Electronic Supplementary Material (ESI) for Environmental Science: Processes & Impacts

Bayesian uncertainty assessment of a semi-distributed integrated catchment model of phosphorus transport

Jostein Starrfelt & Øyvind Kaste.

Supplementary material. MCMC-DREAM parameters, posterior distributions, covariance structure and error model.

Table S 1. Parameters used for the MCMC-DREAM algorithm. For details see Vrugt et al. (2009)

Parameter	Value
N - number of chains	40
n_{CR} - number of crossover values	6
δ - maximum number of pairs of chains from which proposals are affected	3
t_{γ} - Number of iterations between each use of full step-size	5
b - width of uniform distribution of e	0.05
b^* - variance of normal distribution of ε	10e-4

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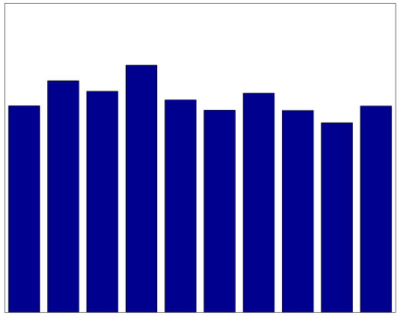
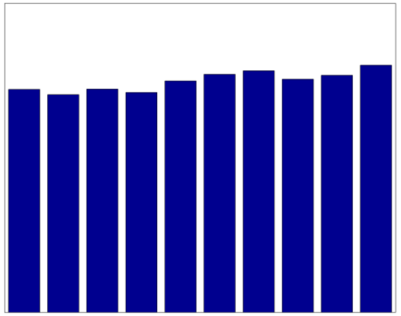
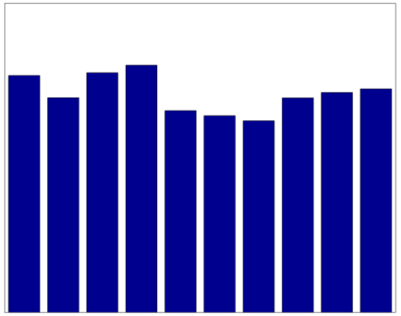
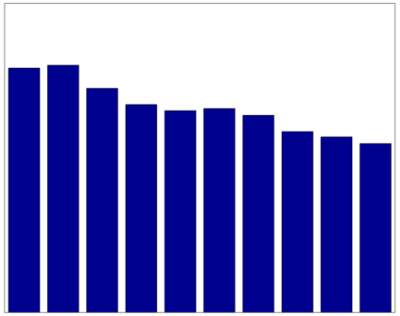
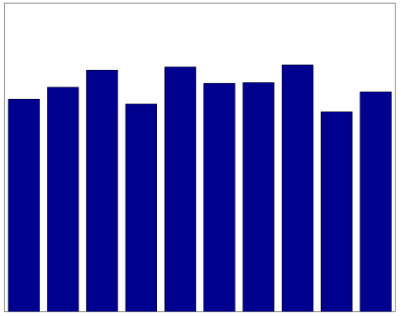
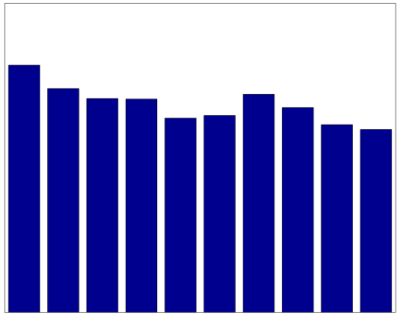
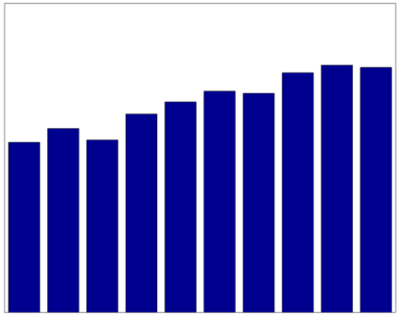
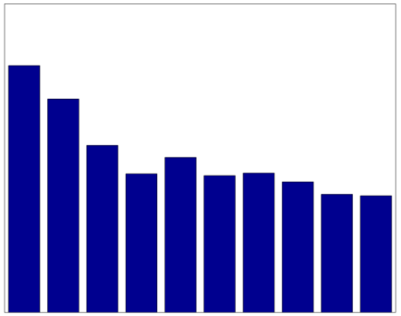
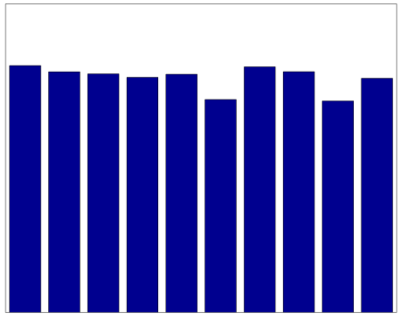
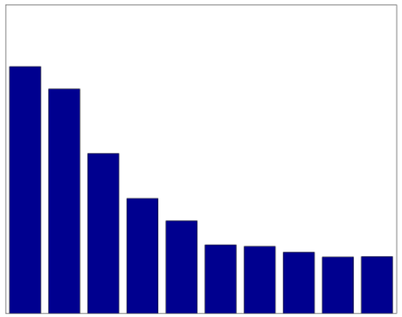
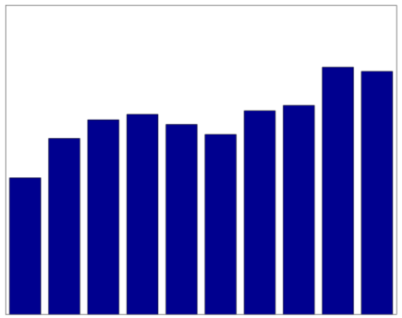
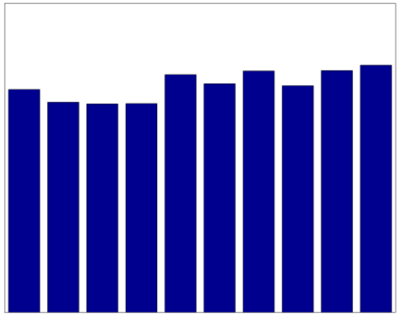
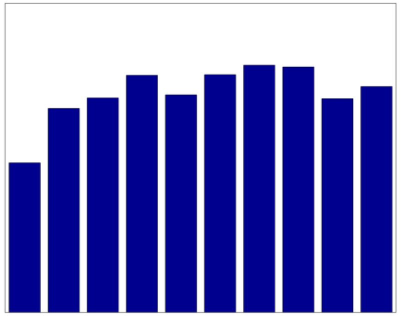
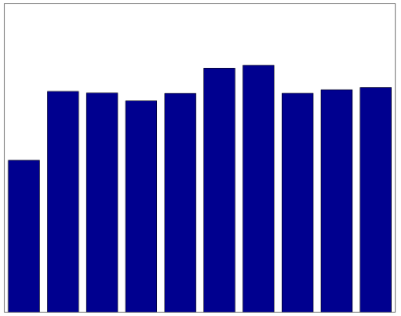
Table S 2: Parameters estimated in the analysis. All priors were given uniform distributions. Histograms of posteriors are plotted using the whole range for the priors with 10 histogram classes. All distributions were collected from converged chains for 2500 iterations, i.e. 100.000 simulations of INCA-P. For reach/subcatchment 5 the parameters estimated for reach 4 was assumed in the posterior predictive simulations.

