E_f	ME	RMSE	E_f	ME	RMSE
5.0	0.997	-0.008	0.010	-1.166	-0.853	2.124
10.0	0.938	0.038	0.039	-0.093	-0.940	1.927
20.0	0.978	0.024	0.026	0.595	-0.716	1.257
50.0	*	*	*	0.892	-1.117	1.159
101.0	0.953	-0.042	0.043	*	*	*

At that time, a spike begins to occur in the statistical parameters. E_f begins to drop, the bias becomes positive which would be expected and the absolute error increased. The spikes in the statistical parameters begin to subside in mid June as ET increases.

To test the model's sensitivity to data anomalies in an air temperature sensor, error in the air temperature input data was manually introduced followed by model simulations. A bias of -5.0 degrees C was manually introduced to the air temperature data set from June to September 2008 followed by model simulations of soil temperature. The model simulation that contained the air temperature bias were compared to the model simulations that did not contain the bias. Figures 5A, 5B and 5C impose the *ME*, *RMSE* and the E_f for the simulations that contained the introduced bias with the simulation that did not contain the introduced bias. In Figure 5A, the *ME*

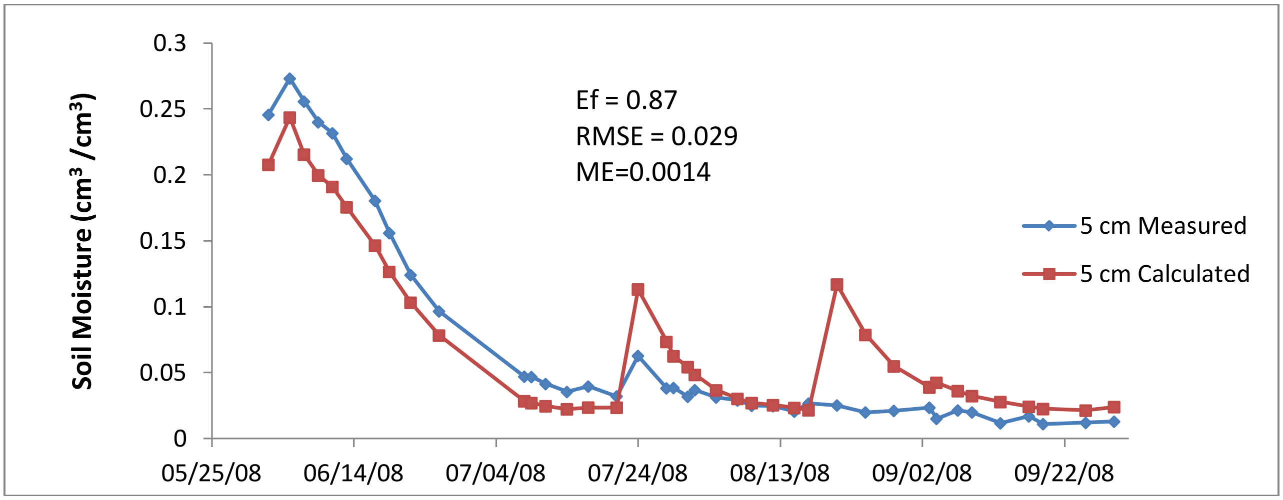

Figure 2A. Depth of 5 cm. Calculated and measured soil moisture during spring snow pack melt.

