Using observed soil moisture to constrain the uncertainty of simulated hydrological fluxes

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Abstract

Using data from five long-term field sites measuring soil moisture, we show the limitations of using soil moisture observations alone to constrain modelled hydrological fluxes. We test a land surface model, MESH/CLASS, with two configurations: one where the soil hydraulic properties are determined using a pedotransfer function (the texture-based calibration) and one where they are assigned directly (the hydraulic properties-based calibration). The hydraulic properties-based calibration outperforms the texture-based calibration in terms of reproducing changes in soil moisture storage within a 1.6 m deep profile at each site, but both perform reasonably well, especially in the summer months. When the models are constrained using observations of changes in soil moisture, the predicted hydrological fluxes are subject to very large uncertainties associated with equifinality. The uncertainty is larger for the hydraulic properties-based calibration, even though the performance was better. We argue that since the pedotransfer functions constrain the model parameters in the texture-based calibrations in an unrealistic way, the texture-based calibration underestimates the uncertainty in the fluxes. We recommend that reproducing observed cumulative changes in soil moisture storage should be considered a necessary but insufficient criterion of model success. Additional sources of information are needed to reduce uncertainties, and these could include improved estimation of the soil hydraulic properties and direct observations of fluxes, particularly evapotranspiration.

1. Introduction

Land surface models simulate the vertical exchanges of water and energy between the land and the atmosphere. These coupled models integrate many different interacting processes and are capable of outputting a large number of state variables and fluxes. Soil moisture is the largest store of water on the land surface (aside from lakes) and is probably the easiest hydrological variable to measure. That is not to say that obtaining representative measurements of soil moisture is straightforward – particular challenges are to measure soil moisture at the appropriate scale and to capture the spatial variability (Vereecken et al., 2008, Peterson et al., 2016, 2019, Pan et al., 2017). On the other hand, Mälicke et al. (2020) looked at networks of soil moisture sensors and showed considerable organization in the spatial response of soil moisture changes, concluding that it is the temporal information from a few sensors, rather than the spatial variation from a large number of sensors, that is most valuable for capturing catchment scale moisture dynamics. Often the most useful metric of soil moisture is field scale (10^4-10^6 m^2 area) root zone (0.5 – 2 m depth) storage, S (mm), where $S=10^3 V_w/A$ and V_w (m^3) is the volume of water and A (m^2) is the land surface area. Such metrics can be useful for irrigation planning, crop yield assessment, and other vegetation productivity measures (Vereecken et al., 2008).

Consider the simple soil water balance equation

$$\frac{dS}{dt}=I-T-E-D \tag{1}$$

Where I, T, E and D are infiltration, transpiration, evaporation and drainage, all with units (mm/d). Changes in soil moisture over some time increment are obtained by

$$\Delta S_i=\int_{t=t_i}^{t_{i+1}} (I-T-E-D)\,dt \tag{2}$$

Subsequent values of storage are given by

$$S_{i+1}=S_i+\Delta S_i \tag{3}$$

The water balance error, ε (mm), over some time increment is given by

$$\varepsilon = \Delta S_i - \int_{t=t_i}^{t_{i+1}} (I - T - E - D)\, dt \qquad (4)$$

Equation 4 may be solved over long-term intervals (monthly, annually or multi-year) for observations and field estimates of fluxes to assess consistency of those data, and large errors (e.g. ¿50 mm/year) can be expected (e.g. Pan et al., 2017). It may also be solved for models over the entire simulation period, to assess model errors in the simulated states and fluxes, and in this case the errors should be very small (e.g. ¿10^{-3} mm/year).

Each of the fluxes in the above equations are simulated by the model – that is to say, they are not boundary conditions (most cannot be directly measured, Vereecken et al., 2008, Li et al., 2019), and they are all conditioned by the assumptions within the model and subject to model errors and uncertainties. It is clear from Equations 1-3 that information about the changes in soil moisture, ΔS, does not uniquely constrain the values that the fluxes should take. Different fluxes can compensate for one another: if the input flux (I) is overestimated then overestimating one or more of the output fluxes can result in the correct change in storage and hence soil moisture; if one output flux is overestimated, this can be compensated for by underestimating another output flux. However, it is also the case that each flux is in some way dependent on the soil storage: the infiltration capacity and soil evaporation rate depend on the level of saturation of the soil at the ground surface; drainage from a free-drainage boundary depends on the saturation of the soil at the base of the soil profile; and transpiration depends on soil water stress, determined by the saturation of the soil over the root zone (Seneviratne et al., 2010). Given all of this, for any given model and particular field site, it is not clear how much information content observations of soil moisture provide for uniquely constraining the model fluxes. We can say that models should be required to reproduce observed changes in soil moisture storage (within some acceptable error tolerance). We cannot say whether a model that does reproduce observed changes in soil moisture storage will necessarily correctly simulate the model fluxes.

