

LARGE SCALE MAPPING OF EVAPOTRANSPIRATION AND RECHARGE FLUXES VIA ASSIMILATION OF GOES LAND SURFACE TEMPERATURE AND SMAP SOIL MOISTURE DATA

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ABSTRACT

Estimation of evapotranspiration and recharge flux are fundamental to sustainable water resource management. These fluxes provide valuable insights for decision-makers, enabling them to implement effective strategies that balance water demand with available resources, promote resilience in the face of climate change, and ensure the long-term sustainability of water ecosystems. In-situ observations of evapotranspiration and recharge are scarce and not representative of large areas. An observation driven variational data assimilation system, named LIDA-2 (Land Integrated Data Assimilation framework) is developed to estimate the key parameters (evaporative fraction, bulk heat transfer coefficient, Brooks-Corey parameter) of evapotranspiration and recharge fluxes by assimilating GOES land surface temperature (LST) and SMAP surface soil moisture observations into a coupled water and dual-source energy balance model. Second order information is used to estimate the uncertainty and guide the model toward a well-posed estimation problem. The algorithm is implemented in part of the US southern great plain, and its performance is evaluated through comparison tests, uncertainty analysis and consistency test. Soil moisture and evapotranspiration estimations are validated against in-situ observations. The spatial pattern of estimated annual recharge map is in good agreement with maps from literature. Overall, the VDA based framework demonstrated its efficacy to do largescale mapping of recharge, and evapotranspiration.

Index Terms— Evapotranspiration, Recharge, Soil moisture, VDA

1. INTRODUCTION

Evapotranspiration and recharge fluxes are key components of global water, energy, and carbon cycles, and influence food production, water management, weather prediction, climate change etc. [1-3]. Evapotranspiration and recharge fluxes are interconnected via soil moisture content. The evaluation of moisture content at the top few centimeters to meters depth of soil holds critical information regarding the partitioning of precipitation which dictates the evapotranspiration and recharge rates [1].

In-situ methods of estimation of evapotranspiration (eddy covariance, Energy Balance Bowen ratio) and recharge

(lysimeters, seepage meters, chemical tracers) fluxes provide good point scale approximation. However, the dynamic nature of the transfer process and land surface heterogeneity do not allow these in-situ observations to represent large areas [4-6]. Remote sensing can be an alternative to in-situ measurement as it provides good spatiotemporal coverage of land surface state observations from different sensors. However, the land surface fluxes cannot be estimated directly through remote sensing. Numerical models can estimate the states and fluxes, but their results are uncertain due to errors of model structure, initial condition, parameters, etc. Data assimilation combines observational data with numerical model output to produce an optimal estimate of the evolving system by taking advantages of both numerical modelling estimates and observations. Different data assimilation methods like Variational data assimilation (VDA) and ensemble Kalman filtering (EnKF) have been used extensively to retrieve land surface fluxes by utilizing remote sensing observation [7-10]. Optimal parameter estimation, robustness and stability of the method make VDA technique more suitable than other data assimilation methods in estimating land surface fluxes [11]. The time evolution of LST data implicitly contains information regarding the partitioning of available energy into turbulent heat fluxes and [7-9,12] The time evolution of surface soil moisture data implicitly contains information regarding the partitioning of precipitation into evapotranspiration, runoff, and infiltration. Remotely sensed surface soil moisture observations have also been utilized to estimate the root zone soil moisture profile and soil effective hydraulic parameters [18-21].

Abdolghafoorian and Farhadi 2019, 2020 [25,4] developed a variational based data assimilation methodology, LIDA (Land Integration Data Assimilation) framework that assimilates land surface soil moisture and land surface soil temperature data into a parsimonious coupled water and energy balance model to effectively estimate flux of evapotranspiration. LIDA contains an uncertainty quantification framework that uses second order information that guides the optimization and evaluates its uncertainty. Mahmood and Farhadi 2022 [26] (LIDA-2) advanced the LIDA framework to estimate recharge flux by including effective soil saturated hydraulic conductivity K_{sat} as an additional parameter of the LIDA. The feasibility and accuracy of the framework were tested in point scales through

a set of synthetic experiments in Mahmood and Farhadi 2022 [26]. In this study the LIDA-2 [26] framework will be validated in the large areas of the US Southern great plain (SGP) and Oklahoma Panhandle region for three years from 2016 to 2018 to estimate the optimal parameters (evaporative fraction, bulk heat transfer coefficient, Brooks-Corey parameter) of evapotranspiration and recharge fluxes by assimilating Geostationary Operational Environmental Satellite (GOES) land surface temperature and Soil Moisture Active Passive (SMAP) surface soil moisture observations into a coupled water and energy balance model. The evapotranspiration and recharge fluxes are estimated using the optimum parameters.