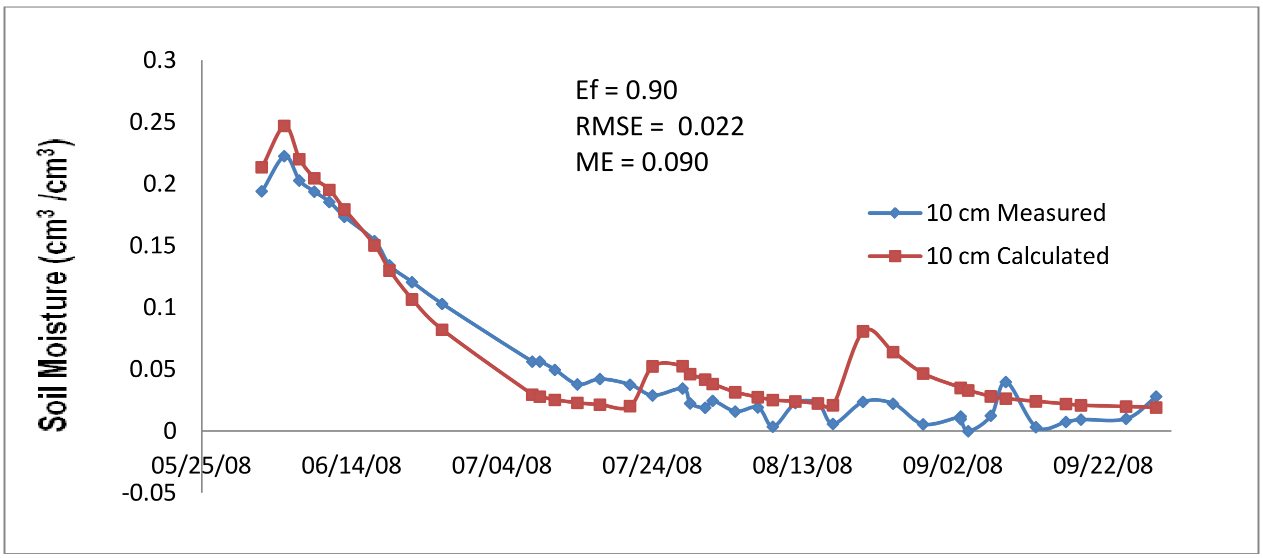

Figure 2B. Depth of 10 cm. Calculated and measured soil moisture during spring snow pack melt.

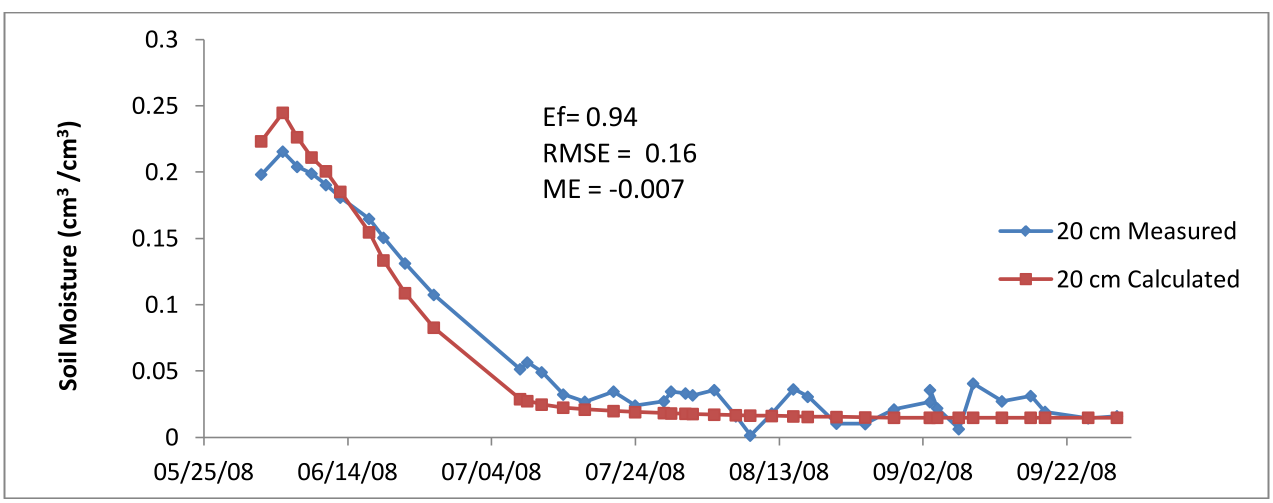

Figure 2C. Depth of 20 cm. Calculated and measured soil moisture during spring snow pack melt.