Many studies have shown the benefits of bringing soil moisture observations to bear on the calibration and validation of hydrological models (Maheu et al. 2018, examples cited by Vereecken et al., 2008, a remote sensing example from Nijzink et al, 2018). Few studies have explicitly looked at the question of how much information is provided by using soil moisture alone to constrain models. Vereecken et al. (2008) do not provide an explicit answer to this question, though they do indirectly address this when they suggest that soil moisture data alone is often insufficient to estimate of soil hydraulic properties, and that inclusion of observed hydrological fluxes will improve the well posedness of the inverse problem. Li et al. (2019) suggested a more positive answer – they suggest that soil moisture observations could be used to estimate hydrological fluxes for a series of irrigated cropped land experiments. However, whilst they did consider uncertainty associated with the observed soil moisture and other data, they did not rigorously look at parameter uncertainty and did not consider the problem of uncertainty associated with equifinality.

In this study, we investigate the question of how useful observations of soil moisture are to calibrate a land surface model and constrain the uncertainty in predictions of runoff, infiltration, evapotranspiration and drainage, all of which are crucial fluxes for use in hydrological and biogeochemical simulations. We apply the MESH/CLASS land surface model to five diverse instrumented field sites along a south-north transect in Saskatchewan, Canada. All sites are seasonally frozen, two are located in the Canadian prairies and three in the southern boreal forest.

2. Methods

2.1 Soil moisture as a metric of model performance

We have available field measurements of volumetric liquid water content, θ (m^3 m^{-3}), at a number of discrete depth intervals, in the profile, z_j (m), and recording at discrete intervals in time, t_i (d). The profile storage, S (mm), is given by

$$S=\int_{z=0}^{z_N} \theta dz=\sum_{j=1}^{N} \theta_j \Delta z_j \tag{5}$$

A more useful metric of storage for use with calibrating models is the cumulative change in storage, Ω (mm). This is defined:

$$\Omega=\int_{t=0}^{t_i} dS=S_i-S_0 \tag{6}$$

We can also define the analogous cumulative change in volumetric water content, Θ (m^3 m^{-3}) as

$$\Theta = \int_{t=0}^{t_i} d\theta = \theta_i - \theta_0 \tag{6}$$

The benefits of calibrating and validating models against Ω or Θ rather than S or θ are twofold. Firstly, observations of soil moisture are made indirectly, and an instrument calibration relationship is required for the probe that relates some measured variable (typically the dielectric constant) to the volumetric (liquid) water content (Gardner et al., 2003). These calibrations can introduce errors, but the errors in the change in water content, measured between two points in time, are smaller than the errors in the absolute water contents. Hence, we have more reliable observations of the changes in water content, and hence changes in storage, than we do of the actual water contents. The second reason is that in most soil moisture models, hydraulic properties are determined using a normalized measure of water content, the effective saturation, given by

$$S_e = \frac{\theta - \theta_r}{\theta_p - \theta_r} \tag{7}$$

where θ_r and θ_p are the residual and saturated water content. The simulated cumulative change in θ (i.e. $\Theta_{¿}$) is the same as the simulated cumulative change in $\theta - \theta_r$ (i.e. from equation 6 we have $\theta_i - \theta_r - \theta_0 + \theta_r = \theta_i - \theta_0 = \Theta_{¿}$). Therefore, any arbitrary value for θ_r can be used to simulate $\Theta_{¿}$ ($\theta_r = 0$ is a sensible choice) and the number of free calibration parameters can be reduced by one. Moreover, after the model has been calibrated to reproduce Θ_{OBS}, if desired, the actual values of $\theta_{¿}$ can be obtained from $\theta_{¿} = \Theta_{¿} - \overline{\Theta_{¿}} + \overline{\theta_{OBS}}$, (and, if desired, the parameters θ_r and θ_p can be rescaled in the same way).

2.2 Field sites

We collected field data at five instrumented sites aligned from south to north in central Saskatchewan, Canada. Saskatchewan has a continental and seasonally frozen climate and a general trend of increasing mean annual precipitation and decreasing mean annual temperature from south to north. Soil type and vegetation cover at each site is summarized in Table 1.

The two prairie sites are in the Moist Mixed Grass ecoregion, which is correlated with semi-arid moisture conditions and Dark Brown Chernozemic soils (Ecological Stratification Working Group, 1996). The Kenaston site, located 90 km southeast of Saskatoon, SK, is in a grazing pasture surrounded by annual crops. The topography is flat to slightly undulating, with slopes of less than 2% (Burns et al., 2016). The water table resides between 3 to 5 m below ground surface (Pan et al., 2017). Mean annual precipitation is about 330 mm (2009 – 2014), of which 70 mm falls as snow. The mean temperature in January and July is −12.9 and 18.8 ◦C, respectively. (Pan et al., 2017).

St. Denis National Wildlife Area (SDNWA) is located east of Saskatoon, SK, and approximately 100 km north of the Kenaston site at the boundary between Moist Mixed Grass and Aspen Parkland ecoregions. The topography of the site and surrounding landscape is hummocky, with local relief of the order of 15 % (Miller et al., 1985). Vegetation at the site is mainly native and non-native grasses, and riparian vegetation or “willow-rings” surrounding numerous ponds. The soil moisture site is in a lowland between two ephemeral ponds. Here, the water table has been observed within 1 m of the ground surface. Annual precipitation is approximately 360 mm, of which 1/3 is snowfall, but is highly variable (Bam et al., 2019). Annual potential evaporation exceeds precipitation in the region, and annual open water evaporation is approximately 700 mm (Parsons et al., 2004). Mean January and July temperatures (1991-2018) are -16.2 and 17.7 ◦C, respectively.

