

Estimating soil hydraulic parameters from lysimeter data: a Bayesian perspective

Marleen Schübl^{1*}, Giuseppe Brunetti¹ and Christine Stumpp¹

Zusammenfassung

Deterministische Modelle sind für die Simulation der Grundwasserneubildung geeignet. Parameter können mittels Messungen des Bodenwassergehalts, Matrixpotenzials und Sickerwassermengen invers geschätzt werden. Inwiefern die Art der für die Modellkalibrierung verwendeten Messungen die Modellunsicherheiten beeinflusst, ist jedoch wenig bekannt und soll in dieser Studie unter Anwendung einer Bayesschen Analyse untersucht werden. Die Daten eines monolithischen Gumpenstein-Lysimeters wurden systematisch zur Modellkalibrierung verwendet und die damit verbundenen Parameter- und Vorhersageunsicherheiten für die Grundwasserneubildung quantifiziert. Basierend auf unseren Ergebnissen für den untersuchten Standort empfehlen wir die Kombination von Sickerwasser- und Matrixpotentialmessungen, um die Unsicherheit in der Grundwasserneubildungsvorhersage zu minimieren. Um eine allgemeingültige Empfehlung für andere Böden oder Klimazonen auszusprechen, ist jedoch eine umfassendere Analyse nötig.

Schlagwörter: Bayessche Statistik, Lysimetermodellierung, Grundwasserneubildung

Summary

Deterministic models are applicable for the simulation of groundwater recharge. Parameters can be inversely estimated using measurements of soil water content, matric potential and seepage. However, it is not well understood how the type of observations used for model calibration affects associated model uncertainties which was specifically assessed in this study applying a Bayesian analysis. Data from a monolithic Gumpenstein lysimeter was systematically used for calibration and quantification of associated parameter and predictive uncertainties in groundwater recharge estimation. Based on our results for the investigated site, we recommend simultaneous assimilation of lysimeter seepage and matric potential measurements to minimize uncertainty in groundwater recharge prediction. However, a more comprehensive analysis is required to make a generally valid recommendation for other soils or climates.

Keywords: Bayesian statistics, lysimeter modelling, groundwater recharge estimation

Introduction

Knowledge on water recharging aquifers through the vadose zone is essential for a sustainable use of groundwater (Taylor et al. 2013). However, groundwater recharge rates are difficult to determine in practice. Lysimeter experiments generally provide an important tool for the estimation of water fluxes combined with physically based models the information from lysimeter experiments can be used for improved model calibration and for the simulation of groundwater recharge rates at the field scale. The improved, inverse model calibration is required for the identification of soil hydraulic properties

¹ University of Natural Resources and Life Sciences (BOKU) Vienna, Institute for Soil Physics and Rural Water Management, Muthgasse 18, A-1190 Vienna

* Ansprechpartner: Marleen Schübl, email: marleen.schuebl@boku.ac.at

(SHP) from in-situ measurements because SHP from laboratory experiments can only be poorly transferred to field conditions. However, inverse calibration can be associated with uncertainties resulting from different sources of systematic or random errors (Beven 2006, Vereecken et al. 2016) which propagate further into the recharge prediction. The extent of the model uncertainty depends for example on the type and combination of data that is assimilated in the model. For an efficient soil water monitoring design that is aimed at the estimation of groundwater recharge, it would therefore be helpful to identify which information is needed or best suited for the reduction of uncertainty in groundwater recharge prediction.

Therefore, a Bayesian framework is used for estimating model uncertainties in HYDRUS-1D in different scenarios when assimilating time series of soil water content, matric potential and seepage data obtained from a monolithic lysimeter experiment in Gumpenstein, Styria, Austria. The uncertainty in groundwater recharge prediction is evaluated accordingly.

Material and Methods

Inverse estimation of soil hydraulic properties in HYDRUS 1-D

The HYDRUS-1D software numerically solves water flow equations in variably saturated porous media accounting for plant water uptake. The relation between soil pressure head and soil water content is given by the van-Genuchten-Mualem model (VGM) (Šimůnek et al. 2008). The SHP can be inversely estimated by minimizing the difference between simulated and the observed variables. Three different types of observations are used for assimilation in this study in different scenarios (*Table 1*): daily measurements of volumetric soil water content and matric potential in two depths (25 and 45 cm), and daily amounts of seepage obtained from the lysimeter in 1.5 m depth. Setting the lower boundary condition to seepage face, the software is used to simulate the seepage flux in 1.5 m depth as approximation to the groundwater recharge flux.

Bayesian analysis

HYDRUS-1D is coupled with a Bayesian framework for estimating model uncertainties. It is used to integrate a priori knowledge of the system in the statistical inference, to combine it with the observed data in order to derive the posterior probabilities of model parameters. Given several measurement types, the resulting data likelihood is aggregated as the product of likelihoods from the individual data types. For each type of measurement, an uncorrelated normally distributed measurement error is assumed and estimated alongside with the model parameters. Different subsets of observed soil water data were included in the Bayesian analysis for the evaluation of the data's effectiveness in constraining model predictive uncertainties similar to Brunetti et al. (2020). The Affine invariant ensemble sampling algorithm emcee (Foreman-Mackey et al. 2013) is used in combination with HYDRUS-1D (Brunetti et al. 2019) to efficiently draw samples from the posterior distribution until a convergence criterion is met.