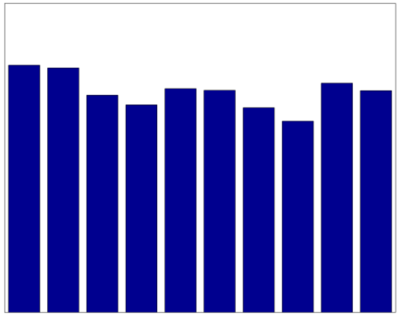
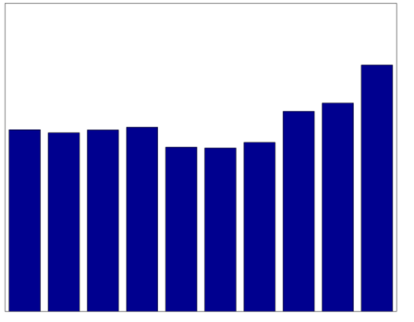
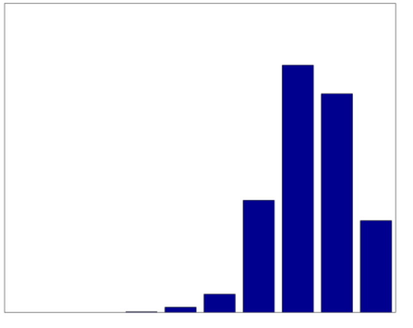
Name	Minimum value	Maximum value	Parameter for which land use, reach or subcatchment.	Posterior distribution
soil inactive P concentration (mg/l)	300	25000	Wetland	
splash detachment soil erodibility parameter ($kg/m^2/s$)	0.0001	0.1	Wetland	