2. METHODOLOGY

2.1. Coupled Energy and Water Model

A grid-based model is used in this study where different processes of energy and water cycle are simulated in each grid separately using a parsimonious coupled water and energy balance model. The energy balance model is based on the dual-source surface energy balance (SEB) model. In this model the contributions from soil and canopy are considered separately. Key parameters of energy balance model to estimate sensible and latent heat fluxes are soil and canopy evaporative fraction and neutral bulk heat transfer coefficient. A simple water balance (SWB) scheme adopted from Schaake et al. 1996 [28] is used to calculate the surface runoff. Brooks-Corey model is used to estimate the hydraulic properties of unsaturated soil [31]. A simple water balance (SWB) scheme adopted from Schaake et al. 1996 [28] is used to calculate the surface runoff.

2.2. VDA Based Modeling Framework

Variational data assimilation (VDA) is based on minimization of cost function that leads to a set of Euler-Lagrange equations to estimate the adjoint variables and parameters. The cost function constitutes of mismatch between simulated state and observations, estimated parameter and its prior estimates. Physical models are added to the cost function using adjoint variables and act as a physical constraint. Parameters of the VDA are daily evaporative fraction for soil EF_s and canopy EF_c , monthly R [$R = \ln(C_{HN}, \text{Neutral bulk heat transfer coefficient})$] and Brooks-Corey parameter B . Physical models in the VDA system are heat diffusion equation and Richard equation. The state observations are land surface temperature (LST) and surface SM.

The Hessian matrix is formed using the gradient of cost function at the optimum point following the Lagrangian method [32]. Hessian matrix at the optimum point must be positive definite (all the eigenvalues are positive). Uncertainty of parameters can be approximated from error covariance matrix which is the inverse of the hessian matrix [11, 33-34]. Uncertainty of fluxes can be estimated using Monte Carlo algorithm [25].

The basic algorithm of the VDA is to make initial guess of unknown parameters, then run the coupled water and energy balance model with these parameters, assimilate the land surface temperature and surface soil moisture, run the adjoint models and estimate the updated parameters. The run continues through the loop until updated parameters reach stabilization. Then the hessian matrix is calculated at this point and if all the eigen values of the hessian matrix are positive it means the solution has reached the optimum point.

3. STUDY AREA AND DATA

A rectangular bounding box [35.5 N to 37.2 N, 97.0 W to 101.4 W] that covers part of the Oklahoma Panhandle regions, and part of Southern great plain (SGP) is selected for this study. Groundwater recharge is very vital in the Panhandle region as 98% of the total water demand in this region comes from groundwater. The adjacent part of Southern great plain (SGP) is also included in the study area due to its higher concentration of in-situ stations that will be used to validate the framework.

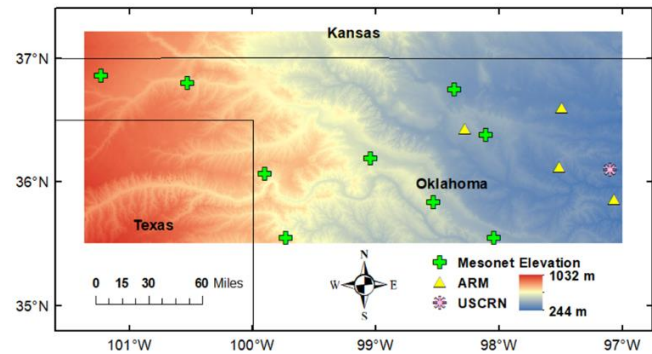


Figure 1: Study area elevation map with station's locations

Detailed descriptions of the data used in this study are reported in Table 1.

A simple look up table with 12 soil classes, GSWP2 [35], is used to estimate the soil hydraulic parameters (except for the Brooks-Corey parameter B) based on the soil texture data that is available for this region. Using a simple look up table makes the framework less dependent on the accuracy of the soil texture data and therefore more applicable for large scale application.

