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Supplement of

Using a surrogate-assisted Bayesian framework to calibrate the runoff-generation scheme in the Energy Exascale Earth System Model (E3SM) v1

Donghui Xu et al.

Correspondence to: Donghui Xu (donghui.xu@pnnl.gov)

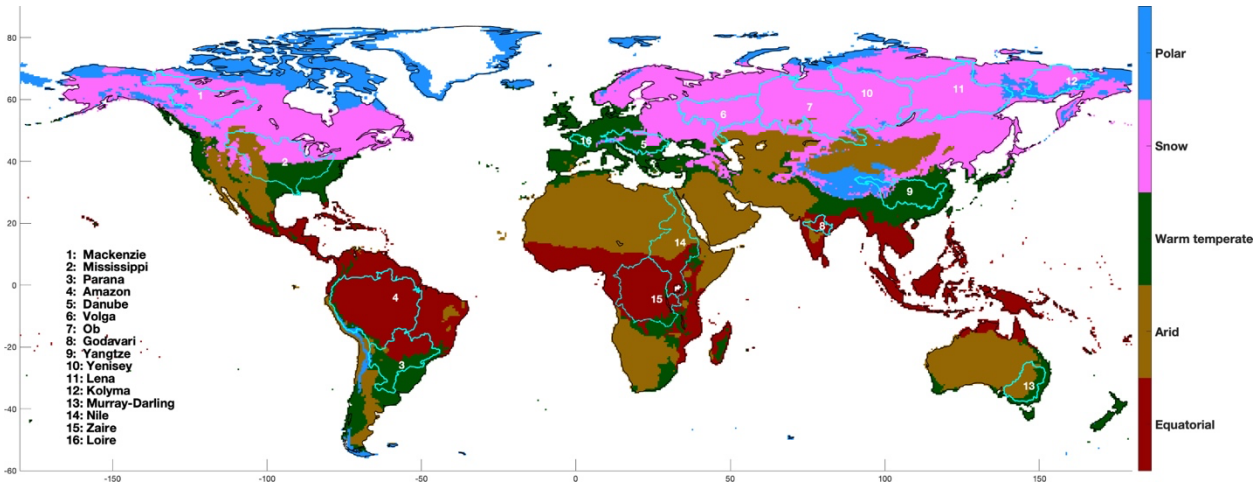

Figure S1. Köppen climate classification with selected major basin boundaries.

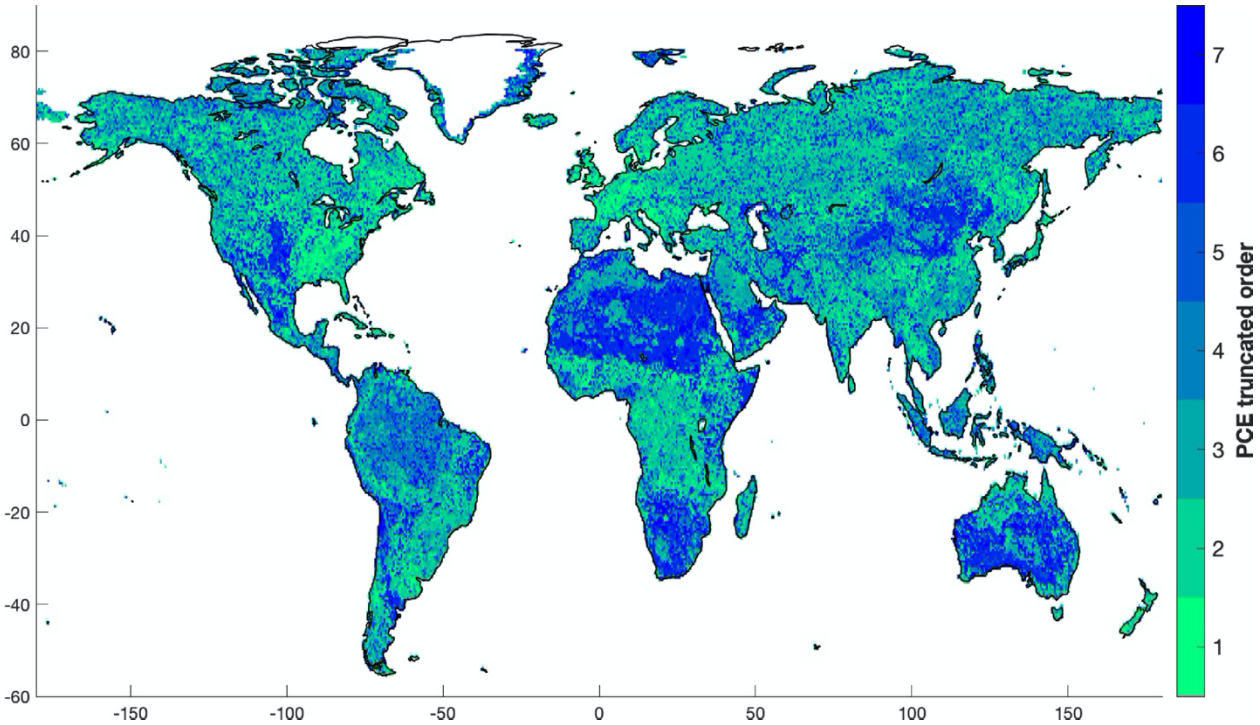

Figure S2. Truncated order of the constructed PCE with best performance.