The BERMS (Boreal Ecosystem Research and Monitoring Sites) study area is approximately 200 km northeast of Saskatoon, SK, in the Mid-Boreal Upland ecoregion, which is characterized by sub-humid climate and mixed coniferous and deciduous forest. The sites are located in three mature forest stands and include flux-towers and soil moisture monitoring sensors. Mean air temperature in January and July in nearby Waskesiu Lake, SK, for the period 1971-2000 are -17.9 and 16.2 ◦C, respectively; during the same period mean annual precipitation was 467 mm, 30% of which fell as snow (Barr et al., 2012).

The Old Aspen site (OAS) and surrounding landscape consists of hummocky terrain and trembling aspen overstory. The underlying geology is glacial till beneath a 10 cm organic layer and 30 cm silt loam mineral horizon. The water table is generally found 1 to 5 m below the ground surface (Barr et al., 2012). The Old Black Spruce site (OBS) has a shallow water table 0 to 1 m below the ground surface, with soil layers that comprise a 20-30 cm deep peat layer overlying poorly-drained sand (Barr et al., 2012). The Old Jack Pine (OJP) site is predominantly jack pine overstory in a well-drained sandy soil. The water table is at least 5 m below the surface at OJP (Barr et al., 2012).

	Prairie sites		**Forest sites**		
	Kenaston	**St. Denis National Wildlife Area**	**Old Jack Pine**	**Old Black Spruce**	**Old Aspen**
Location	51.382°N 106.416°W	52.208°N 106.093°W	53.916°N 104.690°W	53.987°N 105.117°W	53.629 °N 106.200°W
Elevation (m ASL)	596	557.5	579.3	628.9	600.6
Vegetation/ ground cover	Wheatgrasses (*Agropyron* sp.) and needle grasses (*Stipa* sp.)	Native prairie grasses, smooth brome (*Bromus inermis*), cattails (*Typha latifolia*)	Jack pine (*Pinus banksiana* Lamb) with lichen, exposed soil understory	Black spruce (*Picea mariana*) with exposed soil, moss, herbs understory	Trembling aspen (*Populus tremuloides*) with dense hazel understory
Vegetation Type	Grass	Grass, wetland riparian vegetation	Evergreen needle-leaf	Evergreen needle-leaf	Deciduous broad-leaf
Stand density (trees ha^{-1})			1320	4330	980
Canopy height			14 m	11 m	21 m
Soil Layer	Mineral soil: loam to clay loam	Mineral soil: dark brown loam to gravelly-loam soils	Mineral soil: Fine sand	Mineral soil: sandy clay Organic soil: peat	Mineral soil: loam to clay Organic soil: litter, fibric and humic
Drainage	Imperfect to poor	Imperfect to poor	Very well	Imperfect to poor	Well to moderately well

Table 1. Field site characteristics (Pan et al., 2017; Bam et al., 2019; Barr et al., 2012).

FIG 1 HERE

Figure 1. Field site locations (circles) and major cities (stars) in Saskatchewan, Canada. Ecoregions of central Saskatchewan are shown in shading, each aligning with different soils, landforms, and associated plant communities (Ecological Stratification Working Group, 1996).

2.3 Instrumentation and data

In this study, meteorological data were used to drive the model and soil moisture data were used to assess the model performance and constrain the simulated fluxes. The specific instruments and measurement heights/depths are summarized in Table 2.

Variable	**Kenaston**	**SDNWA**	**OJP**	**OBS**	**OAS**
Volumetric water content (m^3/m^3) Depths (cm bgl)	Stevens HydraProbe sensors 0, 20, 50, 75, 100, 130, 160	Stevens HydraProbe sensors 0, 5, 20, 50, 100, 200, and 300	CS615 water content reflectometers 0–15, 15–30, 30–60, 60–90, 90–120, and 120-150	CS615 water content reflectometers 2.5, 7.5, 22.5, 45 and 60-90	Time domain reflectometers 0–15, 15–30, 30–60, 60–90, and 90–120
Air temperature (°C) and Relative humidity (%)	Vaisala HMP45C 4 m above ground	Vaisala HMP45C 1.5 m above ground	Vaisala HMP45C 14 m above canopy	Vaisala HMP45C 14 m above canopy	Vaisala HMP45C 16 m above canopy
Wind speed (m/s)	CS CSAT3 tri-axial sonic anemometer 8 m above ground	CS CSAT3 tri-axial sonic anemometer 10 m above ground	CS CSAT3 tri-axial sonic anemometer 29 m above ground	Gill R3 or R3-50 tri-axial sonic anemometer 26 m above ground	Gill R3 or R3-50 tri-axial sonic anemometer 38 m above ground
Solar radiation (W/m^2)	Kipp and Zonen CNR1 four-component radiometer	Kipp and Zonen CNR4 four-component radiometer	Kipp and Zonen CM11 paired pyranometer 9 - 14 m above canopy	Kipp and Zonen CM11 Paired pyranometer 9 - 14 m above canopy	Kipp and Zonen CM11 paired pyranometer 10 - 16 m above canopy
Longwave radiation (W/m^2)	Kipp and Zonen CNR1 four-component radiometer	Kipp and Zonen CNR4 four-component radiometer	PIR paired pyrgeometer 9 - 14 m above canopy	PIR paired pyrgeometer 9 - 14 m above canopy	PIR paired pyrgeometer 10 - 16 m above canopy
Precipitation (mm)	Geonor T200-B weighing gauge	Geonor T200-B weighing gauge	Belfort 3000 accumulating	Belfort 3000 accumulating	Belfort 3000 accumulating