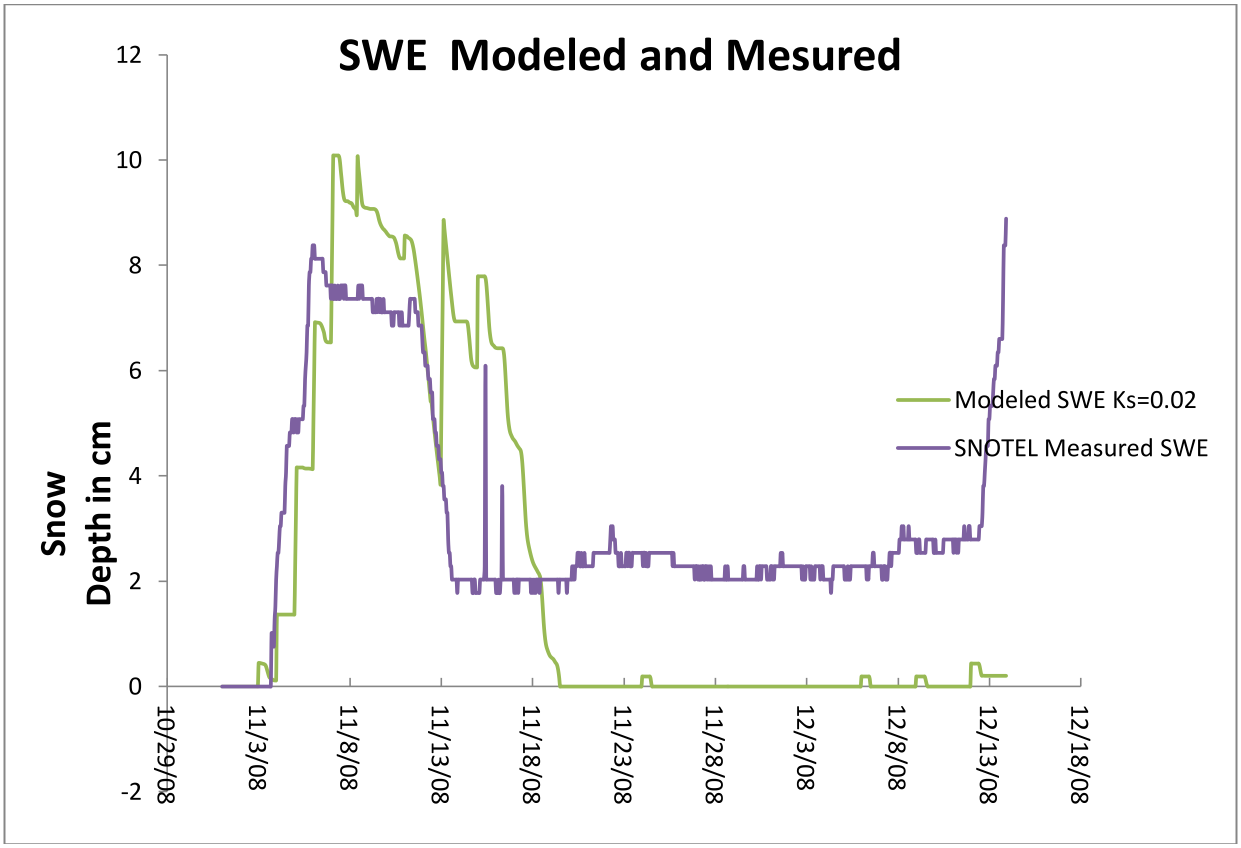

Figure 3 SWE measured at SNOTEL site compared to the modeled SWE with HYDRUS showing that the model has a tendency to over predict from 11/6/2008 11/18/2008 and under predict SWE from 11/18/08 through mid December 2008.