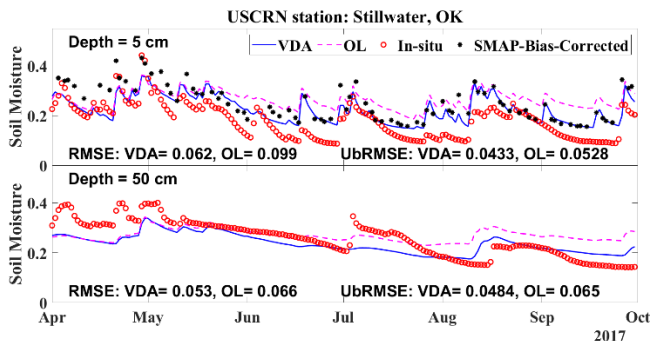
Table 1: Detailed descriptions of data

Data		Source	Spatial Resolution	Temporal Resolution
Assimilated state variables	Soil Moisture	SMAP	9 Km	2-3 days
	Land Surface temperature	GOES	5 Km	1 hr
Input Forcing	Longwave and shortwave radiation, Wind speed, Air temperature	NLDAS-2	0.125°	1 hr
	Precipitation	GPM	10 Km	30 min
Ancillary	Leaf Area Index	MODIS	500 m	8 days
	Soil Texture	SMAP	9 km	
	Land cover	MODIS	500m	1 year
Validation	Latent and Sensible heat fluxes	ARM	point scale	30 min
	Soil moisture	USCRN, Mesonet, ARM	point scale	Daily
	Recharge	Reitz et al. 2017	800 m	Yearly
		Wyatt et al. 2017	point scale	Yearly

4. RESULTS

4.1. Soil Moisture

Soil moisture profiles are validated using in-situ observation shown in Figure 1. Soil moisture profiles from April to September 2017 at two different depths (5 cm and 50 cm) are demonstrated in Figure 2 at the location of USCRN station Stillwater. As seen in the figure, the VDA estimated soil moisture profiles match better with the observed soil moisture profiles than the open loop estimates at both depths in terms of values and trend. The corresponding error metrics RMSE and unbiased RMSE (ubRMSE) both are also reported in the figure for OL and VDA estimated soil moisture profiles. Both the error metrics reduce from OL estimate to VDA estimate which indicates the efficacy of the VDA framework.

**Figure 2: Soil moisture profile at two different depths**

4.2. Recharge

The Gravitational drainage at the bottom of the soil column is taken as the measure of diffuse recharge in this study. Estimated recharge are compared with the annual recharge values reported in literature for this area (Wyatt et al. 2017 [37] and Reitz et al. 2017 [38]). The estimated recharge values for the pixels at those station's location are reported in the table. The estimated annual recharge values are within the range reported in the literature and close to the average annual recharge values reported.

Table 2: Annual Recharge estimations at different Mesonet station's locations

Site Name	Average Recharge (mm/yr): Wyatt et al. 2017	Average Recharge (mm/yr): Reitz et al 2017	Range of Recharge (mm/yr): Reitz et al 2017	Estimated Recharge (mm/yr)
Arnett	17	68.19	13.93-127.34	26.77
Cheyenne	32	81.46	16.83-151.01	90.56
Watonga	88	58.5	22.4-310.4	62.22
Seiling	19	32.46	22.8-50.55	43.94

The spatial pattern of estimated annual recharge are also validated by comparing the maps of estimated recharge with the maps from Wyatt et al. 2017 and Reitz et al. 2017 [37-38]. The spatial pattern of estimated annual recharge matches well with the maps from literature.

4.3. Evapotranspiration

Latent heat flux can be used as a measure of evapotranspiration flux. In-situ latent heat flux observations from two Atmospheric Radiation Measurement (ARM) SGP sites are used to validate the evapotranspiration flux estimated by LIDA-2 framework. Table 3 demonstrates the RMSE of estimated hourly latent heat flux at E13 and E39 ARM stations. Assimilation of LST and surface SM has improved the latent heat flux estimation by reducing RMSE significantly from open loop estimation at both the stations' locations.