			gauge	gauge	gauge

Table 2. Instrumentation at field sites (Pan et al., 2017; Barr et al., 2012; Bam et al., 2019)

The driving data are plotted in Figure 2, which shows the interannual, seasonal and diurnal variation in these datasets. Precipitation is measured at each site with a weighing precipitation gauge that captures both rainfall and snowfall. It is notable that the two prairie sites, Kenaston and SDNWA, have higher windspeeds, which is because the forest sites are more sheltered. As a result, the prairie sites are subject to significant redistribution of snow laterally by the wind, and the snowfall observations from the gauges are not representative of the snow on the ground, which could be higher or lower than the snowfall (Pan et al., 2017). To correct for this, snow survey data from the prairie sites, which measure the peak snow on the ground prior to melt, were used to adjust the snowfall data such that the snow on the ground simulated by MESH would match the snow survey observations. For each winter (typically November to February), every snowfall event was scaled by a constant correction factor that was determined for each year by trial and error. The precipitation data in Figure 2 have been corrected in this way for the prairie sites. Precipitation data at the forest sites were not modified.

FIG 2 HERE

Figure 2. Driving data from meteorological stations. All variables are plotted as average values per time increment dt, where dt is indicated in the plot titles for each column.

The calibration/validation soil moisture data are shown in Figure 3. Soil moisture observations were available at different depths at different sites (Table 2). We used these data to estimate the average volumetric water content in each of the soil depth increments that correspond to the three layers in the model (i.e. 0 – 0.1 , 0.1 – 0.35 and 0.35 – 1.6 m depths), as shown in Figure 3. The data are considered high quality, with minimal gaps or data quality problems. Soil freezing is clearly evident at the prairie sites (Kenaston and SDNWA), where the water content in the first two layers drops rapidly at the start of the winter, and rises rapidly in the spring – this is because the water turns to ice, which is not detected by the dielectric probes. The water content in layer 3 at SDNWA is much higher than at Kenaston, which is because the water table is much closer to the ground surface at SDNWA, and hence the soils are not as free-draining. The same is true of the OBS sites, which is in a low-lying part of the landscape where again the water table is close to the ground surface, and the upper layer has a high organic matter content and a high porosity, with a lot of variation in storage. The OJP site has very sandy soil, which has poor water retention properties, and has a deep water table, and hence the water contents are consistently low, with a small range of variation seasonally. The OAS site has relatively fine grained mineral soils that drain reasonably well.

FIG 3 HERE

Figure 3. Soil volumetric liquid water content observations from the five field sites, averaged over the three model layer depth increments. The shaded cyan areas represent times of the year when the observed soil temperature in layer 1 was below zero °C.

2.4 Model description

MESH (Modélisation Environnementale communautaire - Surface Hydrology) is a physically based hydrological land-surface scheme built by Environment and Climate Change Canada (ECCC) (Pietroniro et al. 2007). MESH is a configuration of the Modelling the Environment Community (MEC) surface model that couples the Canadian Land Surface Scheme (CLASS) (Bartlett at al., 2003, Verseghy, 2017) with hydrological routing scheme WATFLOOD (Kouwen 1988, recently described in Pomeroy, 2016). MESH relies on a mosaic of Group Response Unit's (GRUs) to represent the heterogeneity and hydrological processes of the landscape. A GRU is a grouping of hydrological response units with similar soil and/or vegetation attributes (Xu et al., 2017). In this study, we used a single grid cell with a single GRU to represent the point scale vertical processes. MESH employs CLASS to simulate vertical water fluxes and energy balances for each GRU (Verseghy, 2017). CLASS divides the soil column into three layers and the vertical movement of water between each soil layer is governed by a finite difference solution of one-dimensional Richards' equation for unsaturated flow in porous media (Soulis, 2000). The hydraulic properties in CLASS adopt the Clapp and Hornberger (1978) model to determine the relationship between hydraulic conductivity, K (m/d), matric potential, ψ (m), and soil moisture, where

$$\psi = \psi_s \left(\frac{\theta}{\theta_p} \right)^{-b} \tag{8}$$

$$K = K_s \left(\frac{\theta}{\theta_p} \right)^{2b+3} \tag{9}$$

where ψ_s (m) is the saturated matric potential, θ_p is the saturated water content, K_s (m/d) is the saturated hydraulic conductivity, and b (-) is a shape parameter. Note, temperature corrections are applied to K_s to account for changes in the viscosity of water (Verseghy, 2017, p. 122), and in frozen conditions an additional impedance factor is applied to reduce K_s to account for the ice blockages in the pore space (Verseghy, 2017, p. 146). The parameters in Equations 8 and 9 are normally determined using the empirical pedotransfer functions of Cosby et al. (1984), whereby