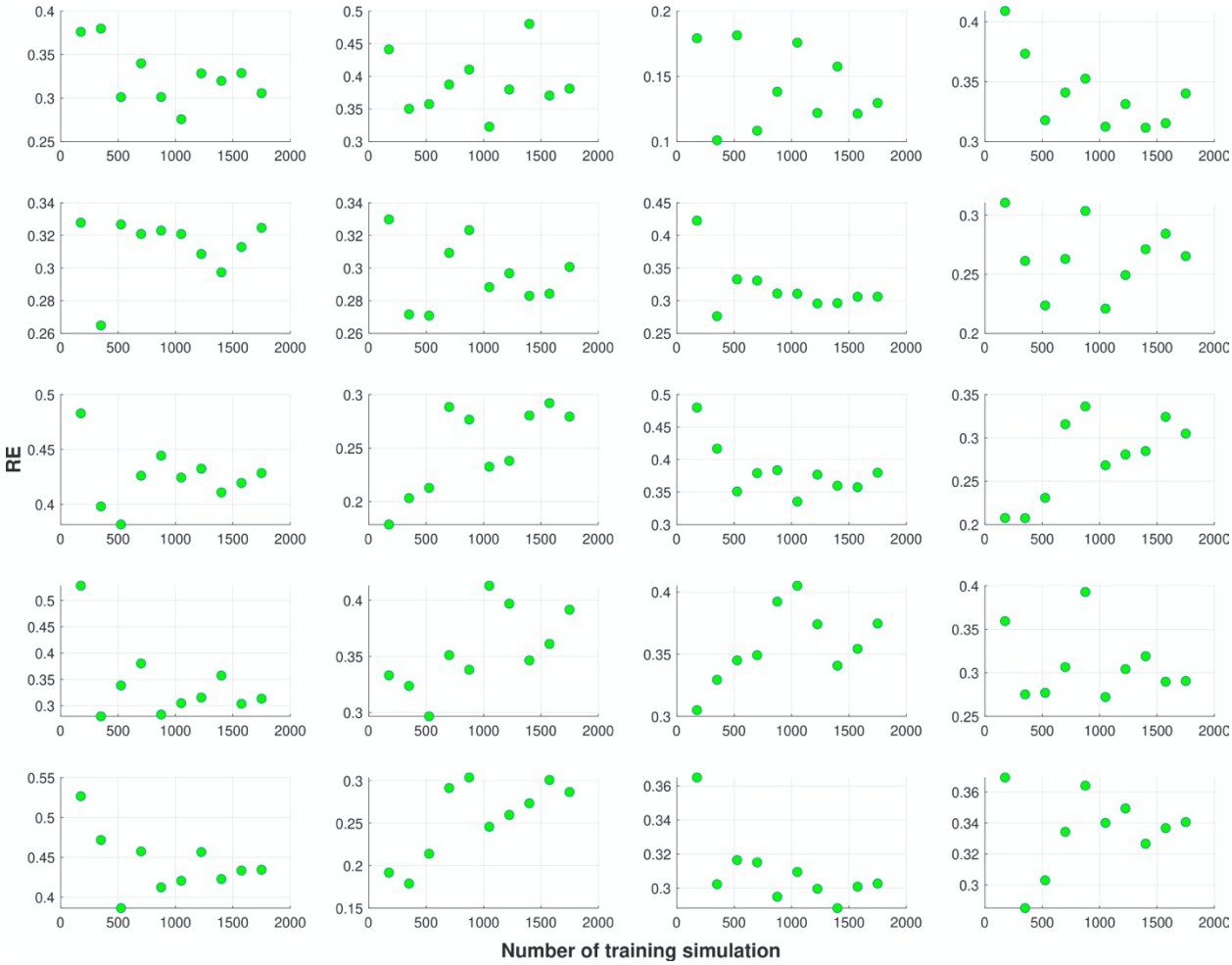

Figure S3. Test the performance of PCE-based surrogate models with different number of training simulation with 20 example grid cells from arid regions.