flow erosion soil erodibility parameter (kg/m²/s)	0.0001	0.5	Wetland	
splash detachment a parameter (s/m)	0.05	15	Wetland	
immobilisation rate	0.005	0.5	Wetland	

equilibrium phosphorus concentration of the soil matrix (mg P/l)	0.002	0.1	Wetland	
direct runoff time constant (days)	0.1	1.2	Wetland	
soil reactive zone time constant (days)	0.8	15	Wetland	

soil water retention volume constant (ø)	1	4	Wetland	
soil inactive P concentration (mg/l)	300	25000	Forest	
splash detachment soil erodibility parameter (kg/m²/s)	0.0001	0.1	Forest	

flow erosion soil erodibility parameter ($kg/m^2/s$)	0.0001	0.5	Forest	
splash detachment a parameter (s/m)	0.05	15	Forest	
immobilisation rate	0.005	0.5	Forest	5 

equilibrium phosphorus concentration of the soil matrix (mg P/l)	0.002	0.1	Forest	
direct runoff time constant (days)	0.1	1.2	Forest	
soil reactive zone time constant (days)	0.8	15	Forest	

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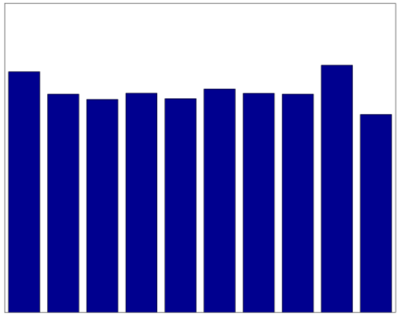
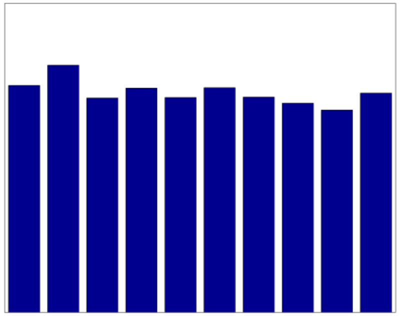
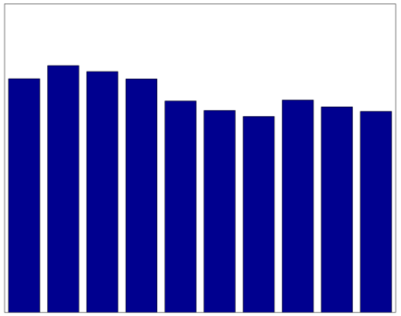
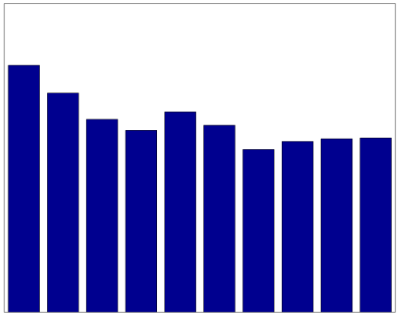
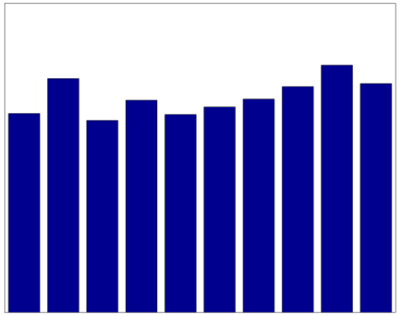
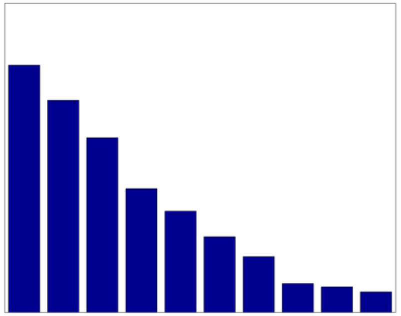
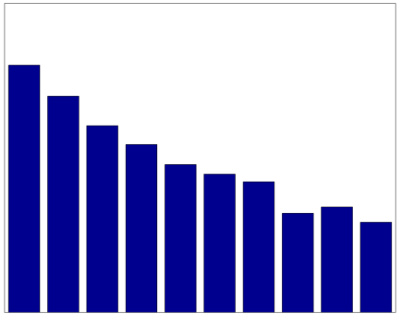
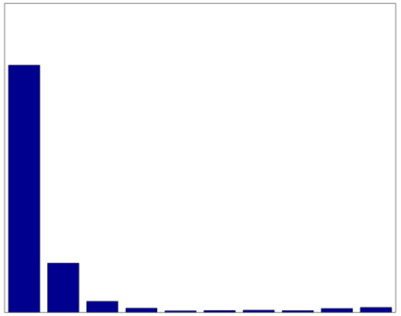
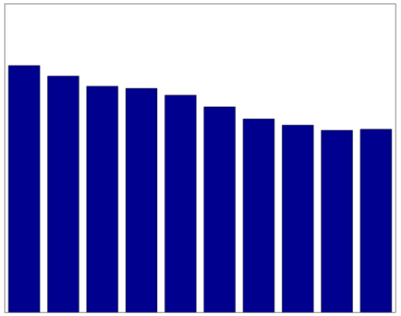
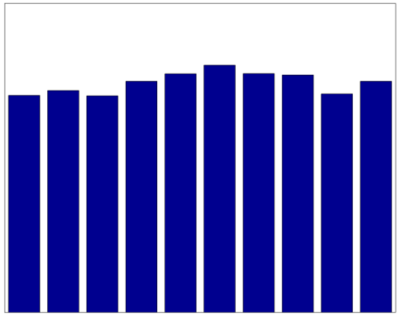
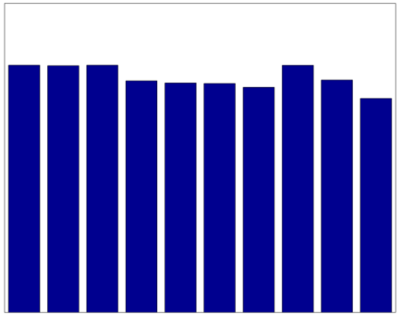
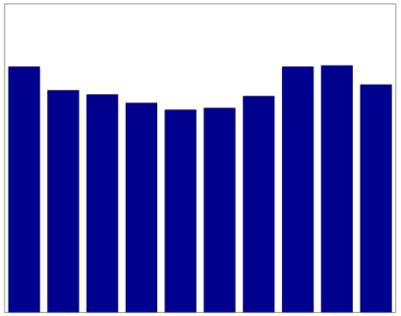
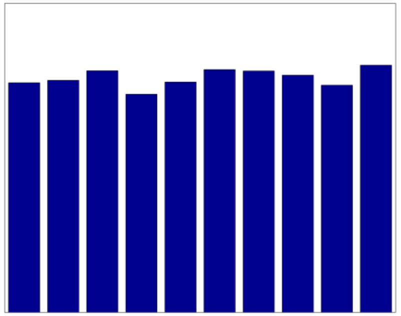
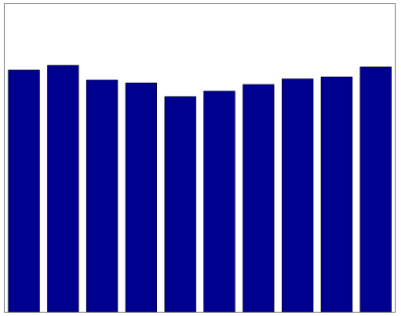
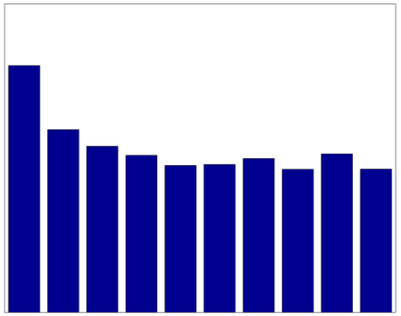
soil water retention volume constant (ø)	1	4	Forest	
soil inactive P concentration (mg/l)	300	25000	Grass	
direct runoff time constant (days)	0.1	1.2	Grass	