$$\theta_p = \frac{-0.126 X_S + 48.9}{100.0} \tag{10}$$

$$b = 0.159 X_C + 2.91 \tag{11}$$

$$\psi_s = 0.01 e^{(-0.0302 X_S + 4.33)} \tag{12}$$

$$K_s = 0.60960384 e^{(0.0352 X_S - 2.035)} \tag{13}$$

Where X_S (%) and X_C(%) are the percentage sand and clay, respectively, of the soil in a particular layer. Note, in Equation 13 K_s is given in units of m/d. The pedotransfer function relationships and the resulting hydraulic properties are shown in Figure 4.

FIG 4 HERE

Figure 4. The pedotransfer functions that define soil hydraulic properties as a function of sand and clay content, and $\psi(\theta)$ and $K(\theta)$ relationships used in CLASS for three example soil textures.

The way that the fluxes in Equation 1 are calculated in CLASS are briefly described in Table 3.

Flux	***Calculation description***
Infiltration	Rainfall and throughfall on the ground are combined with snowmelt to form the potential infiltration flux; the infiltration capacity is calculated by a Green-Ampt model and depends on the soil hydraulic properties; water that cannot infiltrate forms ponding on the ground-surface, where it may later infiltrate unless the surface ponding capacity is exceeded, in which case the excess water forms overland runoff.
Drainage	The bottom of the soil profile, i.e. the base of soil layer 3, has a free drainage boundary condition, (Soulis et al., 2000), where $D=\phi K_3(\theta_3)$, where ϕ is a drainage parameter that restricts free drainage (0-1).
Soil evaporation	Soil evaporation is the sum of evaporation from bare soil and evaporation from soil below the canopy, both of which are driven by a humidity gradient. The humidity at the soil surface, and hence the soil evaporation flux, is reduced as the water content in layer 1 drops below field capacity, and soil evaporation is limited by the availability of water in the top soil layer and surface ponding (Sun and Verseghy, 2019).
Transpiration	Transpiration is extracted from all soil layers, weighted by the root density in each layer, as long as the liquid water content is greater than 0.04. The flux rate depends on the leaf-to-air humidity gradient, the boundary layer resistance and the canopy resistance, which in turn is related to leaf stomatal resistance and leaf area index. The stomatal resistance has a reference value, $r_{s,min}$, and is modified as a function of incoming solar radiation, vapour pressure deficit, soil moisture in the wettest layer, and air temperature. Through the stomatal conductance term transpiration rates are reduced exponentially as the soil suction in the wettest layer reduces below ψ_s, i.e. as the soil moisture reduces (Verseghy, 2017, Sun and Verseghy, 2019).

Table 3. Description of soil flux calculations in CLASS

2.5 Monte Carlo simulations

To investigate how information from soil moisture observations constrains simulated fluxes, we apply a simple Monte Carlo approach. We allow for uncertainty in the model parameters by randomly sampling parameter values from a uniform (or log-uniform) distribution. We generate 10,000 parameter combinations and run the model with each parameter set over a two-year calibration period. The performance of each realization is determined by calculating ϵ_j, the root mean squared error (RMSE) of the cumulative change in liquid water content (equation 6), for each depth, j, as in equation 14, and then averaging these over the three layers, as in equation 15

$$\epsilon_j = \sqrt{\frac{\sum_{i=1}^{n} \left(\Theta_{o(i,j)} - \Theta_{s(i,j)} \right)^2}{n}} \tag{14}$$

$$\epsilon_T = \sum_{j=1}^{3} \frac{\epsilon_j}{3} \tag{15}$$

where $\Theta_{o(i,j)}$ and $\Theta_{s(i,j)}$ are the cumulative change in volumetric liquid water content from the observations and simulations, respectively, at time index i and depth index j, $n$is the number of points in time, and ϵ_T is the overall performance metric, with units of volumetric water content (m^3/m^3). The layer average RMSE was used, so that the performance in each layer would have an equal weighting – if the total storage was used the performance would be biased towards the 3rd soil layer, as this is much thicker (1.25 m) than the 1st (0.1 m) and 2nd (0.25 m) layers.