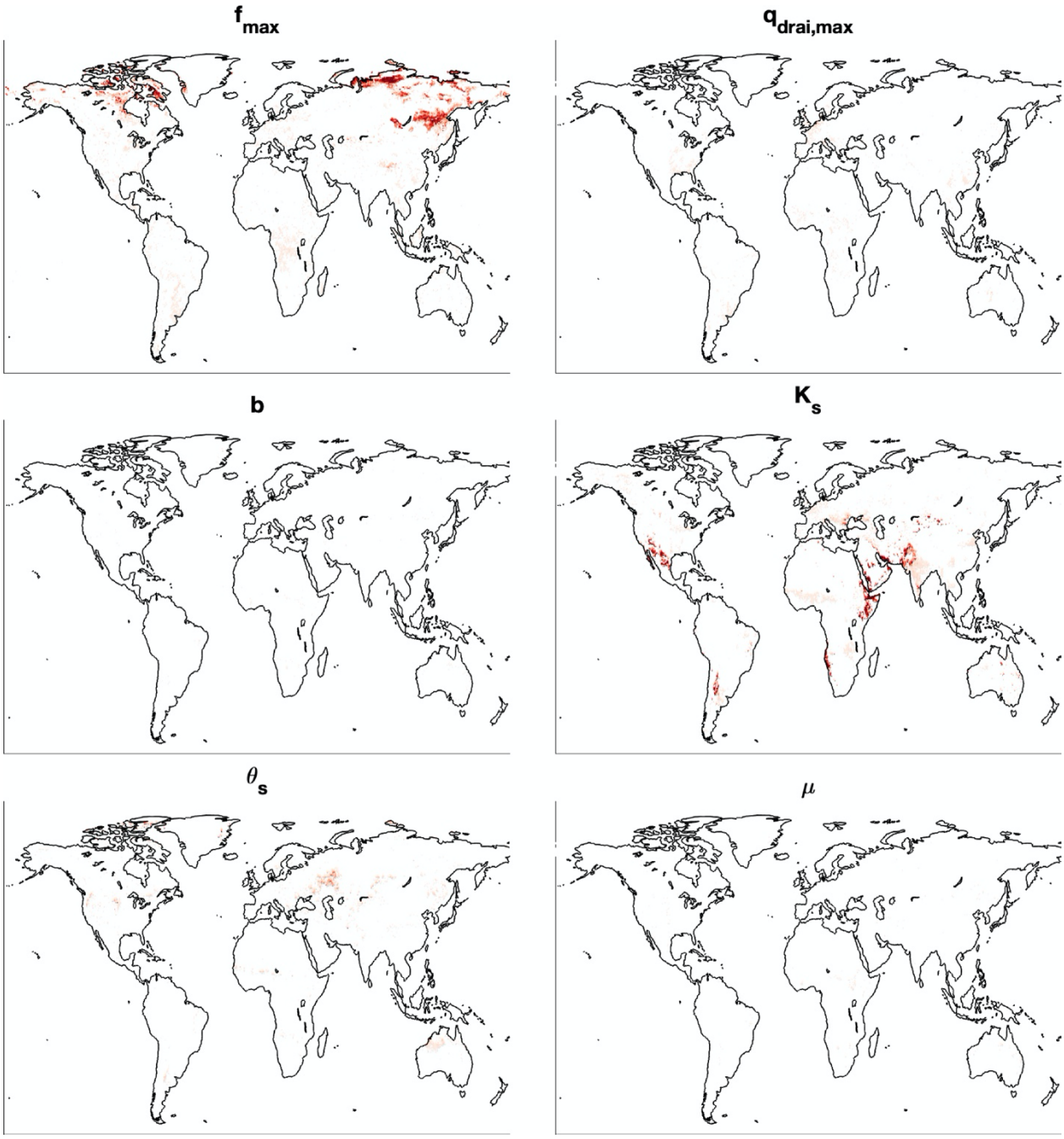

Figure S4. Spatial distribution of main Sobol index for the less sensitive parameters.