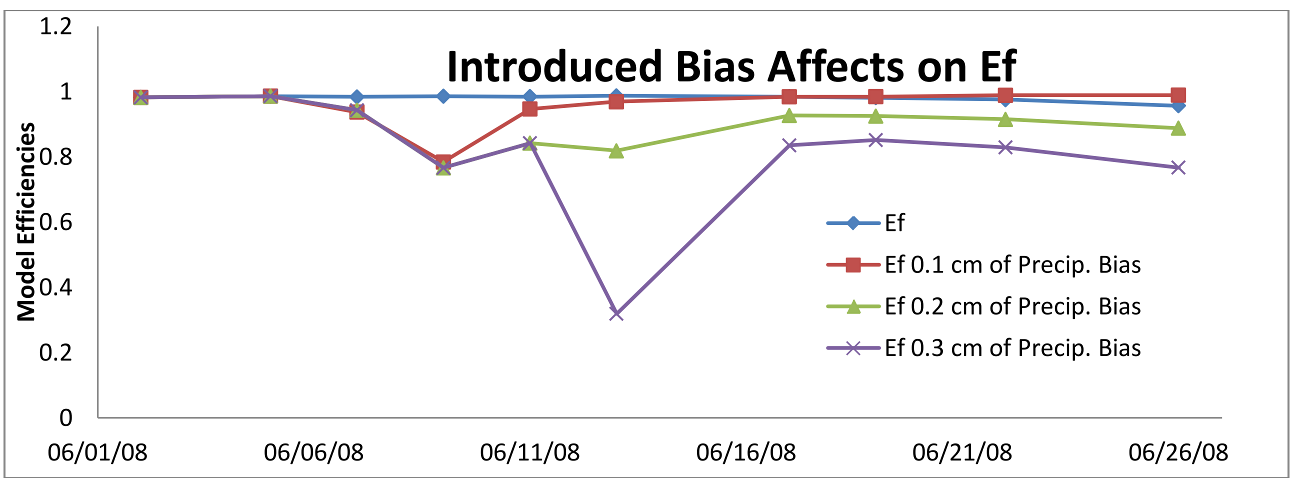

Figure 4A. Model efficiencies for no induced error, induced error of 0.1, 0.2 and 0.3 cm additional hourly precip.

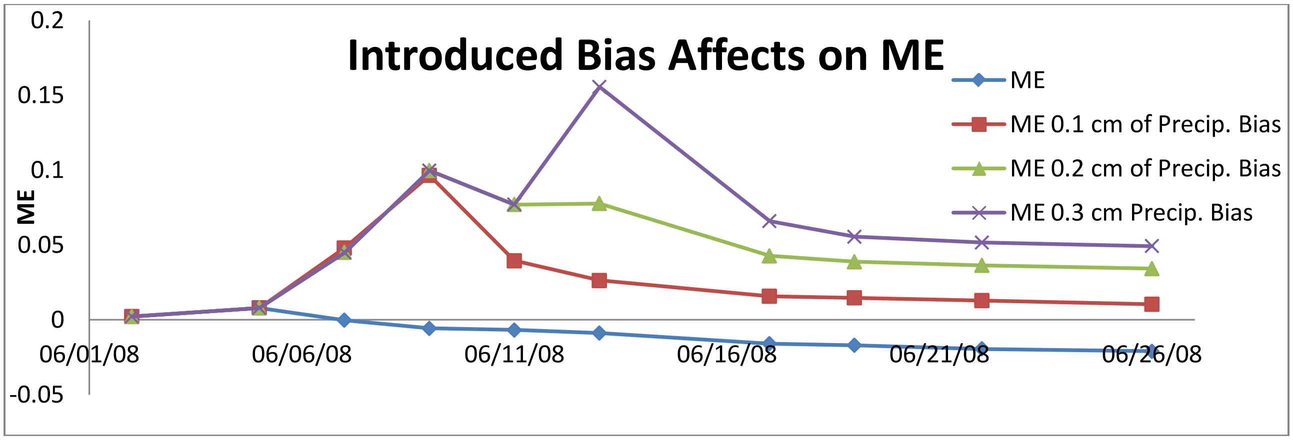

Figure 4B. Mean Error for no induced error, induced error of 0.1, 0.2 and 0.3 cm additional hourly precip.