soil reactive zone time constant (days)	0.8	15	Grass	
soil water retention volume constant (ø)	1	4	Grass	
soil inactive P concentration (mg/l)	300	25000	Crops	

direct runoff time constant (days)	0.1	1.2	Crops	
soil reactive zone time constant (days)	0.8	15	Crops	
soil water retention volume constant (ø)	1	4	Crops	

soil inactive P concentration (mg/l)	300	25000	Vegetables	
direct runoff time constant (days)	0.1	1.2	Vegetables	
soil reactive zone time constant (days)	0.8	15	Vegetables	

soil water retention volume constant (ø)	1	4	Vegetables	
sorption coefficient for the soil matrix (dm^3/day)	100	250	Same for all Land use S	
splash detachment soil erodibility parameter ($kg/m^2/s$)	0.0001	0.1	Same for Grass, Crops and Vegetables	

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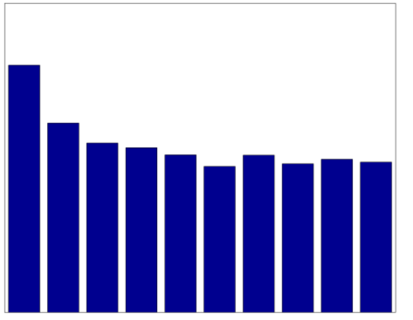
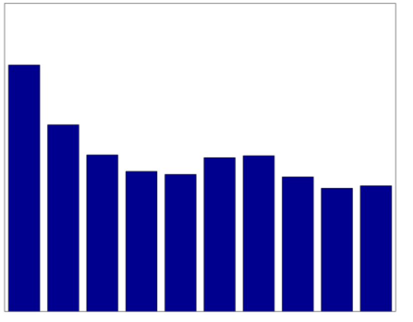