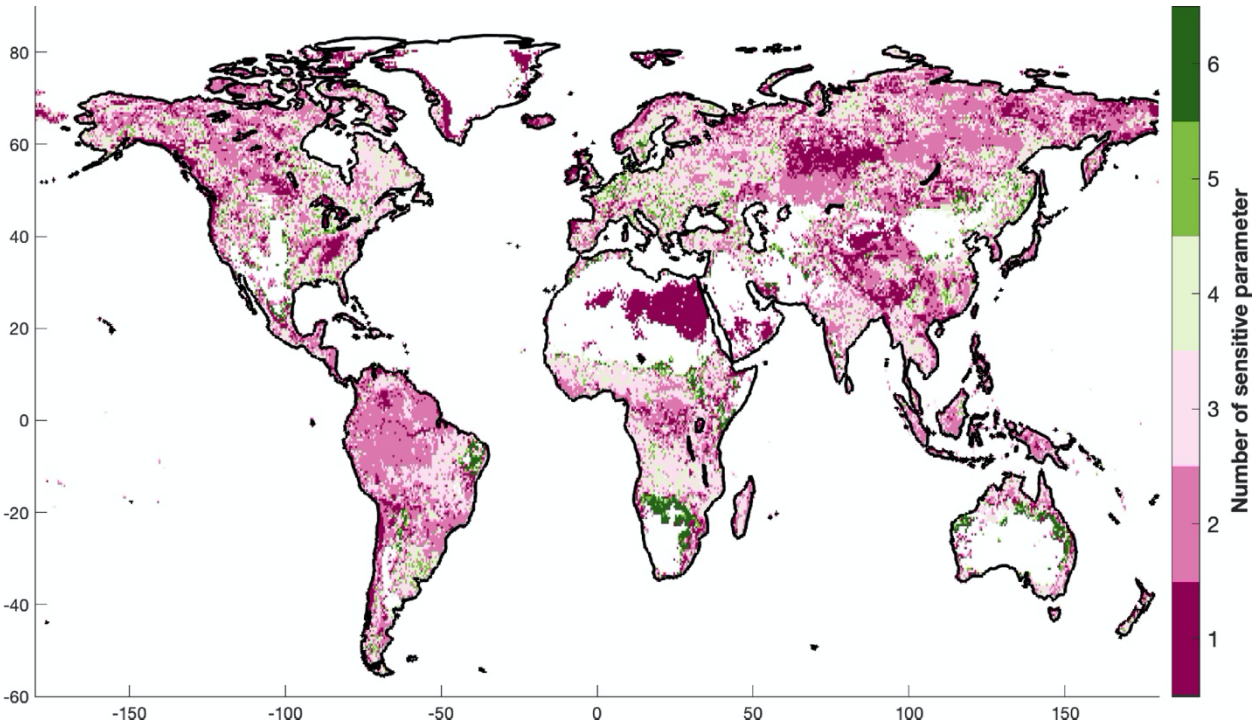

Figure S5. Number of significant parameters for runoff generation. A parameter is regarded as significant if its main Sobol index is larger than 0.05. The cells with relative errors of surrogate models higher than 0.15 are excluded here.

