

Promise and pitfalls of modeling grassland soil moisture in a free-air CO₂ enrichment experiment (BioCON) using the SHAW model



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ABSTRACT

Free-air carbon dioxide (CO₂) enrichment (FACE) experiments provide an opportunity to test models of heat and water flow under novel, controlled situations and eventually allow use of these models for hypothesis evaluation. This study assesses whether the United States Department of Agriculture SHAW (Simultaneous Heat and Water) numerical model of vertical one-dimensional soil water flow across the soil-plant-atmosphere continuum is able to adequately represent and explain the effects of increasing atmospheric CO₂ on soil moisture dynamics in temperate grasslands. Observations in a FACE experiment, the BioCON (Biodiversity, CO₂, and Nitrogen) experiment, in Minnesota, USA, were compared with results of vertical soil moisture distribution. Three scenarios represented by different plots were assessed: bare, vegetated with ambient CO₂, and similarly vegetated with high CO₂. From the simulations, the bare plot soil was generally the wettest, followed by a drier high-CO₂ vegetated plot, and the ambient CO₂ plot was the driest. The SHAW simulations adequately reproduced the expected behavior and showed that vegetation and atmospheric CO₂ concentration significantly affected soil moisture dynamics. The differences in modeled soil moisture amongst the plots were largely due to transpiration, which was low with high CO₂. However, the modeled soil moisture only modestly reproduced the observations. Thus, while SHAW is able to replicate and help broadly explain soil moisture dynamics in a FACE experiment, its application for point- and time-specific simulations of soil moisture needs further scrutiny. The typical design of a FACE experiment makes the experimental observations challenging to model with a one-dimensional distributed model. In addition, FACE instrumentation and monitoring will need improvement in order to be a useful platform for robust model testing. Only after this can we recommend that models such as SHAW are adequate for process interpretation of datasets from FACE experiments or for hypothesis testing.

Key Words: carbon dioxide, FACE experiment, soil water flow, vadose zone, vegetation

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INTRODUCTION

The increasing carbon dioxide (CO₂) concentration in the atmosphere has now passed 410 ppm (410 mg L⁻¹), which is 130 ppm (130 mg L⁻¹) higher than pre-industrial levels. Numerous studies are being conducted to investigate how these increases affect different aspects and components of the Earth system and how well numerical models can represent these impacts. Higher atmospheric CO₂ leads to a decrease in plant transpiration and an increase in water use efficiency by lowering stomatal conductance (Field *et al.*, 1995, 1997; Lee *et al.*, 2009; Adair *et al.*, 2011), consequently enhancing soil moisture storage (Drake *et al.*, 1997; Field *et al.*, 1997). Higher soil moisture in response to higher atmospheric CO₂ environments has been observed in open-top chamber experiments (Field *et al.*, 1997; Fredeen

et al., 1997; Nelson *et al.*, 2004; Dermody *et al.*, 2007) and free-air CO₂ enrichment (FACE) experiments (Adair *et al.*, 2011). The covariance has also been simulated in large ecosystem manipulation models (Grünzweig and Körner, 2001). However, less research has been conducted on the associated subsurface hydrologic processes (Ainsworth and Long, 2005).

In FACE experiments, the atmosphere in controlled plots are enriched with CO₂ (<http://www.bnl.gov/face/>) in order to investigate the effects of higher atmospheric CO₂. Such FACE experiments have been conducted for a number of years in many different ecosystems, but the focus has generally been on the response of plant communities, soil respiration, and microbes to changing conditions (Kimball *et al.*, 2002; Ainsworth and Long, 2005; Adair *et al.*, 2011).

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Comprehensive modeling of vertically-distributed soil moisture and energy balance in FACE experiments is seldom conducted. Using a year's data (2006) from a FACE experiment, the BioCON (Biodiversity, CO₂, and Nitrogen), Adair *et al.* (2011) showed that elevated CO₂ increased volumetric soil water content by 23% on average (113% maximum) and total water storage by 53% on average (182% maximum). They showed that the effect of CO₂ weakened at very low and high volumetric soil water content and at the end of the growing season, when plant activity declined. Also, during post-rainfall events, soil intervals at 0–17 and 42–59 cm depths stayed moist longer in the elevated CO₂ plots than in the ambient CO₂ plots. We expand on the work of Adair *et al.* (2011) by conducting more complex biophysical modeling and considering more recent data.

The overall question this study sought to address was: can the SHAW (Simultaneous Heat and Water) model replicate soil moisture dynamics in plots where vegetation is potentially responding to increasing atmospheric CO₂ concentration? In testing whether SHAW can adequately represent soil moisture dynamics, we also assessed two basic concepts: i) The presence of vegetation contributes to an increase in evapotranspiration and a decrease in soil moisture, and ii) higher atmospheric CO₂ concentrations lead to smaller evapotranspiration values and, consequently, to higher soil moistures. For the first concept, the hydrology of bare and vegetated soils was modeled and compared to each other, while for the second idea, the hydrology of vegetated soils at different atmospheric CO₂ concentrations was modeled and compared. The main point behind the assessment is that if a model such as SHAW succeeds in replicating the soil moisture dynamics and plant water uptake across different treatments in BioCON, then such models have explanatory value and can be used for mechanistic hydrologic-biophysical interpretation of the unique observations offered by a FACE site. These models may also be useful for providing complete spatially distributed, time-series information on soil moisture and fluxes in light of limited measurements in time and space.

The broader objective of this work was, therefore, to characterize and model soil moisture dynamics for different atmospheric CO₂ concentrations and plant presence to ultimately determine how each affects soil moisture simulations on grasslands of central Minnesota, USA. The BioCON experiment data and the SHAW model, which solves the Richards equation for unsaturated zone water flow coupled to a comprehensive energy balance model, are used for this evaluation.

METHODS

Description of the BioCON FACE site

The FACE experiments provide the ideal replicated environment of elevated atmospheric CO₂ around an ecosystem.

In the past, experimental manipulation of enriched concentrations of atmospheric CO₂ was possible only in growth chambers and greenhouses, all of which require containment. These containments alter the ecosystem's relationship to the natural environment, but the FACE setup largely overcomes this problem (Ainsworth and Long, 2005).

The BioCON experiment (Reich *et al.*, 2001b) is a FACE experiment that has been continuously run since 1997 (for more information, visit <http://www.biocon.umn.edu>) in the Cedar Creek Ecosystem Science Reserve in East Bethel, Minnesota (45°24' N, 93°11' E, 218 m above sea level). Mean annual precipitation (1982–2009) at the BioCON experiment site is 800 mm and summer is the wettest season of the year (Adair *et al.*, 2011). The BioCON experiment investigates plant community response to three key environmental variables: increased nitrogen, increased atmospheric CO₂, and decreased biodiversity (Reich *et al.*, 2001a, b, 2004, 2006; Adair *et al.*, 2011; Reich and Hobbie, 2013). The BioCON experiment consists of 371 plots (2 m × 2 m), arranged into six circular areas or "rings" that are 20 m in diameter. Three of the six rings are fumigated with CO₂-enriched air (*ca.* 560 ppm (560 mg L⁻¹) CO₂) during the day throughout the growing season and the remaining rings have ambient atmospheric CO₂ levels (Adair *et al.*, 2009). Elevated CO₂ levels were set to approximately 180 ppm (180 mg L⁻¹) higher than the ambient levels at the start of the experiment and only during the daytime when plants are photosynthesizing. Each of the 371 plots was randomly planted with 0, 1, 4, 9, or 16 species of herbaceous perennial prairie taxa, either native or naturalized to the Cedar Creek area. All sixteen plant species belonged to one of the four following functional groups: C4 grasses, C3 grasses, nitrogen-fixing legumes (C3), or non-nitrogen-fixing herbaceous plants (C3). There were four plant species of each of the four functional groups available for planting (Reich *et al.*, 2001b). The studies at BioCON have investigated the effects of treatments on different plant species' photosynthetic responses (Ellsworth *et al.*, 2004; Crous *et al.*, 2010; Lee *et al.*, 2011). The soils in the region are sandy and primarily classified as Nymore loamy sand, a mixed, frigid Typic Udipsamment, following the United States Natural Resources Conservation Service classification, with low soil organic matter and nitrogen (Dijkstra *et al.*, 2006).