Table 3: RMSE (W/m²) of hourly latent heat flux at ARM stations for the year 2017

Site Name	ARM code	Lat	Lon	VDA	Open Loop (OL)
Lamont, OK	E13	36.60	97.49	81.58	117.64
Morrison, OK	E39	36.37	97.07	83.13	100.64

5. CONCLUSION

A VDA based framework (LIDA-2) has been developed to map the evapotranspiration and recharge flux by assimilating GOES LST and SMAP surface soil moisture into a coupled water energy balance model. Optimum values of essential states (soil temperature and soil moisture) and parameters

(Soil and canopy EF, C_{HN} , B) of evaporative and recharge fluxes are estimated using variational data assimilation method and analyzing second order information. Uncertainty information is estimated from error covariance matrix which is the inverse of hessian matrix at the point of optimum. LIDA-2 framework is used to map a large area of Southern great plain and part of Oklahoma panhandle region for three years from 2016 to 2018. Comparison shows VDA simulated soil moisture profiles match better with the in-situ observation than the open loop estimates in term of values and trend both in case of surface and root zone soil moisture. The annual recharge estimates are within the range of values reported in the literature. The spatial pattern of annual recharge estimates matches well with the maps reported in literature. Comparison with latent heat flux observations from two ARM sites demonstrates improvement due to assimilation of LST and surface soil moisture. Overall, the VDA based framework presented in this study demonstrated efficacy in largescale mapping of recharge, and evapotranspiration. Accurate mapping and estimation of these two important water cycle fluxes provide valuable insights for decision-makers, enabling them to implement effective strategies that balance water demand with available resources, promote resilience in the face of climate change, and ensure the long-term sustainability of water ecosystems.

6. ACKNOWLEDGEMENT

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7. REFERENCES

- [1] Entekhabi, D. & Moghaddam, M. (2007). Mapping recharge from space: Roadmap to meeting the grand challenge, *Hydrogeology Journal*, Vol 15, no. 1, pp. 105–116, DOI 10.1007/s10040-006-0120-6
- [2] Earman, S. & Dettinger, M. (2011). Potential impacts of climate change on groundwater resources - A global review, *Journal of Water and Climate Change*, Vol 2, no. 4, pp. 213-229, <https://doi.org/10.2166/wcc.2011.034>
- [3] Irmak, S., Irmak, A., Jones, J.W. (2003). Solar and net radiation-based equations to estimate reference evapotranspiration in humid climates, *Journal of Irrigation and Drainage Engineering*. ASCE, Vol 129, no. 5, pp. 336-347, [https://doi.org/10.1061/\(ASCE\)0733-9437\(2003\)129:5\(336\)](https://doi.org/10.1061/(ASCE)0733-9437(2003)129:5(336))
- [4] Abdolghafoorian, A., & Farhadi, L. (2020). LIDA: a Land Integrated Data Assimilation Framework for Mapping Land Surface Heat and Evaporative Fluxes by Assimilating Space-Borne Soil Moisture and Land Surface Temperature. *Water Resources Research*, 1–19. <https://doi.org/10.1029/2020WR027183>
- [5] Odhiambo, G. O., & Savage, M. J. (2009). Sensible heat flux by surface layer scintillometry and eddy covariance over a mixed grassland community as affected by Bowen ratio and MOST formulations for unstable conditions. *Journal of Hydrometeorology*, 10, 479–492. <https://doi.org/10.1175/2008JHM1008.1>
- [6] Li, F. & Lyons, T. J. (1999). Estimation of regional evapotranspiration through remote sensing, *Journal Appl. Meteorol.*, vol. 38, no. 11, pp. 1644–1654, [https://doi.org/10.1175/1520-0450\(1999\)038<1644:EORETR>2.0.CO;2](https://doi.org/10.1175/1520-0450(1999)038<1644:EORETR>2.0.CO;2)
- [7] Bateni, S. M., Entekhabi, D., & Jeng, D. S. (2013). Variational assimilation of land surface temperature and the estimation of surface energy balance components. *Journal of Hydrology*, 481, 143–156. <https://doi.org/10.1016/j.jhydrol.2012.12.039>
- [8] Abdolghafoorian, A., Farhadi, L., Bateni S. M., Margulis, S., and Xu, T. (2017). Characterizing the Effect of Vegetation Dynamics on the Bulk Heat Transfer Coefficient to Improve Variational Estimation of Surface Turbulent Fluxes, *Journal of Hydrometeorology*, 321–333. <https://doi.org/10.1175/JHM-D-16-0097.1>
- [9] Caparrini, F., Castelli, F., & Entekhabi, D. (2004). Variational estimation of soil and vegetation turbulent transfer and heat flux parameters from sequences of multisensor imagery. *Water Resources Research*, 40, W12515. <https://doi.org/10.1029/2004WR003358>
- [10] Lu, Y., Steele-Dunne, S. C., Farhadi, L., & van de Giesen, N. (2017). Mapping Surface Heat Fluxes by Assimilating SMAP Soil Moisture and GOES Land Surface Temperature Data. *Water Resources Research*, 53(12), 10858–10877. <https://doi.org/10.1002/2017WR021415>
- [11] Abdolghafoorian, A., & Farhadi, L. (2016). Uncertainty Quantification in Land Surface Hydrologic Modeling: Toward an Integrated Variational Data Assimilation Framework. *IEEE Journal of Selected Topics in Applied Earth Observations and Remote Sensing*, 9(6), 2628–2637. <https://doi.org/10.1109/JSTARS.2016.2553444>
- [12] Bateni, S. M., & Liang, S. (2012). Estimating Surface Energy Fluxes Using a Dual-Source Data Assimilation Approach Adjoined to the Heat Diffusion Equation. *Journal of Geophysical Research*, 117, D17118. <https://doi.org/10.1029/2012JD017618>
- [13] Scanlon, B. R., Healy, R. W., & Cook, P. G. (2002). Choosing appropriate techniques for quantifying groundwater recharge. *Hydrogeology Journal*, 10(1), 18–39. <https://doi.org/10.1007/s10040-001-0176-2>
- [14] Scott, R. L., Shuttleworth, W. J., Keefer, T. O., Warrick A. W. (2000). Modeling multi-year observations of soil moisture recharge in the semi-arid American southwest. *Water Resource Research*, 36 (8):2233–2247, <https://doi.org/10.1029/2000WR900116>
- [15] Allison, G. B., Gee G. W., Tyler, S. W. (1994). Vadose zone techniques for estimating ground-water recharge in arid and semiarid regions. *Soil Science Society of America Journal*, 58(1):6–14. <https://doi.org/10.2136/sssaj1994.03615995005800010002x>
- [16] Van Dam, J.C. (2000). Field-scale water flow and solute transport: SWAP model concepts, parameter estimation and case