Table 1. Scenarios for the assimilation of measured variables (volumetric soil water content and matric potential measured in 25 and 45 cm depth; seepage collected from the lysimeter at 1.5 m depth) using HYDRUS-1D.

Scenario A	Seepage & matric potential
Scenario B	Seepage
Scenario C	Seepage & matric potential & vol. soil water content
Scenario D	Seepage & vol. soil water content
Scenario E	Matric potential & vol. soil water content
Scenario F	Matric potential
Scenario G	Vol. soil water content

Results and Discussion

The scenarios in *Table 1* are sorted by decreasing model response variance (A-G). Posterior predictive checks showed that the lowest uncertainty in groundwater recharge prediction was achieved with the simultaneous assimilation of seepage and matric potential measurements (Scenario A) which provided an improvement compared to the assimilation of seepage measurements alone (Scenario B). Additional information from soil water content measurements (Scenario C) reduced parameter uncertainties, especially in the residual and saturated water content. However, it did not further reduce the uncertainty in groundwater recharge prediction. The marginal and joint parameter uncertainties for Scenario A is shown in *Figure 1*, the resulting uncertainties in groundwater recharge prediction are shown in *Figure 2*. The Scenarios that did not involve assimilation of seepage data (scenarios E-G) resulted in the largest uncertainties in the prediction of groundwater recharge.

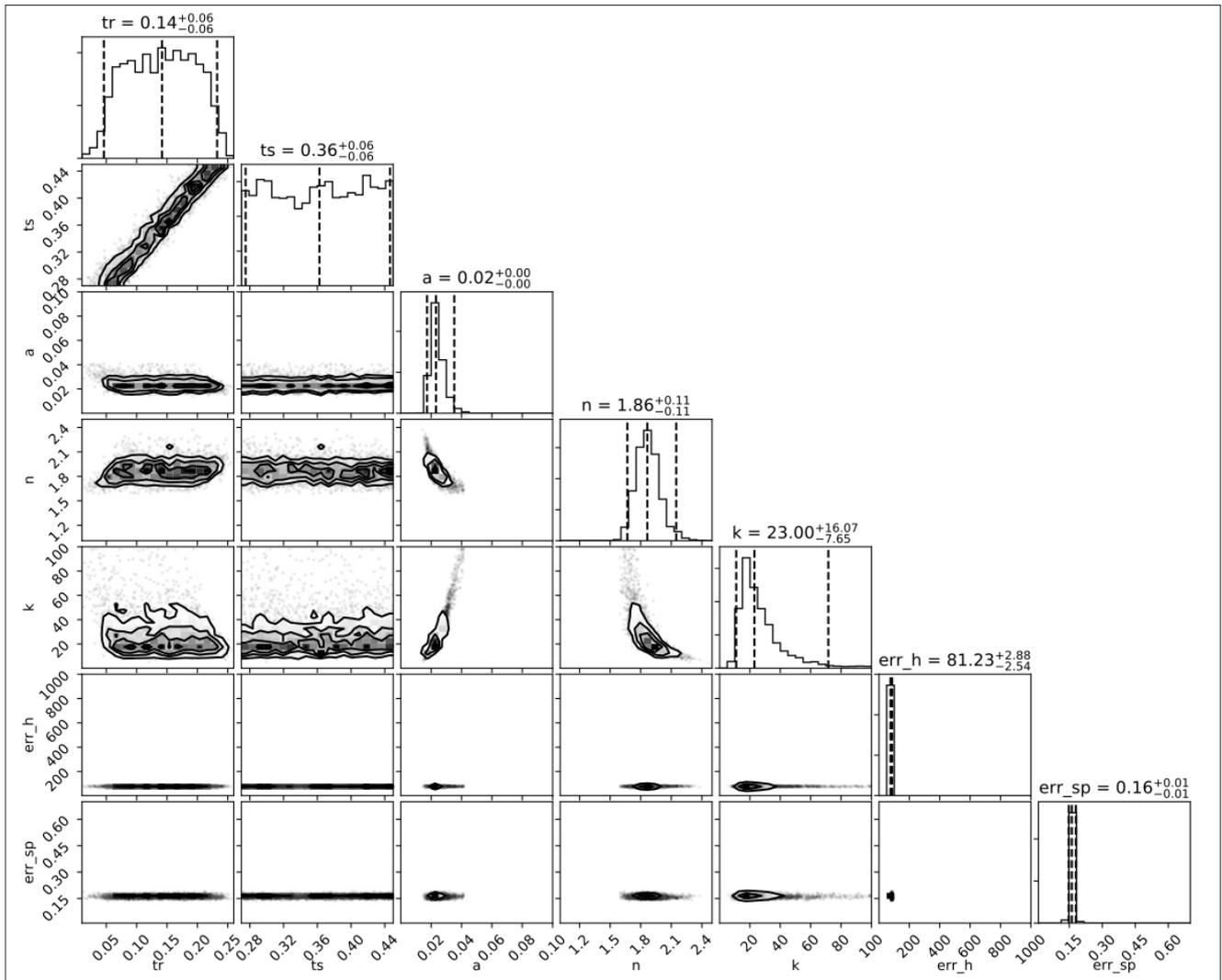
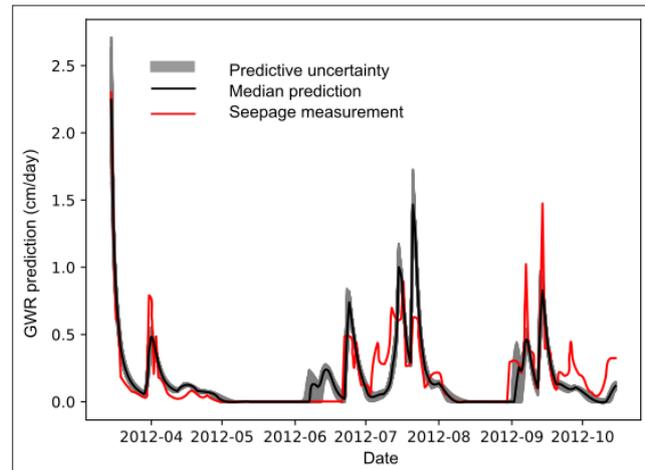