In-situ soil moisture measurements

The field soil moisture was measured in all of the plots by BioCON researchers at four 17-cm intervals (0–17, 22–39, 42–59, and 83–100 cm) multiple times during each growing season from 2007 to 2012. The soil moisture data from a few plots were analyzed and used for comparison with the SHAW simulations.

A Trime FM3 Time Domain Reflectometry (TDR) system, version P3 with a T3 tube-access probe (IMKO Mi-

cromodultechnik GmbH, Ettlingen, Germany), was used for soil moisture measurements (Adair *et al.*, 2011). The TDR measurements were calibrated according to calculated volumetric soil water contents from coincident gravimetric soil moisture and bulk density measurements (Adair *et al.*, 2011). Only a single calibration was done as, according to Dijkstra *et al.* (2006), “Soils (Argic Udipsamments) in this nearly level area are very homogenous, sandy (93% sand, 3% silt, and 4% clay), and poor in soil organic matter.” The volumetric water content measuring range of the instrument was 0.0–0.6 m³ m⁻³. Its measuring accuracy was 0.02 m³ m⁻³ in the 0.0–0.4 m³ m⁻³ range. Due to the measuring accuracy of the equipment, all water content measurement values smaller than or equal to 0.02 m³ m⁻³ were not considered in model performance evaluations.

Soil moisture and energy balance modeling with SHAW

We assessed and used the SHAW model for the hydrologic-biophysical modeling of each of the three plot treatments (Flerchinger and Saxton, 1989a, b; Flerchinger, 2000; Flerchinger *et al.*, 2012). The SHAW model is a vertical one-dimensional heat and water transport numerical model for the soil-plant-atmosphere continuum. It simulates heat, water, and solute transfer through plant cover, dead plant residue, snow, and soil (Flerchinger and Pierson, 1991, 1997). The ability of SHAW to model the soil-plant-atmosphere continuum has been demonstrated in several studies and the reader is referred to these studies for further details and additional examples of its applications (Flerchinger and Pierson, 1997; Wang *et al.*, 2010). Meteorological conditions and soil hydraulic parameters are necessary input parameters. The iterative Newton-Raphson technique is used to numerically solve the implicit finite-difference energy and water balance equations for each time step (Flerchinger and Saxton, 1989a).

The SHAW model Version 3.0 (Flerchinger, 2013) was selected for these detailed small-scale hydrologic simulations because it allows for plant-water uptake and uses a water and energy balance approach to represent freeze-thaw processes (Flerchinger and Saxton, 1989a), which occur at BioCON. The model was parameterized using a combination of field and laboratory estimates of soil properties. The following sections describe the boundary conditions and some important equations used in the model. More detailed information on the components of the model can be found in its manual (Flerchinger, 2000).

Soil water flux modeling

The SHAW model solves the modified Richards equation for water flow in the unsaturated zone. This equation takes into account freezing and thawing of the soil (Flerchinger and Saxton, 1989a) and reads as:

$$\frac{\partial \theta_l}{\partial t} + \frac{\rho_i}{\rho_l} \frac{\partial \theta_i}{\partial t} = \frac{\partial}{\partial z} \left[K \left(\frac{\partial \Psi}{\partial z} + 1 \right) \right] + \frac{1}{\rho_l} \frac{\partial q_v}{\partial z} + U \quad (1)$$

where θ_l is the volumetric liquid water content (m³ m⁻³), θ_i is the volumetric ice content (m³ m⁻³), ρ_i is the density of ice (kg m⁻³), ρ_l is the density of liquid water (kg m⁻³), t is the time (s), z is the soil depth (m), K is the unsaturated hydraulic conductivity (m s⁻¹), Ψ is the soil matric potential (m), q_v is the vapor flux through the soil (kg m⁻² s⁻¹), and U is the sink term representing root water extraction (m³ m⁻³ s⁻¹).

The SHAW model calculates the energy and water fluxes at the land surface based on inputs of daily or hourly weather data of air temperature, wind speed, relative humidity, precipitation, and total solar radiation measured on a horizontal surface. The energy balance at the surface is:

$$R_n - H - L_v E - G = 0 \quad (2)$$

where R_n is the net radiation (W m⁻²), H is the sensible heat flux (W m⁻²), L_v is the latent heat of evaporation (J kg⁻¹), E is the total evapotranspiration from the soil surface and plant canopy (kg m⁻² s⁻¹), and G is the ground heat flux (W m⁻²) (Flerchinger and Saxton, 1989a).

The fluxes through the one-dimensional vertical soil-plant-atmosphere system are computed for each time step by a finite-difference approximation between model nodes. Adjustments for precipitation, snowmelt, settling of the snowpack, interception, and infiltration are made at the end of each time step (Flerchinger and Saxton, 1989a). Evaporation from the soil or residue surface is computed directly from the gradient in vapor density between the surface and the bottom canopy node (Flerchinger and Pierson, 1997).

Water flux through the plant residue is described by the following equation:

$$\frac{\partial \rho_v}{\partial t} = \frac{\partial}{\partial z} \left(K_v \frac{\partial \rho_v}{\partial z} \right) + \frac{\partial}{\partial z} \left(\frac{h_r \rho'_{vs} - \rho_v}{r_h} \right) \quad (3)$$

where ρ_v is the vapor density within the residue layer (kg m⁻³), K_v is the convective vapor transfer coefficient within the residue (m s⁻¹), h_r is the relative humidity within the residue elements, ρ'_{vs} is the saturated vapor density at the temperature of the residue elements, and r_h is the resistance (s m⁻¹).

Water flow through plants is physically dependent on the soil-plant-atmosphere continuum, as plants draw water stored in the soil and transpire it through the stomata. This flux is regulated by atmospheric demand but also by resistances directly related to the soil, roots, plant xylem, and leaf water potential. It is calculated according to the equation below (Flerchinger and Pierson, 1997):

$$T_r = \sum_{m=1}^{NS} \frac{\Psi_{s,m} - \Psi_x}{r_{r,m}} = \sum_{i=1}^{NC} \frac{\Psi_x - \Psi_{l,i}}{r_{l,i}}$$

$$= \sum_{i=1}^{NC} \frac{\rho_{vs,i} - \rho_{v,i}}{r_{s,i} + r_{h,i}} L_i \quad (4)$$

where T_r is total transpiration rate ($\text{kg m}^{-2} \text{s}^{-1}$) for a given plant species, $\Psi_{s,m}$ is the water potential (m) in layer m of the soil, Ψ_x is the water potential (m) in the plant xylem, $\Psi_{l,i}$ is the water potential (m) in the leaves of canopy layer i , NS is the number of the soil layer, NC is the number of the canopy layer, $r_{r,m}$ is the resistance to water flow ($\text{m}^3 \text{s kg}^{-1}$) through the roots of layer m and xylem up to location x , $r_{l,i}$ is the resistance to water flow ($\text{m}^3 \text{s kg}^{-1}$) through the xylem above location x and through the leaves of layer i , L_i is the leaf area index within canopy layer i , $\rho_{vs,i}$ is the vapor density within the stomatal cavities, $\rho_{v,i}$ is the vapor density of the air within the canopy layer, $r_{s,i}$ is the stomatal resistance (s m^{-1}), and $r_{h,i}$ is the resistance to convective transfer (s m^{-1}).

Water flow within the plant is dependent mainly on the stomatal resistance (r_s), typically the largest of the above-mentioned resistance variables:

$$r_s = r_{so} \left[1 + \left(\frac{\Psi_l}{\Psi_c} \right)^n \right] \quad (5)$$

where r_{so} is the stomatal resistance with no water stress (m s^{-1}), Ψ_c is the critical leaf water potential (m), and n is an empirical coefficient (Flerchinger and Pierson, 1991).