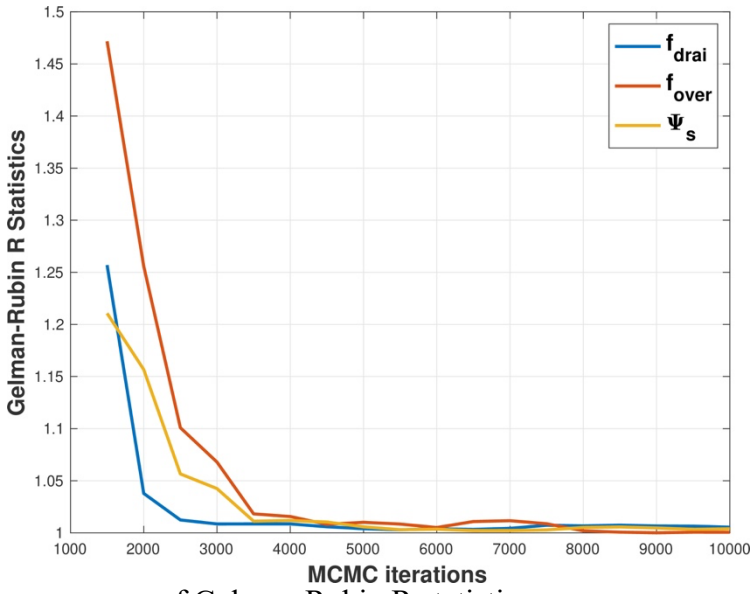

Figure S6. Convergence curve of Gelman-Rubin R statistics

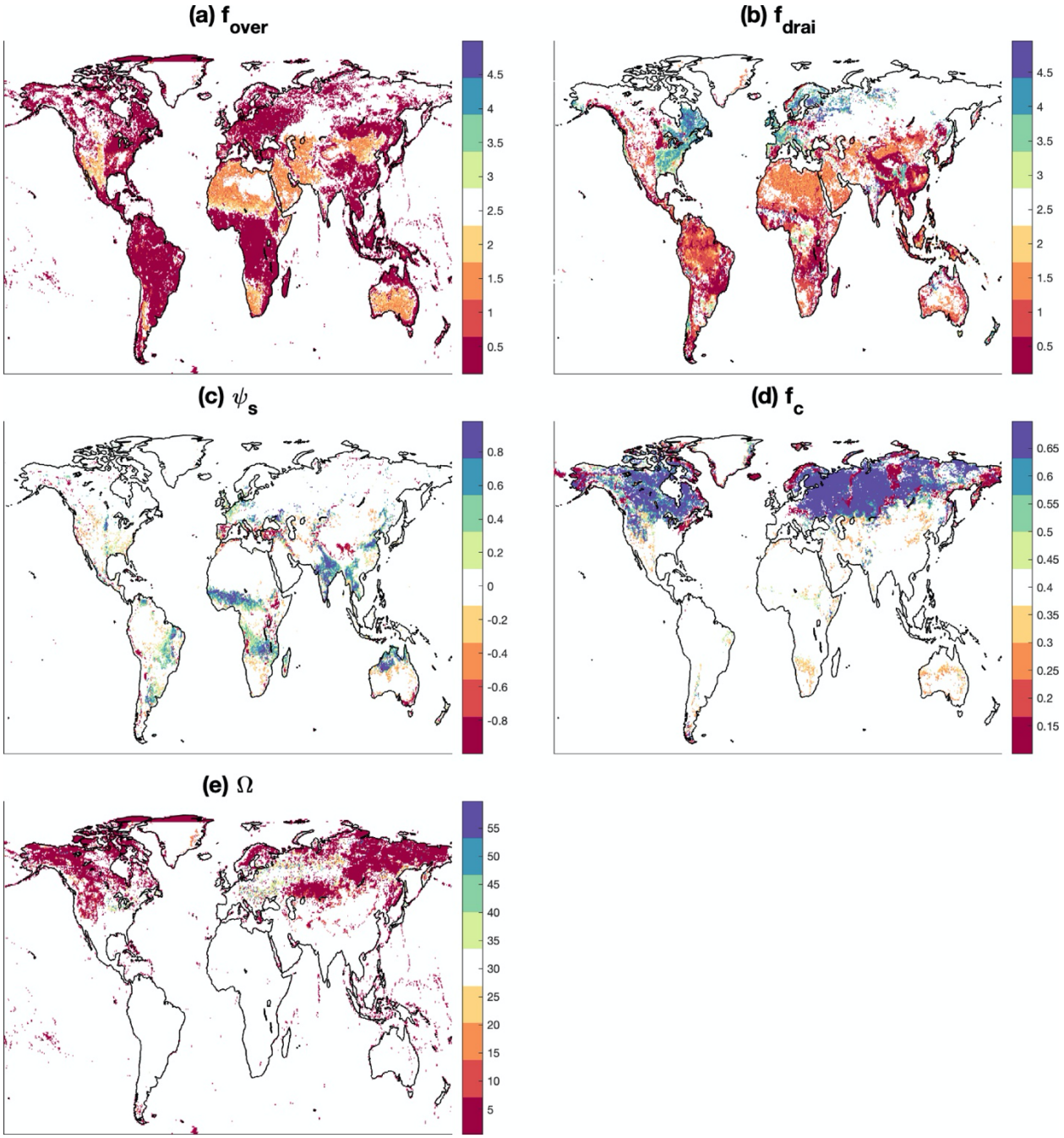

Figure S7. Parameter values at 5% of the posterior. There are no certainty bounds for ψ_s from different grid cells because it is determined by the soil properties. Therefore, the values of ψ_s are scaled to [-1, 1] in subplot (c) for each grid cell with the corresponding upper bound ($\psi_{s,max}$) and lower bound ($\psi_{s,min}$): $\frac{2}{\psi_{s,max}-\psi_{s,min}}\psi_s - \frac{\psi_{s,max}+\psi_{s,min}}{\psi_{s,max}-\psi_{s,min}}$.