As described in section 2.3, the CLASS model is typically run using the Cosby et al (1984) pedotransfer function, which determines the soil hydraulic properties from soil texture – specifically sand percentage, X_S and clay percentage X_C. We perform two separate calibration experiments here: the first using these pedotransfer functions samples the parameters X_S and X_C for each soil layer – i.e. six free parameters; the second does not use the pedotransfer functions, and samples the four hydraulic properties (θ_p, b, ψ_s, K_s) directly for each soil layer – i.e. twelve free parameters. Hereafter we describe these two experiments as the texture-based calibration and hydraulic properties-based calibration. In addition to the six/twelve soil parameters, we also sample four additional parameters that are understood to have a strong control on the simulated fluxes (Nazarbakhsh et al., 2020): the minimum and maximum annual leaf area index, L_{min} and L_{max} (-), the minimum stomatal conductance, $r_{s,min}$ (s/m) and a drainage index, ϕ (-) (Table 4). To prevent the random parameter sampling procedure from generating $L_{min} > L_{max}$ we instead sample L_{max} and the factor f_L such that $L_{min} = min\left(L_{max}, L_{max} f_L\right)$. f_L is randomly sampled from a uniform distribution between 0.5 – 1.25, which ensures that around one-third of combinations will have $L_{min} = L_{max}$. For the texture sampling, we need to specify ranges in sand (X_S¿, clay (X_C) and silt (X_L) and ensure that the sum of the three equals 100%, which is done by randomly sampling X_S, X_C and X_L from uniform distributions (see ranges in Table 4), and then rescaling each by the same scale factor such that $X_S + X_C + X_L = 100$. The texture-based and hydraulic properties-based calibrations sample 10 and 16 free parameters, respectively. The parameter ranges considered for each site were based on knowledge of the soils and vegetation characteristics at each site, and are shown in Table 4.

	Kenaston	**SDNWA**	**OJP**	**OBS**	**OAS**
Texture-based calibration parameters:					
X_S (%)	$20-70$	$20-70$	$45-100$	$20-70$	$20-70$
X_L (%)	$30-80$	$30-80$	$0-55$	$30-80$	$0-50$
X_C (%)	$0-60$	$0-60$	$0-55$	$0-60$	$5-35$
Hydraulic properties-based calibration parameters:					
θ_p (-)	$0.2-0.5$	$0.2-0.5$	$0.1-0.4$	$0.2-0.7$	$0.2-0.5$
b (-)	$3-18$	$3-18$	$3-18$	$3-18$	$3-18$
ψ_s (m)	$0.05-3$	$0.05-3$	$0.05-3$	$0.05-3$	$0.05-3$
K_s (m/s)	$10^{-7}-10^{-4}$	$10^{-7}-10^{-4}$	$10^{-7}-10^{-4}$	$10^{-7}-10^{-4}$	$10^{-7}-10^{-4}$
Additional parameters:					
L_{max} (-)	$0.5-3$	$0.5-3$	$2-4$	$2-4$	$1-4$
f_L (-)	$0.5-1.25$	$0.5-1.25$	$0.5-1.25$	$0.5-1.25$	$0.5-1.25$
$r_{s,min}$ (s/m)	$50-300$	$50-300$	$50-300$	$50-300$	$50-300$
ϕ (-)	$0-1$	$0-1$	$0-1$	$0-1$	$0-1$

Table 4. Parameter ranges considered. All parameters are sampled from a uniform distribution except K_s which is sampled from a log-uniform distribution.

The models were all initialized on 1st August 2013, and the calibration period ends on 30th September 2015 (two complete hydrological years) while the validation period ends on 30th September 2017 (two additional complete hydrological years). Initializing the models in August eliminates the need to specify initial soil ice content or the initial snowpack. The initial water content of the model was based on observed estimates of the initial saturation, combined with the current realization value of θ_p, i.e.

$$\theta_{j,ini} = \frac{\theta_{O,j,ini} - min\left(\theta_{O,j}\right)}{max\left(\theta_{O,j}\right) - min\left(\theta_{O,j}\right)} \theta_{p,j} \quad (16)$$

where θ_O is the observed liquid volumetric water content, and subscripts j is the depth index and ini is the initial time. This approach ensures that the initial relative saturation is always the same, regardless of the porosity value that was sampled randomly in the Monte Carlo simulation.

For the validation run, only the 30 best ranked parameter sets were considered (due to the excessive computational expense of running 10,000 models for a 4 year period). We seek to validate the model validation performance with the Ω observations, and to explore the uncertainty in the model fluxes associated with these runs.

3. Results and Discussion

Figure 5 shows the performance of the model at each of the five sites, for the two sets of Monte Carlo runs: i) sampling the soil texture parameters; and ii) sampling the soil hydraulic properties. The results are shown in units of the cumulative change in storage in the profile (i.e. Ω¿. In the calibration period, the range of Ω from all 10,000 simulations is shown, along with the range from the best 30 simulations, with the ranking based on ϵ_T (equation 14 and 15). Dotty plots for each simulation are provided in the Appendix. The model performance is variable between the different sites, and between the texture based and hydraulic properties-based calibration. The rise in storage in the spring (March-April) is characteristic of seasonally frozen soils, and is a complex combination of snowmelt infiltration and soil thaw (whereby ice becomes liquid water, leading to an apparent observed increase in liquid water content, which may or may not be associated with an actual increase in total, that is ice plus liquid, water content). The timing of this rise is delayed in all models, suggesting there may be some limitations with either the snowmelt, the infiltration flux or the soil thawing. However, the magnitude of the rise, and the overall seasonal changes in storage are generally well captured in the models. The worst performance is at the OJP field site, with the texture-based calibration. The reason this is poor is because the sandy soils at OJP have a very small range of moisture variation, never rising as high as 0.2 (Figure 3). The texture-based properties only allow for a variation in θ_p, the saturated water content, of between 0.36 and 0.49, as shown in Figure 4 (top left), and therefore the model always over-estimates the range of variation of water content. This restriction is removed using the hydraulic properties-based calibration. This improvement in performance using the hydraulic properties-based calibration is true for all field sites. This is because the pedotransfer functions used in the texture-based calibration artificially constrain the agility of the model, as discussed by Mendoza et al (2015). To elaborate, when using pedotransfer functions, for a given parameter value of θ_p there will always be a unique parameter value of K_s, and there is no way to explore deviations in this combination. With the hydraulic properties-based calibration applied here, this constraint is removed, and θ_p and K_s are treated as completely independent of one another. These two cases therefore represent two extreme possibilities in terms of the possible parameter space that is explored by the model.