Parameterization and boundary and initial conditions of the model

The main boundary conditions for the system are temperature and soil water potential at the lower boundary and daily or hourly weather conditions at the upper boundary (Flerchinger and Pierson, 1997). The initial conditions for soil temperature and water content at each node need to be specified. The initial soil water content and temperature for the simulations were based on field measurements and data from the Cedar Creek weather station.

Meteorological information is necessary for forcing the energy balance model and also for defining mass boundary conditions. Initially, we intended to use weather data from the Cedar Creek Ecosystem Science Reserve weather station. Unfortunately, due to malfunctions, data from the station had several gaps and inconsistencies, making its use limited. Therefore, we used hourly National Aeronautics and Space Administration (NASA) Land Data Assimilation Systems (NLDAS) Phase 2 Forcing File A data for the $(1/8)^\circ$ -wide cell containing the study site.

Since 1979, NLDAS-2 data are available for the continental United States. Precipitation is calculated based on a temporal disaggregation of a gauge-only Climate Prediction Center (CPC) analysis of daily precipitation. The other

weather parameters were obtained from the National Centers for Environmental Prediction (NCEP) North American Regional Reanalysis (NARR) based on NCEP data, models, data assimilation systems, and additional datasets (Mesinger *et al.*, 2006). For our study period (2007–2012), the average annual precipitation in the region was 735 mm and the air temperature was 8.3°C . The average January and July air temperatures were -10.6 and 24.8°C , respectively (Fig. 1). In addition to hourly air temperature ($^\circ\text{C}$) and precipitation (mm), similar time-series for wind speed at 10-m height (m s^{-1}), relative humidity (%), and incoming short-wave solar radiation (W m^{-2}) were used in these simulations.

The soil is described by 88.4% sand, 10.7% silt, and 1.0% clay following additional grain-size analysis as part of this study. Table I includes a summary of these analyses. These values are consistent with previous analyses and confirm the homogeneity of the soil at BioCON.

Soil hydraulic parameters were based on the pedotransfer functions defined by Saxton and Rawls (2006), which

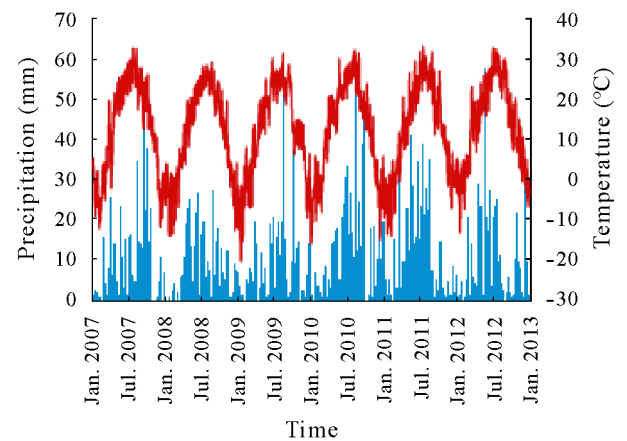


Fig. 1 Daily precipitation (column) and average daily air temperature (line) at the BioCON experiment site in the Cedar Creek Ecosystem Science Reserve in East Bethel, Minnesota, USA. The data were from the National Aeronautics and Space Administration (NASA) Land Data Assimilation Systems (NLDAS) Phase 2 Forcing File A (NLDAS-2).

TABLE I

Grain size statistics for soil samples collected at various depths and adjacent to each ring in the BioCON experiment conducted in the Cedar Creek Ecosystem Science Reserve in East Bethel, Minnesota, USA

Statistics	Clay ($< 2 \mu\text{m}$)	Silt ($> 2 \mu\text{m}$ and $< 50 \mu\text{m}$)	Sand ($> 50 \mu\text{m}$)
%			
10 samples from various depths			
Average	1.0	10.7	88.4
Standard deviation	0.1	1.3	1.3
Maximum	0.9	12.6	90.2
Minimum	0.5	9.3	86.6
6 samples adjacent to each ring			
Average	0.7	11.5	87.9
Standard deviation	0.1	0.9	1.0
Maximum	1.1	12.4	90.9
Minimum	0.8	8.4	86.5
Total average	0.9	11.0	88.2

calculate the parameters for the Brooks and Corey model for soil-moisture retention and saturation-hydraulic conductivity based on soil texture data (Table II).

Plant characteristics and assessment of their conceptualization in SHAW

To simplify the model, the nine random plant species present in the vegetated plots (Table III) were combined and simulated as one “effective” species represented by “generic” grass. This generic grass was used to represent the plant species present in the plot, regardless of which plant species they were.

The parameters of this “generic” grass were obtained from Campbell and Norman (1998), Lee *et al.* (2011), the SHAW User’s Manual, and BioCON data. Some plant characteristics were fixed in time and others varied depending on the season (Fig. 2, Table IV). Monthly time-variant plant parameters included plant height (m), leaf width (cm), dry biomass (kg m⁻²), leaf area index, and effective rooting depth (cm). The following plant residue parameters also changed over time: thickness of the layer (cm), dry weight (kg m⁻²), and fraction of surface area covered by residues.

Three plant parameters differed depending on the CO₂ concentration: stomatal resistance, dry plant biomass, and plant residue dry weight. These differences are likely necessary in order for soil moisture modeled by SHAW to match the observations and, therefore, could help explain any differences across treatments.

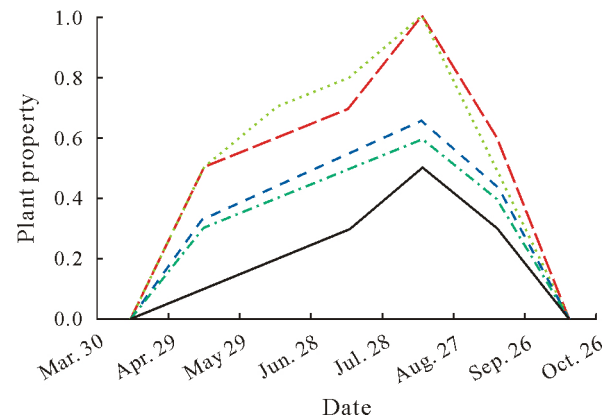


Fig. 2 Time-variable plant properties prescribed in the Simultaneous Heat and Water (SHAW) model simulations for the Biodiversity, CO₂, and Nitrogen (BioCON) experiment conducted in the Cedar Creek Ecosystem Science Reserve in East Bethel, Minnesota, USA: leaf dimension (cm, dot line), effective root depth (m, long-dash line), plant height (m, solid line), and leaf area index (LAI). The LAI values presented have been divided by 10 for both the ambient CO₂ (dash-dot line) and high CO₂ (short-dash line) conditions.