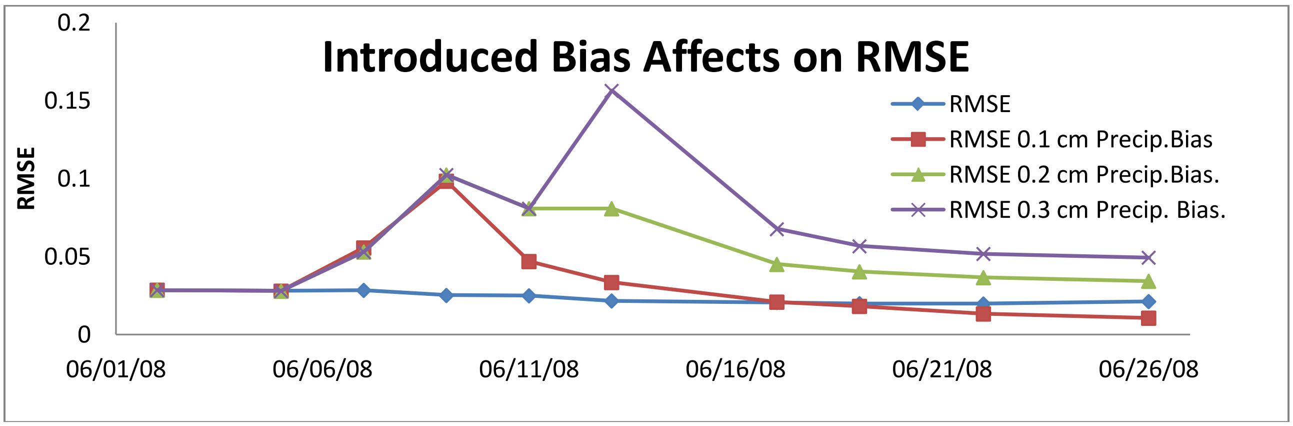

Figure 4C. RMSE for no induced error, induced error of 0.1, 0.2 and 0.3 cm additional hourly precip.

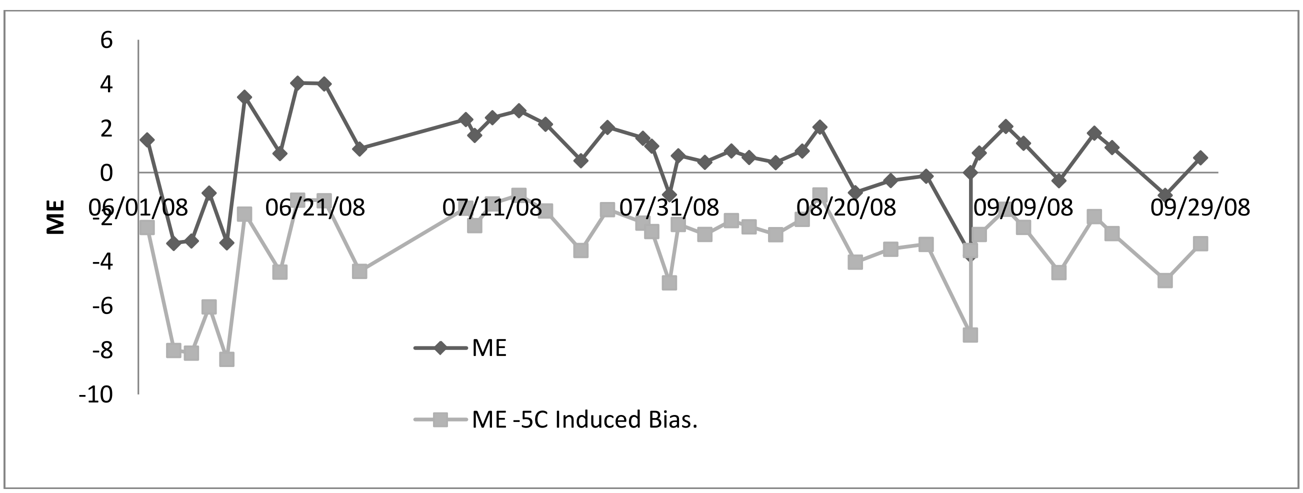

Figure 5A. Mean Error for no induced error, and induced error of -5.0 degrees C.