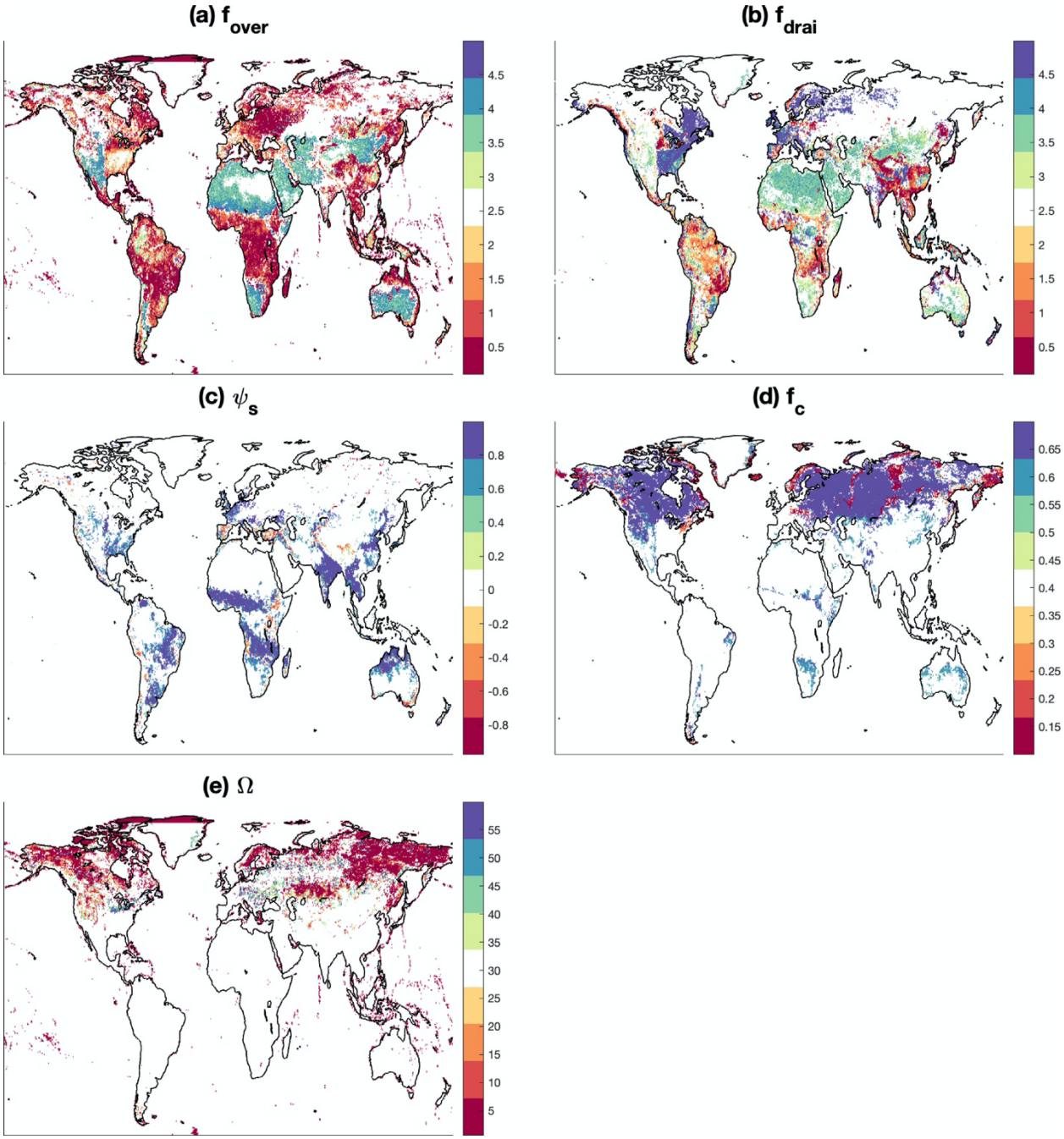

Figure S8. Parameter values at 95% of the posterior. There are no certainty bounds for ψ_s from different grid cells because it is determined by the soil properties. Therefore, the values of ψ_s are scaled to [-1, 1] in subplot (c) for each grid cell with the corresponding upper bound ($\psi_{s,max}$) and lower bound ($\psi_{s,min}$): $\frac{2}{\psi_{s,max}-\psi_{s,min}}\psi_s - \frac{\psi_{s,max}+\psi_{s,min}}{\psi_{s,max}-\psi_{s,min}}$.

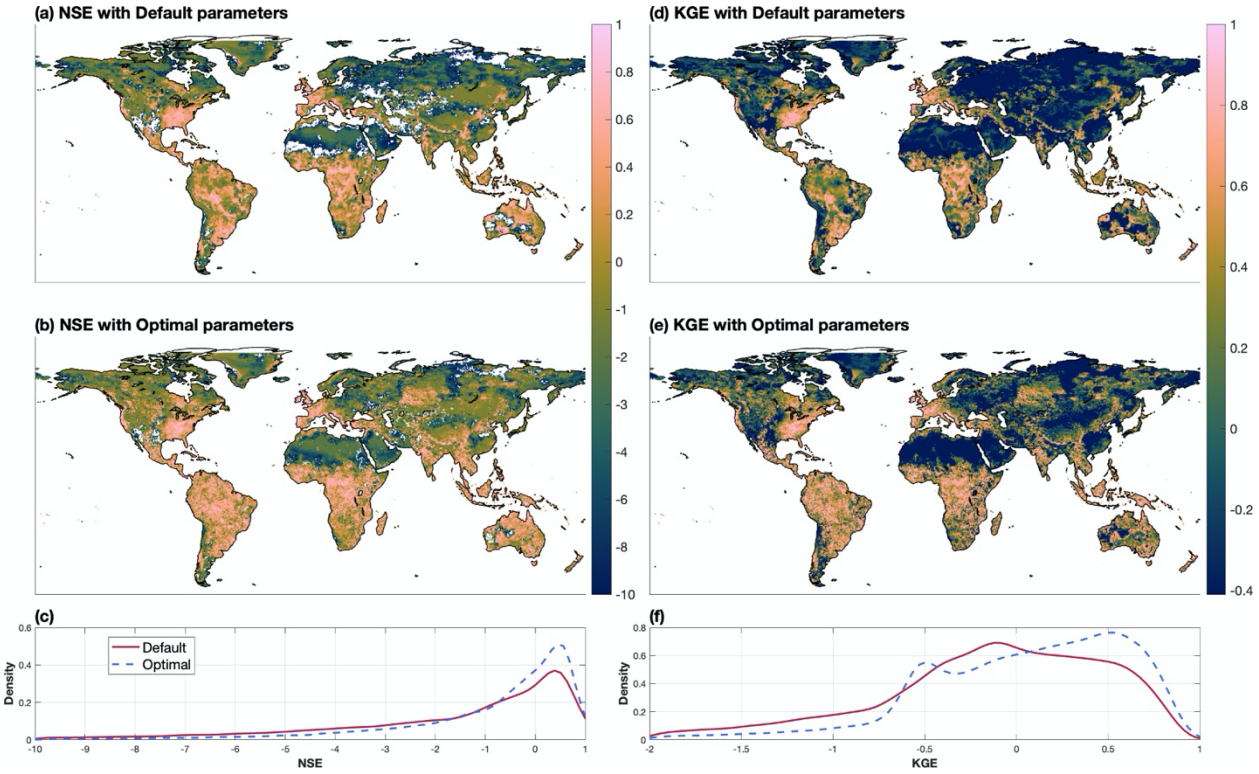

Figure S9. Evaluation of simulated monthly runoff for 2011-2013 at grid level with default and optimal parameters. Subplot (a) and (b) show the NSE metrics between the GRUN runoff and simulated runoff with default and optimal parameter, respectively. Subplot (c) shows the comparison of the probability density function (PDF) of NSE metrics from all the global grid cells. Subplot (d), (e), and (f) illustrate the evolution with KGE metric.