FIG 5 HERE

Figure 5. Model calibration and validation performance in terms of cumulative change in storage over the profile (mm) plotted for all 10,000 runs and the best 30 runs, ranked by ϵ_T

Figure 6 shows box plots of each of the soil water fluxes (Equation 1), plotted as annual fluxes over the calibration period of the model, for both all simulations and the best 30. In the box plots, the whiskers represent the complete range of the data, i.e. minimum to maximum data points, which is taken as a simple measure of the overall uncertainty. The range of the “all” plots represents the uncertainty of the simulated flux in the absence of any constraints, while the range of the “best” plots represents the uncertainty of the simulated flux when constrained by observed changes in soil moisture (as in Figure 5 and the dotty plots in the appendix). If we consider each of the 30 best realizations as equally credible, then the spread in the fluxes from these models is attributable to equifinality – that is, different parameter sets that provide the same performance in one metric, but provide different outcomes in terms of some other state or flux. The texture-based calibration, which had a lower performance, appears to be slightly better at constraining the fluxes than the hydraulic properties-based calibration. For example, at Kenaston, the range of uncertainty in soil evaporation, E, is reduced from 300 mm/year (unconstrained) to 176 mm/year (constrained) using soil texture-based calibration. Using the hydraulic properties-based calibration, uncertainty was reduced from 394 mm/year (unconstrained) to 327 mm/year (constrained). We consistently see higher uncertainties when we calibrate the hydraulic properties rather than the texture, which is expected because there are more degrees of freedom in the hydraulic properties-based calibration. The infiltration flux has the highest value and the lowest uncertainty of all of the fluxes, though the uncertainty increases markedly for the hydraulic properties-based calibration. This is because the infiltration capacity of the soil depends on the hydraulic properties directly, and these properties are overly restricted in the texture-based calibration. At different sites for the constrained (best) simulations the relative size of uncertainty in the soil evaporation, transpiration and drainage does vary, but is in almost all cases too large to be useful. The possible exception to this is at OBS for the texture-based calibration – where the fluxes are most effectively constrained. Here the median/uncertainty range values for the constrained fluxes are: I 443/27 mm/year; E 90/36mm/year; T 347/39 mm/year; D 0/1 mm/year. These uncertainties are perhaps low enough that the model predictions could be considered useful, but note that we are only reporting here the uncertainty based on soil moisture observations, and an assessment of the performance of these fluxes against flux observations is still needed.

FIG 6 HERE

Figure 6. Box plots of annual modelled soil fluxes including infiltration, I, soil evaporation, E, transpiration, T, and drainage, D, for all 10,000 runs and the best 30 runs, ranked by ϵ_T. The whiskers represent the entire range of the data (i.e. minimum to maximum) and the boxes represent the 1st, 2nd and 3rd quartiles.

Figure 7 shows cumulative fluxes of evapotranspiration (which includes soil evaporation plus transpiration plus canopy evaporation and snow sublimation), runoff and drainage, for both the calibration and validation period. As in Figure 6, this plot shows that soil moisture overall is acting as a poor constraint on all of these fluxes. In the prairie sites (Kenaston and SDNWA) we see evapotranspiration is the dominant flux; simulated runoff is associated with the melt period; and drainage is relatively small but highly uncertain. At OJP we see the largest uncertainties, particularly in the drainage fluxes that could be anywhere from zero to > 200 mm/year. At OBS, where again the uncertainties are lowest overall, evaporation is relatively well constrained, but drainage and runoff are still quite uncertain, especially in

2017. At OAS, the evaporation is somewhat well constrained, runoff is small, but drainage is highly uncertain.

FIG 7 HERE

Figure 7. Simulated cumulative fluxes from the unconstrained (all 10,000) and constrained (best 30) model runs for the calibration and validation periods.