At higher CO₂ concentrations, stomatal resistance, dry plant biomass, and plant residue dry weight have been shown to increase (Drake *et al.*, 1997; Field *et al.*, 1997; Lee *et al.*, 2011). This occurs as plants have more CO₂ to photosynthesize and grow and can increase stomatal resistance as CO₂ is abundant. The values for stomatal resistance under ambient and elevated CO₂ conditions were based on BioCON data from Lee *et al.* (2011). For maximum dry plant biomass,

TABLE II

Brooks and Corey soil hydraulic parameters used in the SHAW model simulations for the BioCON experiment conducted in the Cedar Creek Ecosystem Science Reserve in East Bethel, Minnesota, USA

Parameter	Symbol	Value	Source
Saturated hydraulic conductivity (cm h ⁻¹)	K_s	12.73	Modshell SHAW interface (Saxton and Rawls, 2006)
Air-entry pressure (m)	h_b	-0.16	Modshell SHAW interface (Saxton and Rawls, 2006)
Saturated volumetric water content (m ³ m ⁻³)	θ_s	0.27	Modshell SHAW interface (Saxton and Rawls, 2006)
Pore-size distribution parameter	λ	0.30	Modshell SHAW interface (Saxton and Rawls, 2006)
Residual volumetric water content (m ³ m ⁻³)	θ_R	0.02	Based on field measurements
Pore-connectivity parameter	τ	2.0	Original Brooks and Corey equation

TABLE III

Plants present in each vegetated plot investigated in the BioCON experiment conducted in the Cedar Creek Ecosystem Science Reserve in East Bethel, Minnesota, USA

Plant species	Present in the ambient CO ₂ plot (Ring 2, plot 106)	Present in the high CO ₂ plot (Ring 1, plot 26)	Photosynthetic pathway
<i>Achillea millefolium</i>	No	Yes	C3
<i>Agropyron repens</i>	Yes	Yes	C3
<i>Amorpha canescens</i>	No	Yes	C3
<i>Andropogon gerardi</i>	Yes	No	C4
<i>Asclepias tuberosa</i>	Yes	No	C3
<i>Bouteloua gracilis</i>	Yes	Yes	C4
<i>Koeleria cristata</i>	Yes	Yes	C3
<i>Lupinus perennis</i>	Yes	Yes	C3
<i>Poa pratensis</i>	Yes	Yes	C3
<i>Schizachyrium scoparium</i>	Yes	Yes	C4
<i>Sorghastrum nutans</i>	Yes	Yes	C4

TABLE IV

Main vegetation and residue parameters used in the SHAW model simulations for the BioCON experiment conducted in the Cedar Creek Ecosystem Science Reserve in East Bethel, Minnesota, USA

Parameter	Value	Source
Fixed plant characteristics		
Wind-profile surface-roughness parameter for momentum transfer (cm)	9	Thick grass, 50 cm high (Campbell and Norman, 1998)
Albedo	0.25	Grass (Campbell and Norman, 1998)
Stomatal resistance with no water stress for the ambient CO ₂ condition (s m ⁻¹)	216	BioCON data of 2007 and 2008 (Lee <i>et al.</i> , 2011)
Stomatal resistance with no water stress for the high CO ₂ condition (s m ⁻¹)	289	BioCON data of 2007 and 2008 (Lee <i>et al.</i> , 2011)
Time-varying plant characteristics (seasonal maximum)		
Maximum plant height (m)	0.5	Grass, estimated
Maximum leaf width (cm)	1	Grass, estimated
Maximum dry biomass for the ambient CO ₂ condition (kg m ⁻²)	6	Grass (Flerchinger, 2013)
Maximum dry biomass for the high CO ₂ condition (kg m ⁻²)	6.6	10% higher based on BioCON data
Maximum leaf area index	1	Grass (Flerchinger, 2013)
Maximum effective rooting depth (m)	0.6	BioCON
Varying plant residue characteristics		
Maximum thickness of the layer (cm)	2.0	Flerchinger (2013)
Maximum dry weight for the ambient CO ₂ condition (kg m ⁻²)	0.3	Flerchinger (2013)
Maximum dry weight for the high CO ₂ condition (kg m ⁻²)	0.45	Flerchinger (2013)
Maximum fraction of surface area covered by residues	0.8	Flerchinger (2013), estimated

the ambient CO₂ condition value was based on grass values from the SHAW User's Manual and Documentation. The maximum dry plant biomass for elevated CO₂ conditions was 10% higher than for ambient CO₂ conditions. Moreover, the leaf area index (LAI) was also modified accordingly. This variation was based on dry biomass variations measured at BioCON under the different CO₂ conditions. For the maximum plant residue dry weight, the ambient and elevated CO₂ conditions values were based on the SHAW User's Manual and Documentation for different grassland disturbance conditions. A list of the main plant parameters and their sources can be found in Table IV, and their time variation is illustrated in Fig. 2.

Energy balance model

Although it is not the focus of this study, SHAW also simultaneously models heat transport within the soil through the heat advection-conduction-dispersion equation. In addition to transport, SHAW includes phase changes (freezing and thawing), which are relevant for our study due to the freezing conditions in winter. The thermal properties of the soil were calculated *via* standard equations following the volumetric proportions of sand, clay, water, and ice (see SHAW Documentation).

General properties of the implemented SHAW model and its application for hypothesis testing

The SHAW simulations were run for the different plot types using the hourly weather NLDAS data for the weather boundary conditions and soil properties obtained from field and laboratory tests. The simulations started in April 2007 and ended in December 2012.

The vertical one-dimensional model consisted of 2-m depth of soil discretized into 18 nodes, which have irregular

spacing denser near the surface. The nodes were located at 0.0, 0.01, 0.02, 0.05, 0.085, 0.1, 0.2, 0.305, 0.4, 0.505, 0.6, 0.7, 0.8, 0.915, 1.0, 1.2, 1.5, and 2.0 m. Unit gradient water flow (*i.e.*, gravity flow) was assumed for the lower boundary condition (2 m). The initial water contents and soil temperatures were based on field measurements and data from the Cedar Creek weather station for the starting date. Additional model details are presented in Table V. Unless otherwise stated, the parameters and properties listed in Tables II–V were kept the same and no calibration or tuning of any parameters was performed.

TABLE V

Inputs of the SHAW model for the BioCON experiment conducted in the Cedar Creek Ecosystem Science Reserve in East Bethel, Minnesota, USA

Input	Value	Source
Number of soil nodes	18	
Total model domain depth (m)	2	
Albedo of dry soil	0.15	Campbell and Norman (1998)
Latitude	45°24' N	BioCON data
Slope (%)	0	BioCON data
Elevation (m)	280.2	BioCON data
Wind-profile surface-roughness parameter for momentum transfer (cm)	0.03	Campbell and Norman (1998) for grass
Measurement height for air temperature and humidity (m)	2	NASA ^{a)} Land Data Assimilation Systems (NLDAS)
Measurement height for wind speed (m)	10	NLDAS
Maximum ponding (m)	0	
Soil bulk density (kg m ⁻³)	1 400	Measured

^{a)}National Aeronautics and Space Administration.

In order to test whether SHAW can model soil moisture dynamics under varied key plant characteristics that change with CO₂ concentration (*e.g.*, stomatal resistance),

we modeled three representative plots from BioCON. These plots represented the following conditions: a bare plot (the base case), a vegetated plot under ambient CO₂ conditions, and a vegetated plot under high CO₂ conditions. Following the naming system at BioCON, these plots correspond to Ring 1-plot 61, Ring 2-plot 106, and Ring 1-plot 26, respectively. Hereafter, these cases are referred to as bare, vegetated-ambient CO₂, and vegetated-high CO₂. The ambient and high CO₂ vegetated plots had a similar mix of C3 and C4 grasses, forbs, and legumes (Table III).

