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A likelihood framework for deterministic hydrological models and the importance of non-stationary autocorrelation

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S1 Synthetic case study: inferring known true parameters

To check if the implemented likelihood and sampling functions are inverses of each other, we produce a streamflow sample with known parameters according to the procedure outlined in Sect. 2.3. Table S1 shows the results when trying to re-infer those known parameters with the error models presented in this study. In all cases, the true value of the parameters are inside the posterior 95%-confidence intervals.

Table S1: Synthetic case study based on parameter values obtained for the Murg river with daily resolution. ML = maximum likelihood estimation, CI = confidence interval.

			E1		E2		E3		E3a		E4		E4a	
Param.	Unit	True value	ML	95%-CI	ML	95%-CI	ML	95%-CI	ML	95%-CI	ML	95%-CI	ML	95%-CI
C_e	-	1.03	1.043	1.027	1.02	0.98	1.02	1.0	1.04	1.007	1.03	1.004	1.04	1.0
				1.063		1.07		1.04		1.075		1.058		1.06
S_{max}	mm	345	352	329	336	298	325	302	330	300	330	307	338	302
				370		373		346		365		356		368
k_u	h^{-1}	8.5e-5	8.59e-5	7.7e-5	9.76e-5	7.44e-5	9.5e-5	8.0e-5	7.95e-5	6.09e-5	9.87e-5	8.14e-5	8.48e-5	7.43e-5
				9.7e-5		1.28e-4		1.1e-4		9.29e-5		1.13e-4		1.08e-4
k_f	h^{-1}	7.59e-4	8.31e-4	7.06e-4	8.82e-5	7.09e-5	8.29e-4	6.6e-4	6.77e-4	5.39e-4	8.83e-4	6.81e-4	7.72e-4	6.65e-4
				9.88e-4		1.19e-4		9.8e-4		7.96e-4		1.00e-3		1.03e-3
a	-	2.04	2.03	1.91	1.82	1.62	1.93	1.81	2.12	1.92	1.96	1.79	1.95	1.77
				2.15		2.16		2.07		2.27		2.14		2.11
b	-	2.0e-2	2.0e-2	1.2e-2	0.017	0.011	1.66e-2	4.6e-3	2.45e-2	1.43e-2	3.44e-2	1.77e-2	1.63e-2	1.05e-2
				3.4e-2		0.042		3.0e-2		4.23e-2		5.17e-2		2.99e-2
τ_{max}	h	393	-	-	297	255	385	335	414	347	374	326	357	300
				-		424		445		497		432		425
τ_{min}	h	48	-	-	-	-	-	-	47.2	41.3	-	-	44.6	38.6
				-		-		-		57.7		-		52.7
γ	-	1.2	-	-	-	-	-	-	-	-	1.21	1.15	1.16	1.10
				-		-		-		-		1.28		1.23
d_f	-	7.39	-	-	-	-	-	-	-	-	6.09	3.97	9.48	5.63
				-		-		-		-		10.2		18.3