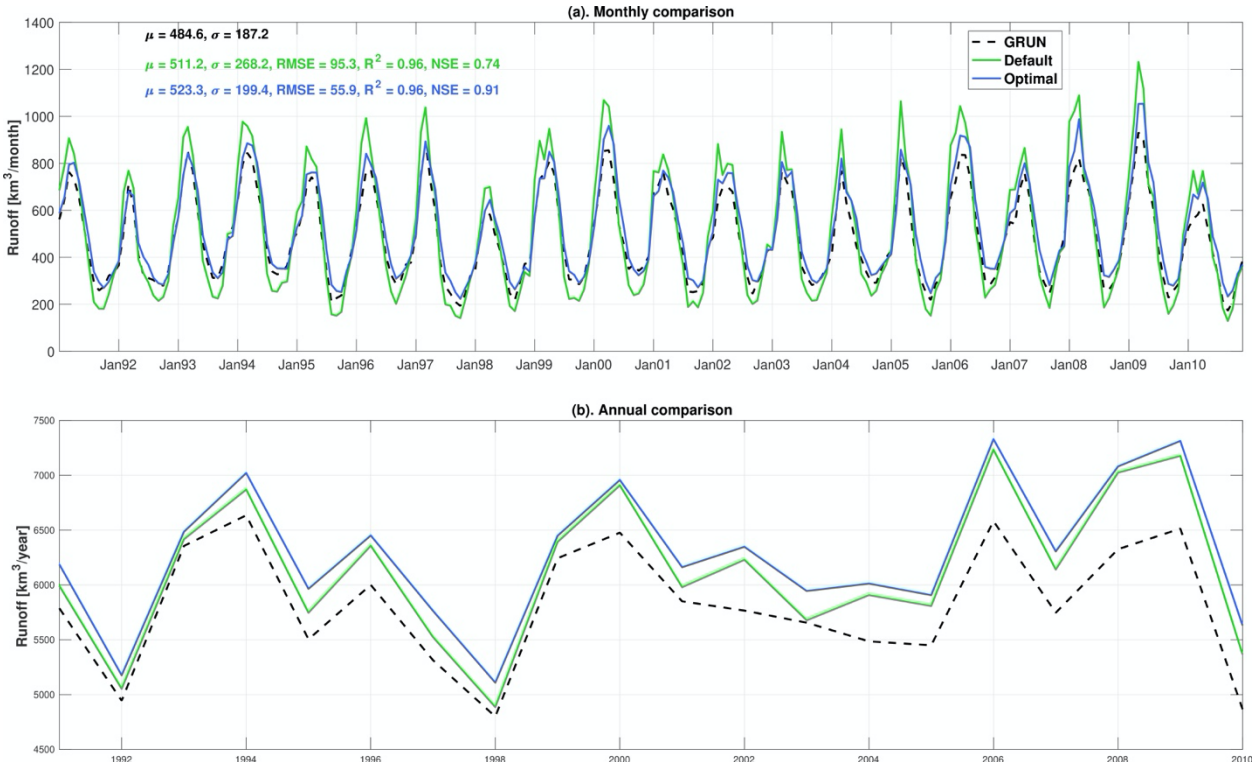

Figure S10. (a). Monthly, and (b) annual time series of reference runoff and simulated runoff for Amazon basin. μ is the mean, and σ is the standard deviation.