RESULTS AND DISCUSSION

Comparison of measured in situ soil moisture (θ) between plots

Each of the three plots had dynamic θ from the top to the bottom of their profiles (Fig. 3). Near the surface ($z =$

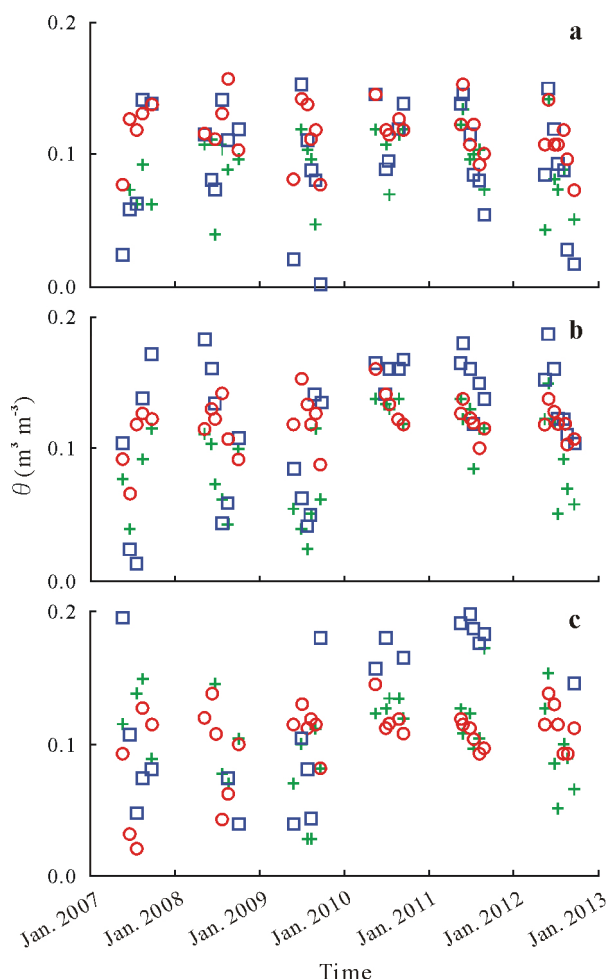


Fig. 3 Comparison of observed volumetric soil moisture (θ) at different soil depths of 8.5 (a), 50.5 (b), and 91.5 cm (c) in the bare plots (circle), vegetated plots with ambient CO₂ (cross), and vegetated plots with high CO₂ (square) of the Biodiversity, CO₂, and Nitrogen (BioCON) experiment conducted in the Cedar Creek Ecosystem Science Reserve in East Bethel, Minnesota, USA.

8.5 cm), θ between the plots were very similar through time and tended to cluster tightly. However, the vegetated-high CO₂ plot tended to be the driest during very dry periods. At intermediate depth ($z = 50.5$ cm), some differences were observed. The vegetated-ambient CO₂ plot was typically the driest, followed by the bare plot, and the vegetated-high CO₂ plot was generally the wettest. However, in all plots and during most observation times, there was substantial variability in θ . These observations support that the differences in θ could be useful for further testing of hydrologic and biophysical processes that are in action and how these are represented in SHAW.

SHAW model results of soil moisture

Some of the observed soil moisture dynamics near the surface were captured by the model simulations. However, the models poorly reproduced observations at the deepest location. The measurements are integrated over 17 cm depth (the length of the TDR probe), while the SHAW model results are for a point or node location. To make the model results and observations comparable, model nodes were precisely positioned to be in the middle of the θ measurement interval.

Bare plots

Soil moisture in the bare plots remained within a narrower and higher range relative to the two vegetated plots (Figs. 4, 5, and 6). The model was able to reproduce θ observations for the bare plot (Fig. 4) only within a narrow range (*ca.* 0.1 to 0.14). The model generally failed to reproduce the driest observed θ (*ca.* 0.05 and less, see scatter plot in Fig. 4). However, like the observations, the model is able to replicate broad drying trends during summer (*e.g.*, around April 2011 and May 2012), except for the deepest location at 91.5 cm. There were some very dry moments in the deepest location (*e.g.*, around June 2007 and July 2008), that the model did not show.

We assessed model performance quantitatively in two ways. The first is through the calculation of the root-mean-square-error (RMSE) for each model depth node. The second is more integrated: *via* scatter plots of all the model results vs. observations and by fitting a line to these with the intercept set at 0. The R^2 and RMSE values are determined for the fits and visually compared with the line of perfect correlation (1:1). Thus, there are two RMSEs, a node-based one and one for the ensemble.

The node RMSE values were 0.017 and 0.020 m³ m⁻³ in the shallow and intermediate depths, respectively; this is similar to the TDR's accuracy, which is 0.02–0.03 m³ m⁻³. However, the RMSE was 0.036 m³ m⁻³ at the deepest measurement location ($z = 91.5$ cm), which is about twice the instrument's accuracy. In general, the SHAW model was

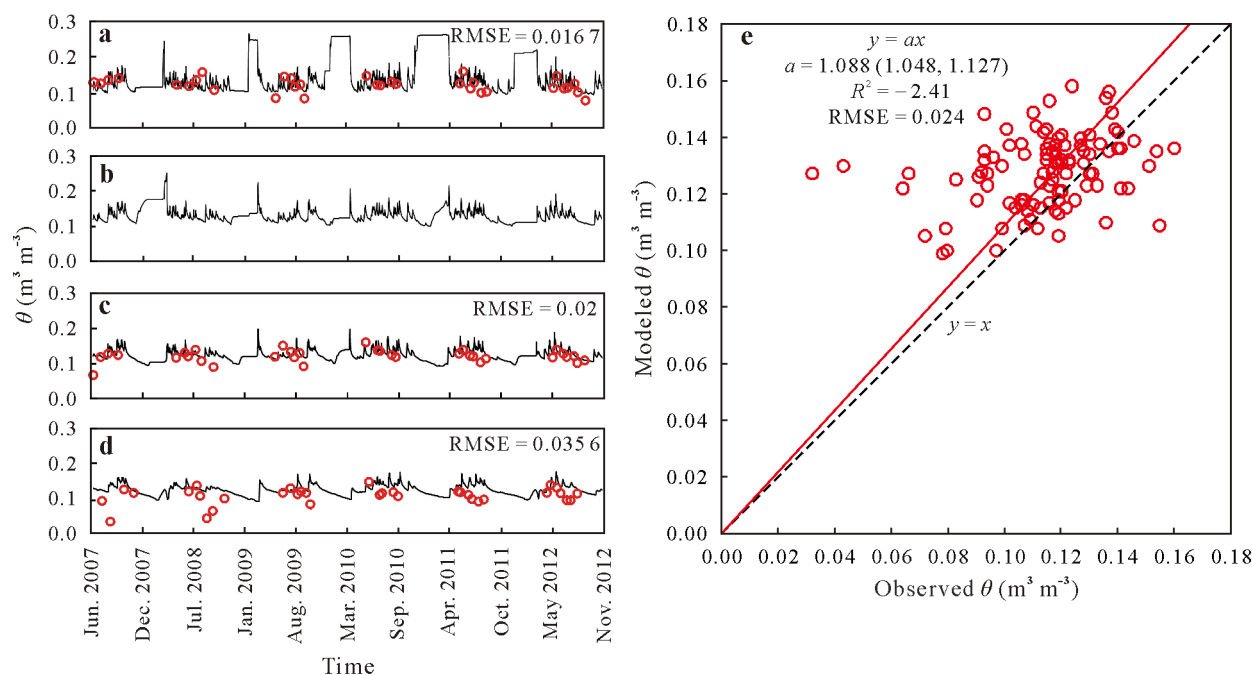


Fig. 4 Comparison of modeled and observed volumetric soil moisture (θ) in the bare plots of the BioCON experiment conducted in the Cedar Creek Ecosystem Science Reserve in East Bethel, Minnesota, USA. The left graphs show the time-series of the modeled (line) and observed (circle) θ for different soil depths of 8.5 (a), 30.5 (b), 50.5 (c), and 91.5 cm (d). Each tick is separated by 180 d and a tick's month and year label does not necessarily denote the start of the month. Also shown in each left panel is the corresponding root-mean-square-error (RMSE) between the modeled and observed θ (not applicable for the 30.5 cm depth as no observed θ for this soil depth). The right graph (e) shows the scatter diagram for θ . In this graph, the solid line is the fitted line, and the dash line is the ideal line (1:1). The graph shows the fitted a , with 95% confidence bounds in the parentheses, and R^2 and RMSE for the fit.

able to simulate wetting and drying events at $z = 8.5$ cm and at the deeper $z = 50.5$ cm. Periods when θ was constant or 'flat-lined' correspond to frozen conditions. These were most apparent at the shallowest location ($z = 8.5$ cm) but were also simulated up to 50.5 cm depth. However, this was not observed at the deepest location ($z = 91.5$ cm), and thus the maximum depth of the freezing front was somewhere between 50.5 and 91.5 cm. The SHAW model generally simulated slightly wetter conditions relative to the observations in the deepest measurement location. However, at this location, the observed wetting and drying events were also captured by SHAW.