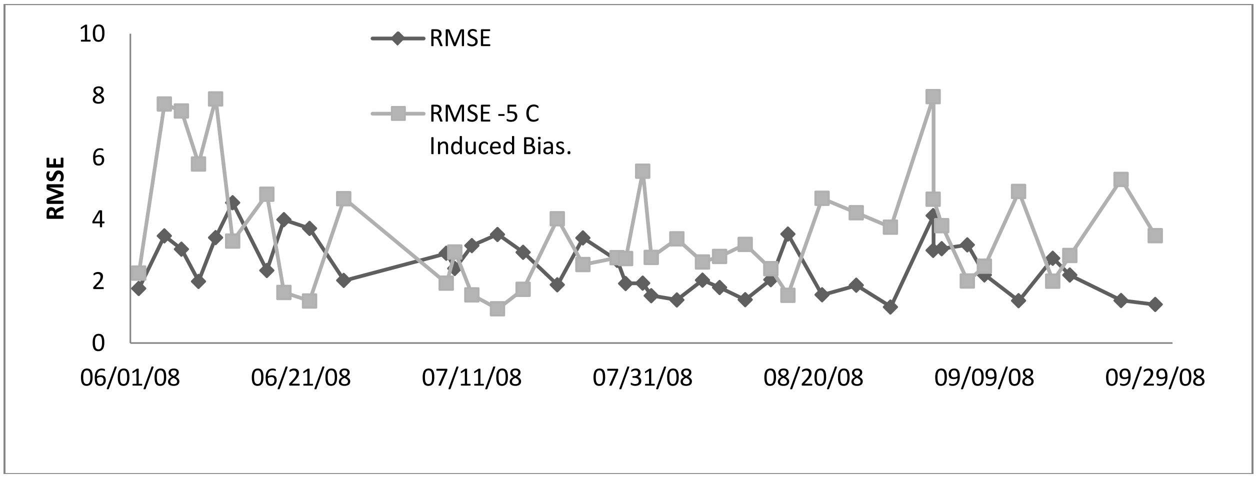

Figure 5B. RMSE for no induced error, and induced error of -5.0 degrees C.

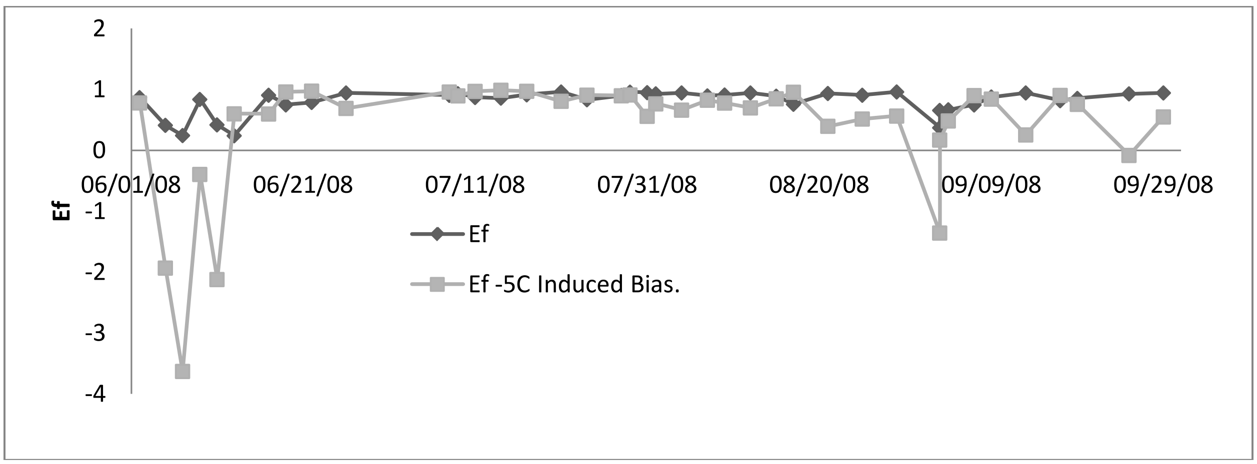

Figure 5C. Model efficiencies for no induced error, and induced error of -5.0 degrees C.

shifts by -2 to -6 over the simulation time frame. The *RMSE* and the E_f shift slightly with strong spikes at various points over the simulated time frame.

Future Work

Future work would include running simulations that take into account the thermal properties of canopy and organic ground litter such as with Simultaneous Heat and Water (SHAW) model (Flerchinger, 1989) to improve model performance. This would provide more reasonable SWE, soil moisture and temperature estimates during time when a snow pack is present. A different use of the statistical parameters may be a better indicator of data anomalies. Also, data anomalies may be better captured on near surface simulation outputs.

SUMMARY

Physically-based hydrological modeling of meteorological station data can be used to detect data anomalies in data sets and could be an indicator for malfunctioning sensors. Physically-based hydrological model simulations were performed using HYDRUS 1D on a data set taken from a SNOTEL station in southern Oregon. The statistical parameters, *ME, RMSE* and E_f, between the model output and the soil moisture and temperature data collected with the Hydra Probe soil sensors were used as quantitative indicators of data set anomalies. The simulations revealed a potential data anomaly in the soil moisture data at 50 cm. While HYDRUS 1D provide accurate model simulation outputs during the summer months, HYDRUS 1D's degree day method for calculating SWE lead to model deviations for periods when a snow pack was present at this particular alpine site. When data anomalies were manually introduced into the data sets, the statistical parameters of the model simulation had a visible response.

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