studies. Ph.D. diss. Wageningen Univ., Wageningen, the Netherlands.

[17] Das, N.N., Mohanty, B.P. & Njoku, E.G. (2008). A Markov chain Monte Carlo algorithm for upscaled soil-vegetation-atmosphere-transfer modeling to evaluate satellite-based soil moisture measurements. *Water Resources Research*, Vol. 44, W05416, <https://doi.org/10.1029/007WR006472>

[18] Reichle, R., McLaughlin, D., Entekhabi, D. (2002). Hydrologic data assimilation with the ensemble Kalman filter. *Monthly Weather Review* 130(1):103–114, [https://doi.org/10.1175/1520-0493\(2002\)130<0103:HDAWTE>2.0.CO;2](https://doi.org/10.1175/1520-0493(2002)130<0103:HDAWTE>2.0.CO;2)

[19] Margulis, S. A., McLaughlin, D., Entekhabi, D. & Dunne S. (2002). Land data assimilation and estimation of soil moisture using measurements from the Southern Great Plains 1997 Field Experiment, *Water Resources Research*, 38(12), 1299, <https://doi.org/10.1029/2001WR001114>

[20] Ines, A.V.M., Mohanty, B.P. (2009). Near-surface soil moisture assimilation for quantifying effective soil hydraulic properties using genetic algorithms: II. Using airborne remote sensing during SGP97 and SMEX02. *Water Resources Research*, 45, W01408. doi:10.1029/2008WR007022

[21] Shin, Y., Mohanty, B. P., and Ines, A. V. M. (2013). Estimating Effective Soil Hydraulic Properties Using Spatially Distributed Soil Moisture and Evapotranspiration. *Vadose Zone Journal*, 12(3), vzj2012.0094. <https://doi.org/10.2136/vzj2012.0094>

[22] Liu, Y., & Gupta, H. V. (2007). Uncertainty in hydrologic modeling: Toward an integrated data assimilation framework. *Water Resources Research*, 43, W07401. <https://doi.org/10.1029/2006WR005756>

[23] Dimet, L., F.-X., Navon, I. M., and Daescu, D. N. (2002). Second-order information in data assimilation. *Monthly Weather Review*, 130(3), 629–648. [https://doi.org/10.1175/1520-0493\(2002\)130<0629:SOIIDA>2.0.CO;2](https://doi.org/10.1175/1520-0493(2002)130<0629:SOIIDA>2.0.CO;2)