The scatter plot shows a general over-estimation of θ by SHAW. The poor and negative R^2 shows that there is little predictive capacity of the observations. This indicates that the mean is just as predictive as any of the actual model results. However, the RMSE based on all the results of $0.024 \text{ m}^3 \text{ m}^{-3}$ is small and within the accuracy of the TDR measurements as noted above. The metrics suggest that the SHAW model may be able to capture the mean behavior or the mean soil moisture state, but inaccurately captures the instantaneous point values.

Vegetated plots under ambient CO_2 conditions

The vegetated plots under ambient CO_2 conditions had more dramatic changes in θ across all depths (Fig. 5). Compared with the bare plots, there were more pronounced drying

and wetting events in the summers. The SHAW model was able to capture the dynamics of these events, with drying and wetting at the same times and of similar magnitudes (*e.g.*, in June/July 2007, July 2008, and June/July 2012). However, the model failed to capture the observed dynamics in the deepest location ($z = 91.5$ cm). The node RMSE values for the vegetated-ambient CO_2 plots (Fig. 5) were also generally low ($0.032\text{--}0.069 \text{ m}^3 \text{ m}^{-3}$) but a little higher than those in the bare plot (Fig. 4). The RMSE values were nonetheless similar to that of the measurement error of the TDR probe, but slightly outside the range. The simulated and observed θ was more dynamic in the vegetated-ambient CO_2 plots relative to the bare plots. The drying and wetting events led to a broader θ range. Nonetheless, the SHAW model was able to qualitatively capture these events for the first three measurement depths. However, the deepest location displayed larger differences between the simulated and measured θ , and this is also reflected by the highest RMSE of $0.069 \text{ m}^3 \text{ m}^{-3}$. The SHAW model simulated relatively wetter conditions at the deepest location. Flat-lining θ (frozen) was also simulated only in the shallower three locations, similar to the bare plots.

The scatter plot analysis showed that SHAW tends to over-estimate θ when the soil is drier (*ca.* $0.05 \text{ m}^3 \text{ m}^{-3}$ and less), similar to the model behavior for the bare plots. There were five observations that fell outside the range illustrated

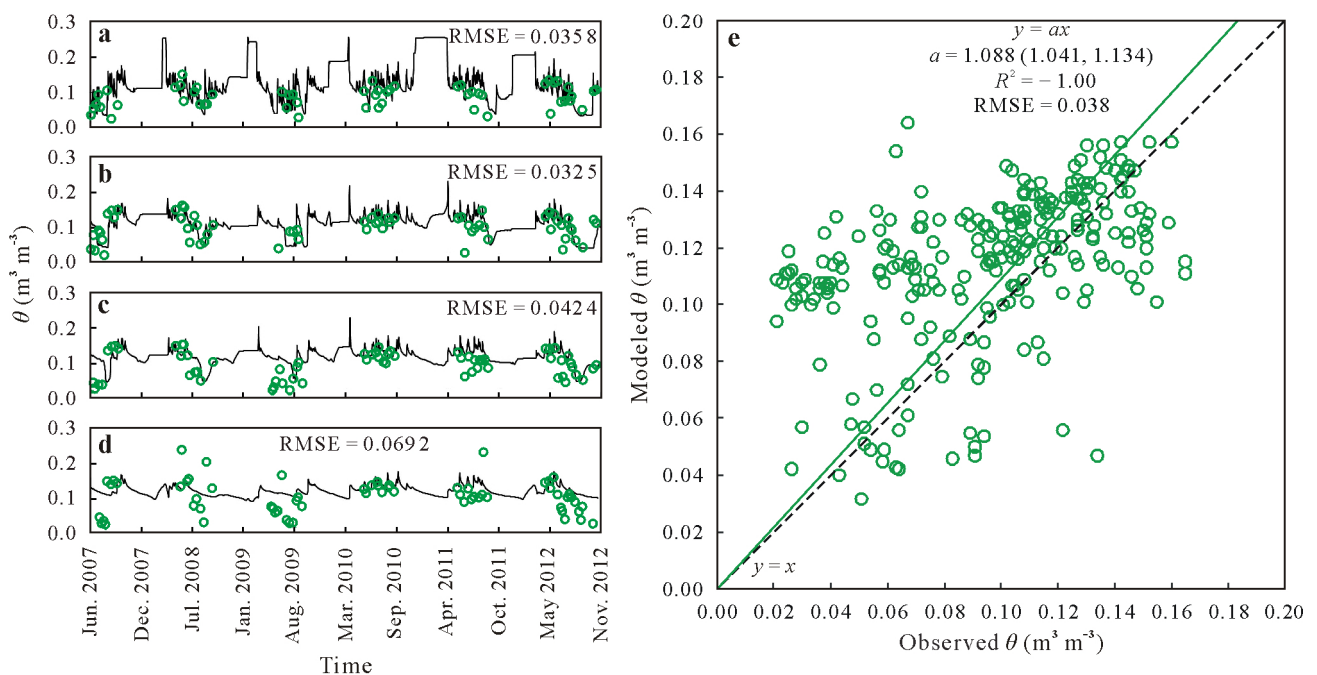


Fig. 5 Comparison of modeled and observed volumetric soil moisture (θ) in the vegetated ambient CO₂ plots of the BioCON experiment conducted in the Cedar Creek Ecosystem Science Reserve in East Bethel, Minnesota, USA. The left graphs show the time-series of the modeled (line) and observed (circle) θ for different soil depths of 8.5 (a), 30.5 (b), 50.5 (c), and 91.5 cm (d). Each tick is separated by 180 d and a tick's month and year label does not necessarily denote the start of the month. Also shown in each left panel is the corresponding root-mean-square-error (RMSE) between the modeled and observed θ . The right graph (e) shows the scatter diagram for θ . In this graph, the solid line is the fitted line, and the dash line is the ideal line (1:1). The graph shows the fitted a , with 95% confidence bounds in the parentheses, and R^2 and RMSE for the fit.

in Fig. 5, ranging from 0.20 to 0.46 m³ m⁻³. However, the corresponding modeled values did not reach this range and stayed between 0.12 to 0.15 m³ m⁻³. The SHAW model failed to reproduce these few high θ values and drastically under-estimated them. Similar to the bare plot comparison, the negative R^2 shows that there is little predictive capacity of the observations. The over-all RMSE of 0.038 m³ m⁻³ is higher than that of the bare plots, but still close to the range of the TDR accuracy.

Vegetated plots under elevated CO₂ conditions

The simulated θ values in the vegetated-high CO₂ plots were very similar to those in the vegetated-ambient CO₂ plots (Figs. 6 and 5). This is expected since the only difference between the two model scenarios is the decreased stomatal resistance, which resulted in slightly wetter soil conditions. However, the differences are not visibly obvious in the time-series plots of θ . In this case, SHAW was able to replicate the observed drying and wetting events. The SHAW model resulted in similar node RMSE values of around 0.03–0.04 m³ m⁻³ as the previous two plots at the first three depths, and higher RMSE in the deepest location. However, in this case, the RMSE of 0.084 m³ m⁻³ for the deepest location was relatively much higher, with observations showing much wetter and more dynamic conditions than what SHAW simulated. In general, the observed θ values were higher

than what the model produced. Nonetheless, the node RMSE values here, as in the other two cases, indicate that the dominant dynamics are captured by the SHAW simulations.

The scatter plot further highlights that SHAW tends to over-estimate θ in drier conditions, and under-estimates them in wetter conditions (Fig. 6). The R^2 for the fitting was similarly poor and also negative, indicating almost no predictive capacity. However, the over-all RMSE of 0.036 m³ m⁻³ was reasonably low, again indicating that SHAW is mostly representing the mean conditions.