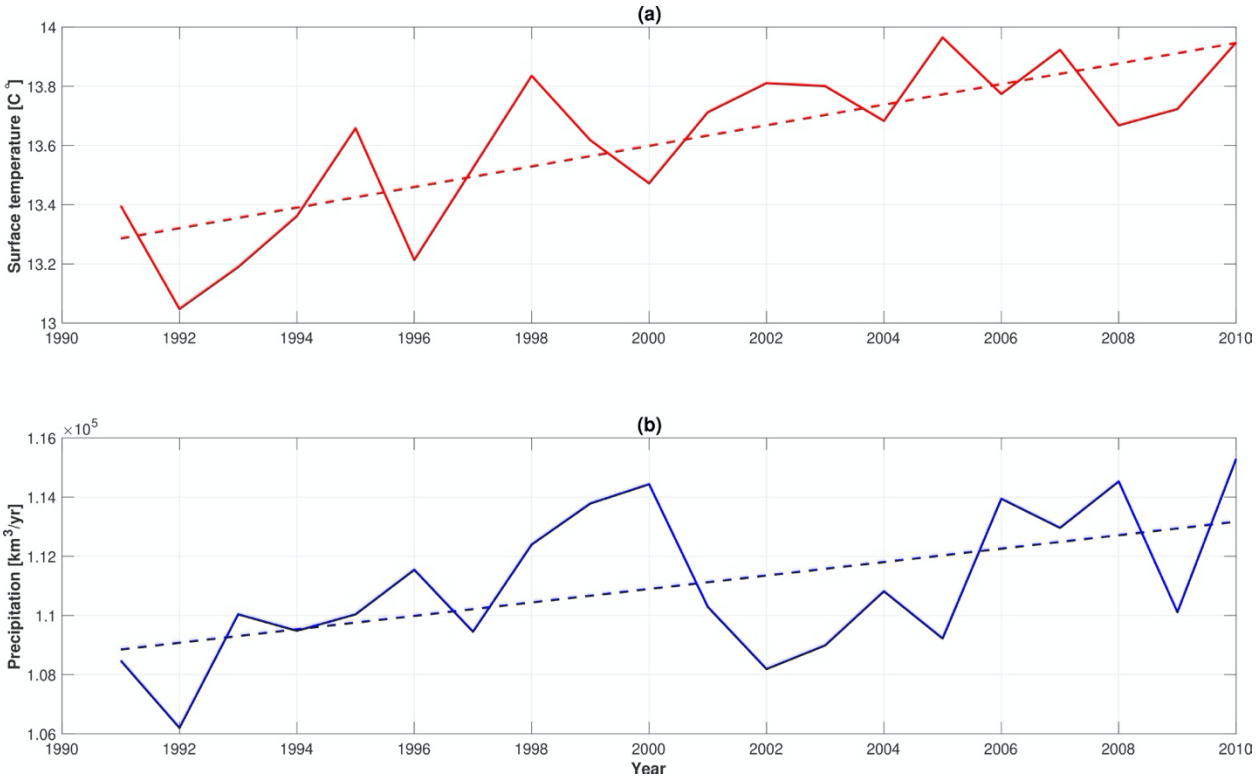

Figure S11. Global annual (a). temperature, and (b). precipitation trend for the simulation period using GSWP3v1 data. The blue and red dashed lines represent the linear trend.

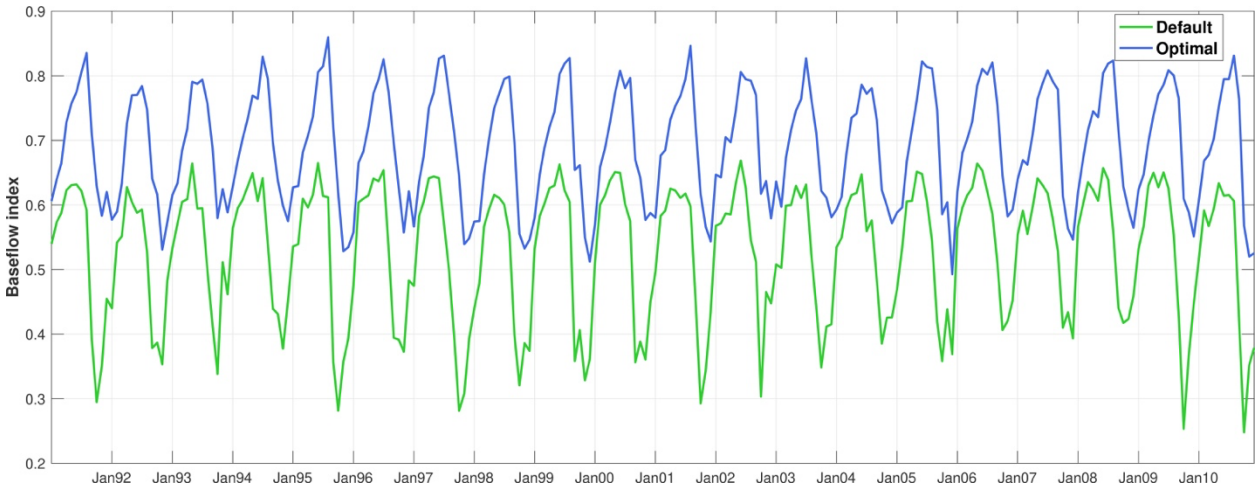

Figure S12. Monthly time series of baseflow index (i.e., ratio between subsurface runoff and total runoff) for Amazon basin.

Table S1. Model relative error at basin scale with default and optimal parameters.

Basin	Relative error	
	Default	Optimal
Mackenzie	-40.5%	-31.4%
Mississippi	18.1%	17.2%
Parana	1.5%	10.1%
Amazon	5.5%	9.6%
Danube	6.0%	7.4%
Volga	48.9%	65.8%
Ob	21.9%	30.2%
Godavari	44.6%	26.6%
Yangtze	61.1%	66.6%
Yenisey	25.3%	33.5%
Lena	3.3%	13.5%
Kolyma	-13.1%	-3.8%
Murray	-24.9%	-15.1%
Nile	-41.1%	-20.0%
Congo	-14.9%	-5.9%
Loire	11.4%	4.0%