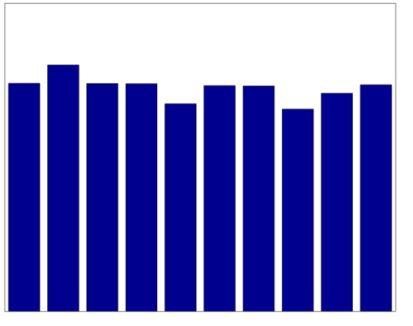
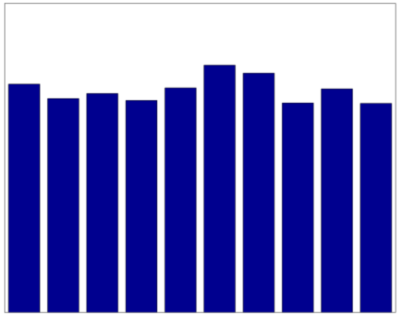
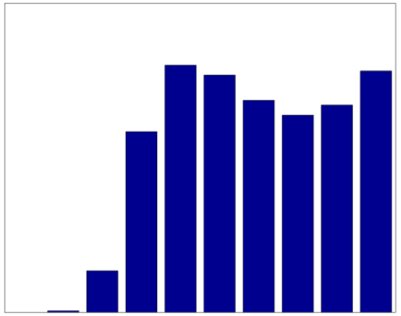
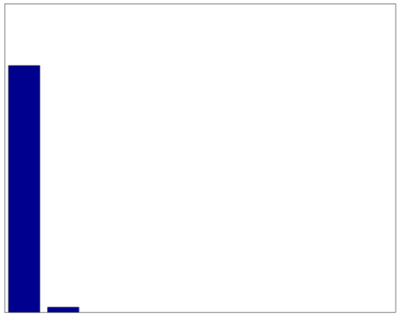
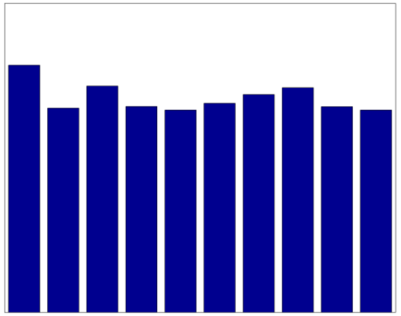
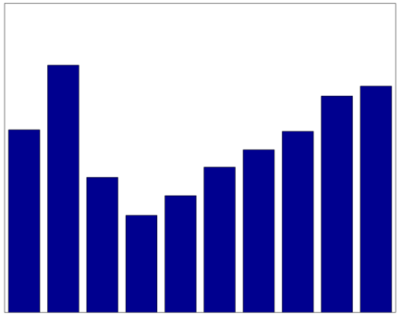
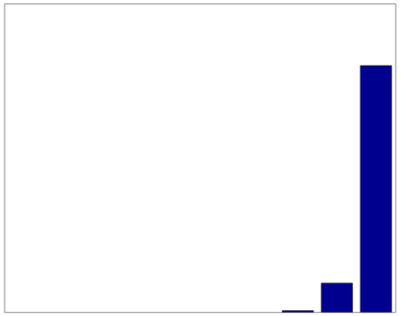
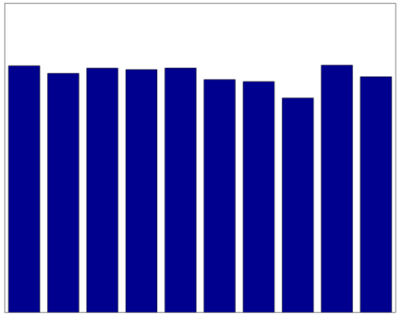
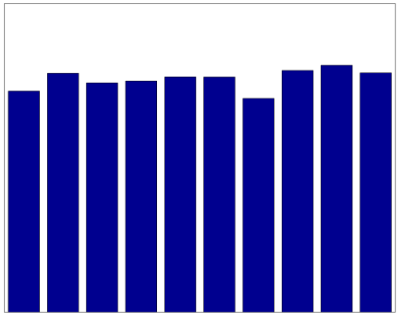
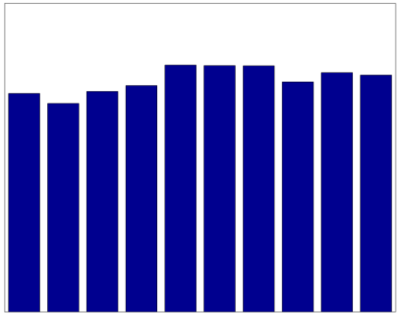
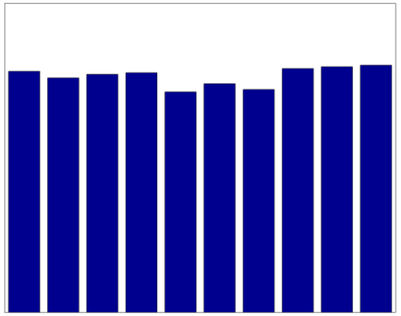
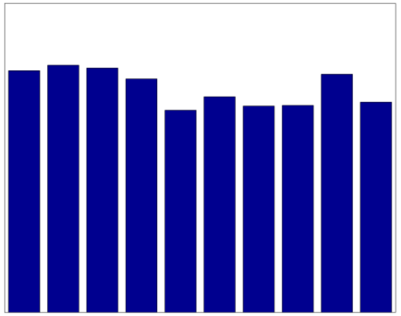
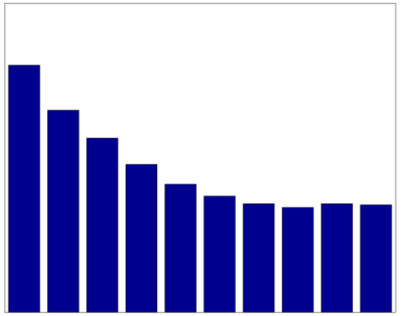
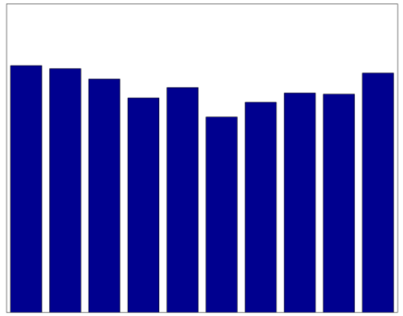
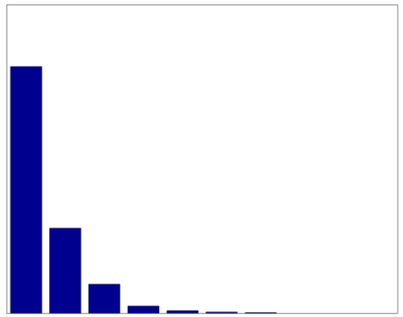
flow erosion soil erodibility parameter ($kg/m^2/s$)	0.0001	0.5	Same for Grass, Crops and Vegetables	
splash detachment a parameter (s/m)	0.05	15	Same for Grass, Crops and Vegetables	
immobilisation rate	0.005	0.5	Same for Grass, Crops and Vegetables	