Total water storage and fluxes modeled by SHAW

In order to further highlight and analyze the differences in the simulation results, here we focus on the total amount of water stored and the evaporation and transpiration fluxes. One representative year, 2012, is chosen for this analysis.

The total amount of water stored over the model domain of 2 m is calculated by vertical integration of the simulated θ profile, ranging from 0.2–0.3 m of water (Fig. 7), with increases and decreases in the summer due to precipitation input and evapotranspiration output. The bare plot always stored the most water, but all the plots had more similar, if not the same, amount of water during the wet period (early spring). However, after the period of peak wetness, the vegetated plots dried up more, reducing soil water storage. This increasing dryness is clearly driven by transpiration

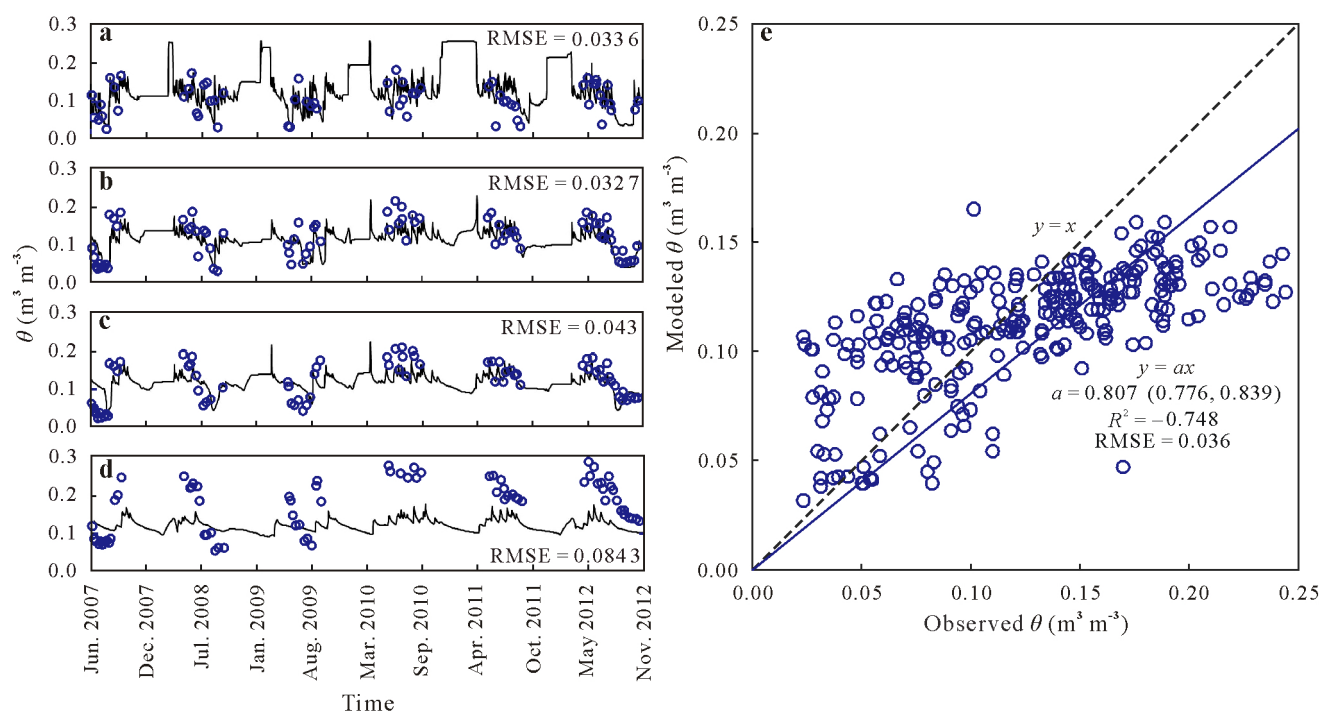


Fig. 6 Comparison of modeled and observed volumetric soil moisture (θ) in the vegetated high CO_2 plots of the Biodiversity, CO_2 , and Nitrogen (BioCON) experiment conducted in the Cedar Creek Ecosystem Science Reserve in East Bethel, Minnesota, USA. The left graphs show the time-series of the modeled (line) and observed (circle) θ for different soil depths of 8.5 (a), 30.5 (b), 50.5 (c), and 91.5 cm (d). Each tick is separated by 180 d and a tick's month and year label does not necessarily denote the start of the month. Also shown in each left panel is the corresponding root-mean-square-error (RMSE) between the modeled and observed θ . The right graph (e) shows the scatter diagram for θ . In this graph, the solid line is the fitted line, and the dash line is the ideal line (1:1). The graph shows the fitted a , with 95% confidence bounds in the parentheses, and R^2 and RMSE for the fit.

(Fig. 7c). During the mid-to-late summer period of late July to early August, the transpiration fluxes generally exceeded evaporation fluxes in the vegetated plots. As expected, the ambient CO_2 plots showed slightly higher transpiration during this period, and generally throughout the period of active transpiration. However, the differences between the vegetated-ambient CO_2 and high CO_2 are relatively small compared to the overall evapotranspiration differences between the bare soil and vegetated plots.

Note that Fig. 7 compares transpiration between the SHAW simulations only. It shows that transpiration rates for the vegetated-ambient CO_2 conditions are higher than for the vegetated-elevated CO_2 conditions. Table VI also presents time-averaged values for evaporation and transpiration. The observations show this in a much more accentuated manner. As the observed soil moisture for the vegetated-ambient CO_2 is smaller than the simulation, the transpiration in this case is probably even higher than what was simulated. For the vegetated-elevated CO_2 conditions, the observed soil moisture was higher than the simulation, suggesting that the real transpiration rates were even smaller than what was simulated.

Potential reasons for the mixed results of the comparison and recommendations

The main sources of uncertainty in this study were

related to temporally limited field soil moisture data, soil hydraulic properties, and plant properties. On average, field soil moisture was only measured and results were available for eight times each year, with each measurement taken at different months. This limitation generates uncertainty in our comparison of field data to the simulations. For future work, it would be interesting to have continuous daily soil moisture observations. The plant species present in each plot were simplified to an "effective" grass. In the future, if sufficient data become available, it would be beneficial to represent each species separately and to see how this affects the model results. The lack of local weather data adds some uncertainty to this study.

The two decades of observations from the BioCON FACE experiments have led to substantial insights into the effects of various perturbations on grassland ecosystems. However, BioCON was not expressly designed for testing hydrologic-biophysical process models, although it clearly offers some potential for this. This is what we set out to test and our analysis has revealed some issues. Overall, the SHAW models we set up seem to capture primarily the mean soil moisture state of the plots. However, there are persistent discrepancies when point and instantaneous results are observed. These suggest that the current monitoring design of the BioCON site is not adequate for a robust test. Our modeling has