4. Conclusions

We have shown that the MESH/CLASS model is capable of simulating the changes in soil moisture within a 1.6 m deep profile at five diverse prairie/forest field sites relatively well, albeit with some limitations associated with the timing of the rise in liquid water content during the spring melt period. However, this relatively good performance at simulating water content did not result in well constrained predictions of hydrological fluxes. From a simple and qualitative assessment of Figure 6 and 7 we conclude that the information content in soil moisture data is relatively low. The texture-based calibration is apparently slightly better at constraining the fluxes than the hydraulic properties-based calibration, which demonstrates that uncertainties in models can be reduced by embedding assumptions within the models. However, this also requires that these embedded assumptions are reasonable. In this case, the embedded assumption is that the hydraulic properties can be determined from pedotransfer functions. Since we see in Figure 5 that doing this degrades the performance of the model in reproducing observed changes in soil moisture storage, this is not deemed a reasonable assumption in this case; the reduction in uncertainty is considered misleading. We therefore conclude that the very wide uncertainty bounds predicted by the hydraulic properties-based calibration are in fact a more accurate reflection of the true uncertainty in the system. It is important to recognize that we are only looking at one form of uncertainty here: uncertainty associated with parameters. There are still other sources of uncertainty, most importantly uncertainty in the input data and uncertainty in the model structure, that are not addressed here. We conclude that soil moisture observations, while valuable in combination with other data, on their own are inadequate for calibration of land surface models. Reproducing the cumulative change in soil moisture storage is a necessary but insufficient criterion for model success. Uncertainty is reduced by bringing in more information. If we had knowledge of the hydraulic properties, for example from direct field observations, we would have a reduction in the parametric uncertainty, resulting in less spread in the simulated fluxes. However, representative parameter values are hard to obtain. Another valuable source of information comes from observations of fluxes, which can be used to better constrain the model, and we recommend that multi-objective calibration, using ET estimates from flux towers, will improve the situation.

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Data Availability Statement

On acceptance of the paper, all field data used will be uploaded to the Canadian Federated Research Data Repository at: https://www.frdr-dfdr.ca/repo/ and assigned a DOI number.

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Appendix: Parameter identifiability

Figures A1 – A10 present the dotty plots for the texture-based and hydraulic properties-based calibrations for each of the five sites. On the x-axes are plotted the parameter values (refer to sections 2.4 and 2.5 for symbols), and on the y-axes are plotted the objective function values, i.e. ϵ_T (Equations 14 and 15). For all sites, we see that the parameter identifiability is better for the texture-based calibration than for the hydraulic properties-based calibration. For the hydraulic properties-based calibration, the parameters are often completely unidentifiable. One notably exception is at OJP (Figure A6) where the porosity is identifiable and low values are clearly preferred. This poor identifiability is associated with the equifinality in the model, and further shows that additional observations are needed to constrain the parameters.

FIG A1 HERE

Figure A1. Dotty plots for the Monte Carlo runs at Kenaston using the texture based soil parameterisation. RMSE is the root mean squared error between the observed and simulated cumulative change in water content for the unfrozen period, averaged between the three layers, in units of volumetric water content.

FIG A2 HERE

Figure A2. Dotty plots for the Monte Carlo runs at Kenaston using the hydraulic properties based soil parameterisation. RMSE is the root mean squared error between the observed and simulated cumulative change in water content for the unfrozen period, averaged between the three layers, in units of volumetric water content.

FIG A3 HERE

Figure A3. Dotty plots for the Monte Carlo runs at St Denis using the texture based soil parameterisation. RMSE is the root mean squared error between the observed and simulated cumulative change in water content for the unfrozen period, averaged between the three layers, in units of volumetric water content.

FIG A4 HERE

Figure A4. Dotty plots for the Monte Carlo runs at St Denis using the hydraulic properties based soil parameterisation. RMSE is the root mean squared error between the observed and simulated cumulative change in water content for the unfrozen period, averaged between the three layers, in units of volumetric water content.

FIG A5 HERE

Figure A5. Dotty plots for the Monte Carlo runs at OJP using the texture based soil parameterisation. RMSE is the root mean squared error between the observed and simulated cumulative change in water content for the unfrozen period, averaged between the three layers, in units of volumetric water content.

FIG A6 HERE

Figure A6. Dotty plots for the Monte Carlo runs at OJP using the hydraulic properties based soil parameterisation. RMSE is the root mean squared error between the observed and simulated cumulative change in water content for the unfrozen period, averaged between the three layers, in units of volumetric water content.

FIG A7 HERE

Figure A7. Dotty plots for the Monte Carlo runs at OBS using the texture based soil parameterisation. RMSE is the root mean squared error between the observed and simulated cumulative change in water content for the unfrozen period, averaged between the three layers, in units of volumetric water content.

FIG A8 HERE

Figure A8. Dotty plots for the Monte Carlo runs at OBS using the hydraulic properties based soil parameterisation. RMSE is the root mean squared error between the observed and simulated cumulative change in water content for the unfrozen period, averaged between the three layers, in units of volumetric water content.

FIG A9 HERE

Figure A9. Dotty plots for the Monte Carlo runs at OAS using the texture based soil parameterisation. RMSE is the root mean squared error between the observed and simulated cumulative change in water content for the unfrozen period, averaged between the three layers, in units of volumetric water content.

FIG A10 HERE

Figure A10. Dotty plots for the Monte Carlo runs at OAS using the hydraulic properties based soil parameterisation. RMSE is the root mean squared error between the observed and simulated cumulative change in water content for the unfrozen period, averaged between the three layers, in units of volumetric water content.