equilibrium phosphorus concentration of the soil matrix (mg P/l)	0.002	0.1	Same for Grass, Crops and Vegetables	
threshold soil zone flow (m3/s)	0.02	0.2	Same for all subcatchments	
Base Flow Index (ø)	0.1	0.8	Same for all subcatchments	

flow erosion scaling factor (ø)	7	15	Same for all subcatchments	
Flow a (/m²)	0.02	0.5	Same for all subcatchments	
Flow b (ø)	0.1	1	Same for all subcatchments	

equilibrium phosphorus concentration of the aquifer matrix (mg P/l)	0.01	0.5	Subcatchment 1	
equilibrium phosphorus concentration of the aquifer matrix (mg P/l)	0.01	0.5	Subcatchment 2	
equilibrium phosphorus concentration of the aquifer matrix (mg P/l)	0.01	0.5	Subcatchment 3	

equilibrium phosphorus concentration of the aquifer matrix (mg P/l)	0.01	0.5	Subcatchment 4	
Water column equilibrium phosphorus concentration (mg P/l)	0.001	1	Same for all reaches	
Stream bed equilibrium phosphorus concentration (mg P/l)	0.001	1	Same for all reaches	

P exchange (water column/pore water) ***(/day)***	0.001	4	Same in all reaches	
Effluent scaling (ø)	0.5	2	For effluent inputs in all reaches.	

Covariance structure

When only inspecting the probability distributions (table S 2) in one dimension at a time, the full level of information gathered by our Bayesian inference scheme is often not appreciated. All these parameter distributions also have a covariance (and higher moments), which can easily be seen from the figure below. Here we have plotted parameters 'direct runoff time constant' for land use category 2 and 'flow a' from the list above against each other. The smoothed density plot in the upper left panel shows clearly that higher values of the flow a parameter is most often associated with higher values of the time constant, which cannot be seen from single parameter distributions. This covariance is taken into account in our posterior predictive simulations by always sampling parameters from the chains themselves and not from the single parameter distributions.