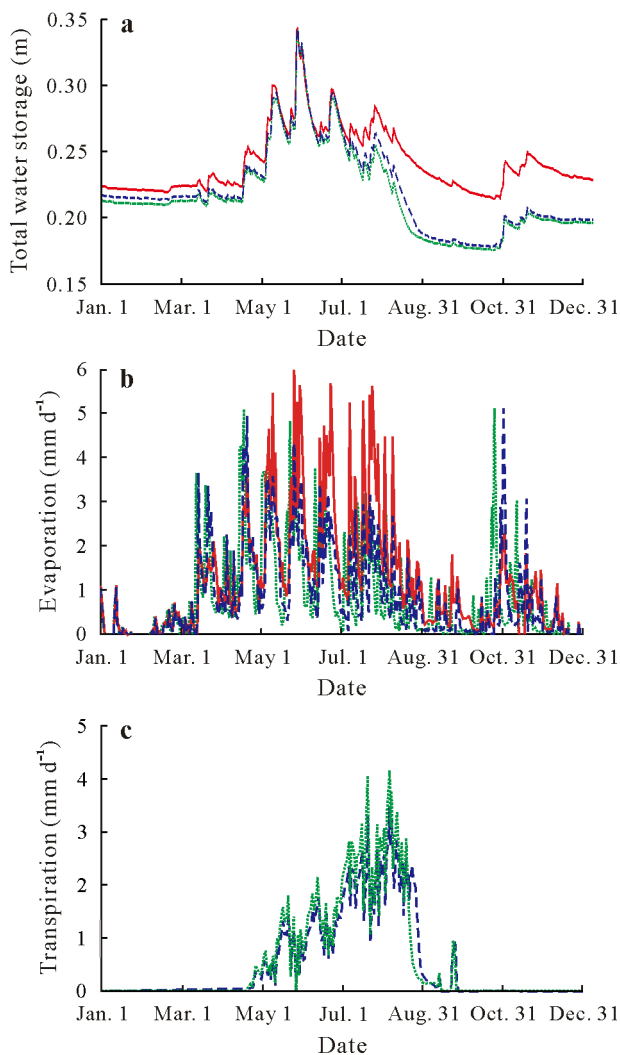


Fig. 7 Modeled total water storage (a), evaporation (b), and transpiration (c) in 2012 for the bare plots (solid line), vegetated-ambient CO₂ plots (dot line), and vegetated-high CO₂ plots (dash line) of the BioCON experiment conducted in the Cedar Creek Ecosystem Science Reserve in East Bethel, Minnesota, USA.

attempted to minimize calibrations and varying parameters. The most logical values of input parameters were assumed when they were not constrained by observations. While these are also reasons for the discrepancies, analysis of each of the potentially dozens of parameters is beyond the scope of this study. We attempted to be as parsimonious as possible in the model design and construction, given the limited observations. Following this, here we speculate on other sources of error.

The plots at BioCON are 2 m wide. It is possible that there is lateral soil moisture transport between each plot, especially when there are lateral soil moisture gradients. Given the observed differences between the bare and vegetated plots, such lateral gradients and variability are likely. The one-dimensional (vertical) formulation of SHAW does not represent such effects. However, attempting to assess

TABLE VI

Comparison of simulated evaporation (E) and transpiration (T) fluxes in the bare plots, vegetated-ambient CO₂ plots, and vegetated-high CO₂ plots of the BioCON experiment conducted in the Cedar Creek Ecosystem Science Reserve in East Bethel, Minnesota, USA

Flux	Bare	Vegetated-ambient CO ₂	Vegetated-high CO ₂
	mm d ⁻¹		
Average summer E (Apr. 15–Aug. 15)	2.49	1.59	1.63
Average winter E (Dec. 1–Mar. 1)	0.10	0.07	0.07
Annual average E	1.17	0.80	0.82
Average summer mean daily T (Apr. 15–Aug. 15)	0.00	1.60	1.34
Average winter mean daily T (Dec. 1–Mar. 1)	0.00	0.00	0.00
Average mean daily T	0.00	0.56	0.51

plot-plot soil moisture transport would require a fully three-dimensional model since there are several plots within one ring at BioCON.

The soil columns and other soil hydraulic and thermal properties are considered homogeneous. While grain-size analysis of samples from BioCON has indicated relative consistency in soil texture across plots and rings, it is likely that the soil columns have individually evolved through time, and of course, that there had always been inherent vertical and lateral variability that was not mapped. Moreover, BioCON, because it was designed to assess vegetation, obviously has roots. Some roots were also plucked for analysis. The roots and root extraction produced macropores. Our SHAW models do not represent any macropores. Mapping centimeter to perhaps decimeter scale variability in soil physical properties was not an early goal of the initial characterization of the sites, and monitoring any changes is close to impossible given all other measurements being done. Unfortunately, this is the scale over which such models such as SHAW are implemented, and some inputs may even vary over finer scales in the real world. One indicator of these issues in spatially varying soil hydraulic properties is the very dynamic soil moisture in the deepest location at 91.5 cm. This location goes from very wet to very dry, both aspects missed by the SHAW models. Since this behavior is unlikely driven by plants given the depth, this is likely the outcome of a unique combination of soil hydraulic properties. Soil water has to be able to go through this zone like a relative fast piston, which would indicate a texture that is coarser than prescribed.

The plant properties we imposed (*e.g.*, those in Fig. 2) may also vary from year to year and could exhibit some higher frequency variations, but the latter is less likely. Inter-annual variations could possibly lead to memory effects with signals from previous years affecting those of the following year. One of the critical plant parameters in SHAW, and any

biophysical model, is the stomatal resistance. The values we used here are based on limited measurements. Thus, there is some uncertainty introduced with imposing the measured stomatal resistance values. They may have also varied through time and the values imposed may not be the most representative.

The FACE sites offer a unique but challenging opportunity for testing distributed models of soil water flow across the soil-plant-atmosphere continuum. However, the typical instrumentation and monitoring design of a site like BioCON may prevent a robust test for whether models are representing the myriad processes correctly and where improvements are needed. Doing so would, unfortunately, require more detailed measurements of soil moisture and soil physical properties in space and time. These are not only time- and resource-intensive, but their invasive nature may run counter to the primary goals of the FACE experiments.

The detailed representation of many physical and physiological processes within models such as SHAW results in endless possibilities of parameter combinations. This led us to the strategy of simply imposing most parameters following observations or standard values representative for the specific vegetation and soils present in the studied plots. This study is certainly just a start. We recommend that a more robust test of a soil water flow model includes frequent, if not continuous, soil moisture monitoring and a broad analysis of some parameters *via*, *e.g.*, Monte Carlo simulations.

Some biophysical implications following the model results

The higher water use efficiency by vegetation at high CO₂ levels is not a surprise, as it is a prescribed feature of the SHAW models implemented. However, here we showed that the observed differences in stomatal resistance can produce noticeable differences in the modeled soil water budget, even when LAI is higher than what was observed independently and empirically in the field experiment (Adair *et al.*, 2011). Thus, our study further suggests that CO₂ fertilization leads to less transpiration and potentially wetter soils in the grassland ecosystems of Minnesota, and likely in ecosystems where the relative shifts in stomatal resistance and LAI are of comparable magnitudes. However, increasing CO₂ levels imply other changes, *e.g.*, increasing temperatures. Temperature increases could lead to higher evapotranspiration rates, which could completely counteract the increase in soil moisture caused by the higher water use efficiency of plants. The SHAW model is a potentially useful modeling framework for investigating these changes.

CONCLUSIONS

We simulated soil moisture at the BioCON FACE site using the SHAW numerical model. Three representative sites

were considered: a bare plot, a vegetated plot with ambient CO₂, and a vegetated plot with high CO₂. The simulations were populated by field-observed parameters and boundary conditions. The SHAW model qualitatively reproduced patterns of observed soil moisture dynamics across a vertical soil section without any calibration. However, quantitative comparisons revealed that the model inadequately predicted point and instantaneous values of soil moisture. The model mostly captured the mean state and behavior.

The SHAW model was able to simulate the expected result of higher evapotranspiration and lower total water content for vegetated soil than for bare soil. The higher total water content for the bare plots occurs due to the lack of the transpiration. Evapotranspiration at high CO₂ conditions was smaller and water content was higher when compared to ambient CO₂ conditions. The difference is primarily due to higher imposed stomatal resistance at elevated CO₂ conditions as well as higher plant and residue biomass. Thus, given that SHAW reproduces soil moisture patterns for the different vegetation-CO₂ treatments, the simplified biophysical representation of transpiration and the soil-plant-atmosphere continuum in SHAW appears to be adequate and holds promise for future applications in assessing the impacts of increasing atmospheric CO₂. However, the limited measurements available for model testing so far indicate some delinquencies in the model or how they are parameterized. The available soil moisture measurement and observations of input parameters prevent a robust and conclusive analysis of whether SHAW is capturing or missing certain local, instantaneous or broad dynamics for the right reasons. We conclude that a hydrologic-biophysical model such as SHAW remains a promising complement for FACE and other manipulation experiments, given that the pitfalls can be overcome.

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