Figure 1. Uncertainties in SHP and measurement errors for Scenario A (assimilation of seepage and matric potential measurements): tr = residual water content ($\text{cm}^3 \text{cm}^{-3}$), ts = saturated water content ($\text{cm}^3 \text{cm}^{-3}$), a = VGM shape parameter α (cm^{-1}), n = VGM shape parameter n (-), k = saturated hydraulic conductivity (cm d^{-1}), err_h = measurement error in matric potential (hPa), err_sp = measurement error in seepage measurement (cm). Upper panels of each column depict the marginal posterior distributions of each parameter. Numbers are given for the median value and the 95% uncertainty range, drawn as dashed lines. The lower panels in each column show the joint posterior distribution of two parameters each.

Figure 2. Posterior uncertainty in groundwater recharge (GWR) prediction according to Scenario A compared to lysimeter measurements (red) for the model calibration period.



Conclusion and Outlook

This study provides an example for the applicability of a Bayesian analysis with real data from a lysimeter experiment for determining uncertainties in the inverse estimation of SHP and the associated uncertainty in groundwater recharge prediction. Based on our results for the investigated site, we recommend simultaneous assimilation of lysimeter seepage and matric potential measurements to minimize uncertainty in groundwater recharge prediction. In order to make general recommendations for an efficient soil water monitoring design for the simulation of groundwater recharge, a more comprehensive analysis is required for other soils or climates.

References

- Beven K. (2006) A manifesto for the equifinality thesis. *Journal of Hydrology*, 320(1-2), 18-36.
- Brunetti G., Šimůnek J., Bogena H., Baatz R., Huisman J.A., Dahlke H., Vereecken H. (2019) On the Information Content of Cosmic-Ray Neutron Data in the Inverse Estimation of Soil Hydraulic Properties. *Vadose Zone Journal*, 18(1), 1-24.
- Brunetti G., Papagrorgiou I.A., Stumpp C. (2020) Disentangling model complexity in green roof hydrological analysis: A Bayesian perspective. *Water Research*, 182.
- Foreman-Mackey D., Hogg D.W., Lang D., Goodman J. (2013) emcee: The MCMC Hammer. *Publications of the Astronomical Society of the Pacific*, 125(925), 306-312.
- Šimůnek J., van Genuchten M.T., Šejna M. (2008) Development and Applications of the HYDRUS and STANMOD Software Packages and Related Codes. *Vadose Zone Journal*, 7(2), 587-600.
- Taylor R.G., Scanlon B., Döll P., Rodell M., Van Beek R., Wada Y., Longuevergne L., Leblanc M., Famiglietti J.S., Edmunds M., Konikow L., Green T.R., Chen J., Taniguchi M., Bierkens M.F.P., Macdonald A., Fan Y., Maxwell R.M., Yechieli Y., et al. (2013) Ground water and climate change. *Nature Climate Change*, 3(4), 322-329.
- Vereecken H., Schnepf A., Hopmans J.W., Javaux M., Or D., Roose T., Vanderborght J., Young M.H., Amelung W., Aitkenhead M., Allison S.D., Assouline S., Baveye P., Berli M., Brüggemann N., Finke P., Flury M., Gaiser T., Govers G., et al. (2016) Modeling Soil Processes: Review, Key Challenges, and New Perspectives. *Vadose Zone Journal*, 15(5), vzj2015.09.0131.