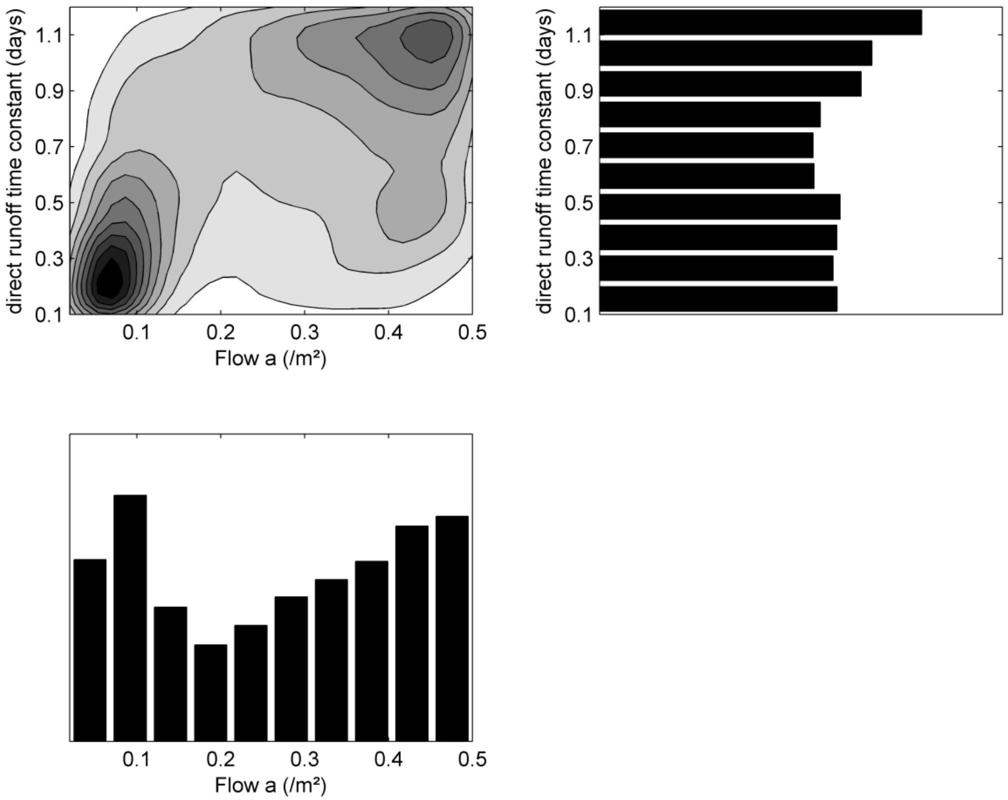
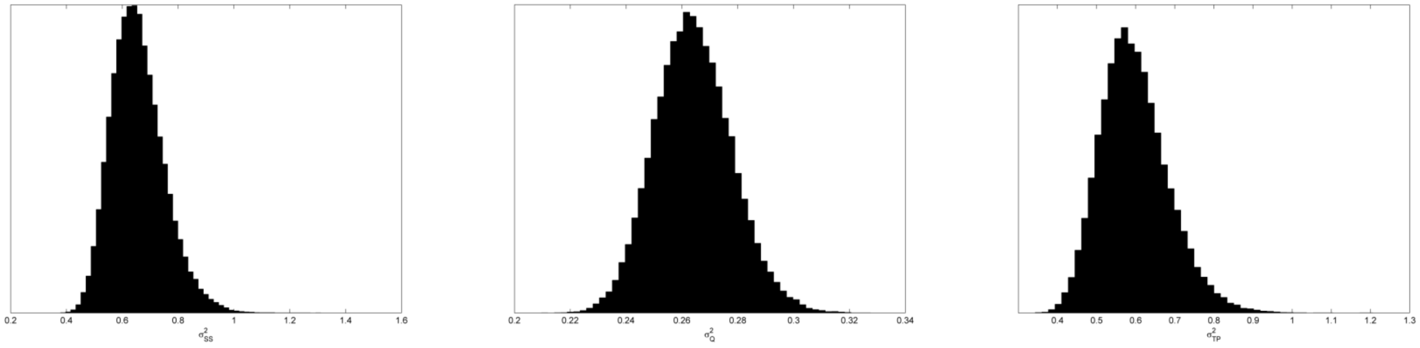


Figure legend Supplementary material, figure S.1.

Distribution of the converged chains for parameters 'Flow a' (m^{-2}) for all reaches and the time constant scaling the resident time of the direct runoff box in the land phase for land use category 2. Top left shows the smoothed probability density of the converged chains in two dimensions, where darker areas indicate higher probability. Top right shows the marginal distribution for the time constant alone and bottom left shows the marginal distribution for the 'Flow a' parameter. The strong covariance is not visible from the single parameter marginal distributions alone.

Parameters of the error model.

In addition to the parameters estimated by the MCMC-DREAM algorithm the error variances (i.e. the expected deviation from the model predictions) was sampled by Gibbs sampling. By assuming a particular shape (here Gamma distributed) of the inverse prior of the error variances we can derive a posterior distribution using values from imaginary (pseudo-) observations and sum of squares of deviations from a particular parameter set. See the pseudocode for the definition of the posterior.



Refernces

Vrugt JA, ter Braak CJF, Diks CGH, Robinson BA, Hyman JM, Higdon D. Accelerating Markov Chain Monte Carlo Simulation by Differential Evolution with Self-Adaptive Randomized Subspace Sampling. International Journal of Nonlinear Sciences and Numerical Simulation 2009; 10: 273-290.