[24] Crow, W. T., & Kustas, W. P. (2005). Utility of assimilating surface radiometric temperature observations for evaporative fraction and heat transfer coefficient retrieval. *Boundary-Layer Meteorology*, 115(1), 105–130. <https://doi.org/10.1007/s10546-004-2121-0>

[25] Abdolghafoorian, A., & Farhadi, L. (2019). Estimation of Surface Turbulent Fluxes From Land Surface Moisture and Temperature Via a Variational Data Assimilation Framework, *Water Resources Research*. 1–20. <https://doi.org/10.1029/2018WR024580>

[26] Mahmood, A., & Farhadi, L. (2022). A Variational Framework for Coupled Estimation of Evapotranspiration and Recharge Fluxes by Assimilating Land Surface Soil Moisture and Temperature, *IEEE Journal of Selected Topics in Applied Earth Observations and Remote Sensing*, vol. 15, pp. 3246–3257, 2022, doi: 10.1109/JSTARS.2022.3168485

[27] S'imunek, J., M. T. van Genuchten and O. Wendroth (1998), Parameter estimation analysis of the evaporation method for

determining soil hydraulic properties, *Soil Sci. Soc. Am. J.*, 62, 894–905, <https://doi.org/10.2136/sssaj1998.03615995006200040007x>

[28] Schaake, J. C., V. I. Koren, Q.-Y. Duan, K. Mitchell, and F. Chen (1996), Simple water balance model for estimating runoff at different spatial and temporal scales, *J. Geophys. Res.*, 101(D3), 7461–7475, doi:10.1029/95JD02892

[29] Lievens, H. et al. 2015, SMOS soil moisture assimilation for improved hydrologic simulation in the Murray Darling Basin, Australia. *Remote Sens. Environ.* 168, 146–162.

[30] Richards, L. A. (1931). Capillary conduction of liquids through porous mediums. *Journal of Applied Physics*, Vol. 1, no. 5, pp. 318–333, <https://doi.org/10.1063/1.1745010>

[31] Clapp, R. B., and Hornberger, G.M. (1978). Empirical equations for some soil hydraulic properties. *Water Resources Research*, 14(4), 601–604. <https://doi.org/10.1029/WR014i004p00601>

[32] Burger, J., Le Brizaut, J. S., and Pogu, M. (1992). Comparison of two methods for the calculation of the gradient and of the Hessian of cost functions associated with differential systems. *Mathematics and Computers in Simulation*, 34, 551–562. [https://doi.org/10.1016/0378-4754\(92\)90041-E](https://doi.org/10.1016/0378-4754(92)90041-E)

[33] Gejadze, I., Copeland, G., Le Dimet, F. X., & Shutyaev, V. (2011). Computation of the Analysis Error Covariance in Variational Data Assimilation Problems with Nonlinear Dynamics. *Journal of Computational Physics*, 230(22), 7923–7943. <https://doi.org/10.1016/j.jcp.2011.03.039>

[34] Shutyaev, V., Le Dimet, F. X., & Gejadze, I. (2008). On Optimal Solution Error Covariances in Variational Data Assimilation. *Journal of Computational Physics*, 23(2), 197–205. <https://doi.org/10.1515/156939806776369492>

[35] Dirmeyer, P., Gao, X. and Oki, T. (2002). The Second Global Soil Wetness Project (GSWP2), International GEWEX Project Office Publication, V-37.

[36] Cosby, B. J., Hornberger, G. M., Clapp, R. B. & Ginn, T. R. A Statistical Exploration of the Relationships of Soil Moisture Characteristics to the Physical Properties of Soils. *Water Resour. Res.* 20, 682–690 (1984).

[37] Wyatt, B. M., Ochsner, T. E., Fiebrich, C. A., Neel, C. R. & Wallace, D. S. Useful Drainage Estimates Obtained from a Large-Scale Soil Moisture Monitoring Network by Applying the Unit-Gradient Assumption. *Vadose Zo. J.* 16, vzj2017.01.0016 (2017).

[38] Reitz, M., Sanford, W. E., Senay, G. B. & Cazenias, J. Annual Estimates of Recharge, Quick-Flow Runoff, and Evapotranspiration for the Contiguous U.S. Using Empirical Regression Equations. *J. Am. Water Resour. Assoc.* 53, 961–983 (2017).