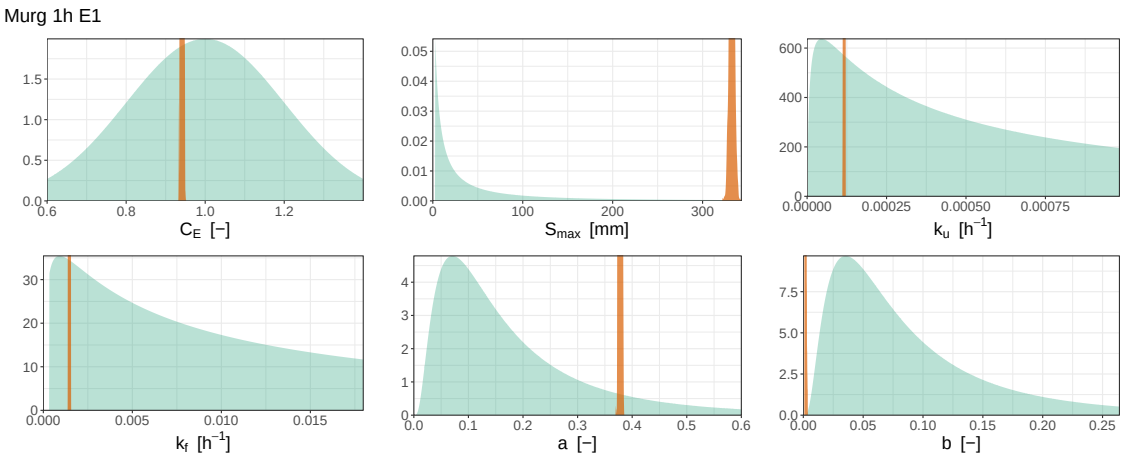

Figure S1: Marginal prior (blue) and posterior (orange) densities of hydrological and error model parameters. The combination of catchment, temporal resolution and error model is given in the top left corner.

S2 Complete results

S2.1 Marginal prior and posterior densities

This section contains the marginal density plots of the prior and the posterior parameter distributions for all tested error models at hourly and daily resolution in the Murg catchment. Note that the lognormal distribution type chosen to represent the prior knowledge of non-negativity of parameter values, together with the assumed large standard deviation to allow the distribution to span multiple orders of magnitude, can result in pronounced peaks of the prior near the lower end. This is especially the case for $S_{\max}$, $\tau_{\max}$ and $\tau_{\min}$.

S2.2 Kullback-Leibler divergence

The Kullback-Leibler divergence of the marginal posterior parameter distributions from the prior were calculated using the 10 nearest neighbours and a sample size of 10000 for the posterior and the prior. Figure S13 and S14 show those divergences for the hydrological model and the error model parameters, respectively.

S2.3 Standardized innovations

The standardized innovations are defined as:

$$\chi(t_i) = \frac{\eta(t_i) - \eta(t_{i-1}) \exp(-\frac{\Delta t}{\tau(t_i)})}{\sqrt{1 - \exp(-2\frac{\Delta t}{\tau(t_i)})}} \tag{S1}$$

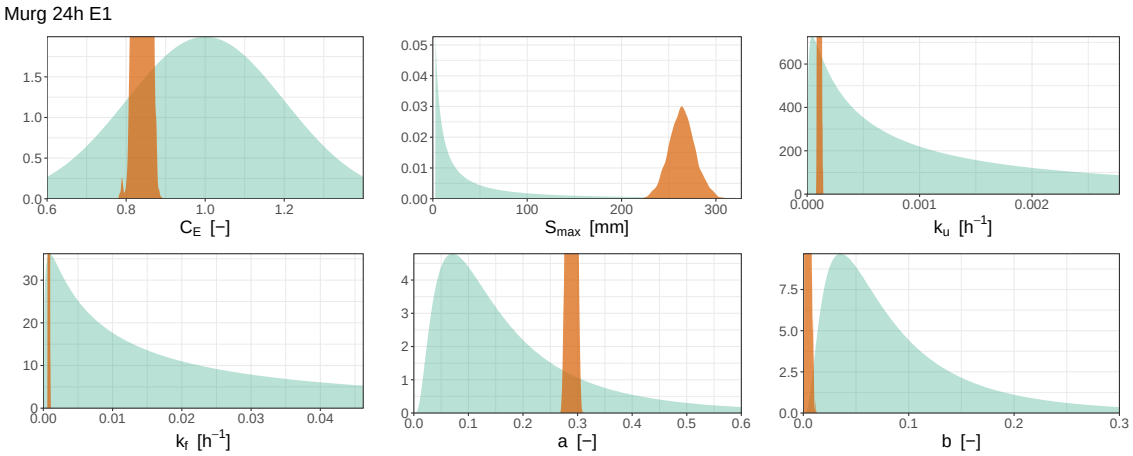

Figure S2: Marginal prior (blue) and posterior (orange) densities of hydrological and error model parameters. The combination of catchment, temporal resolution and error model is given in the top left corner.

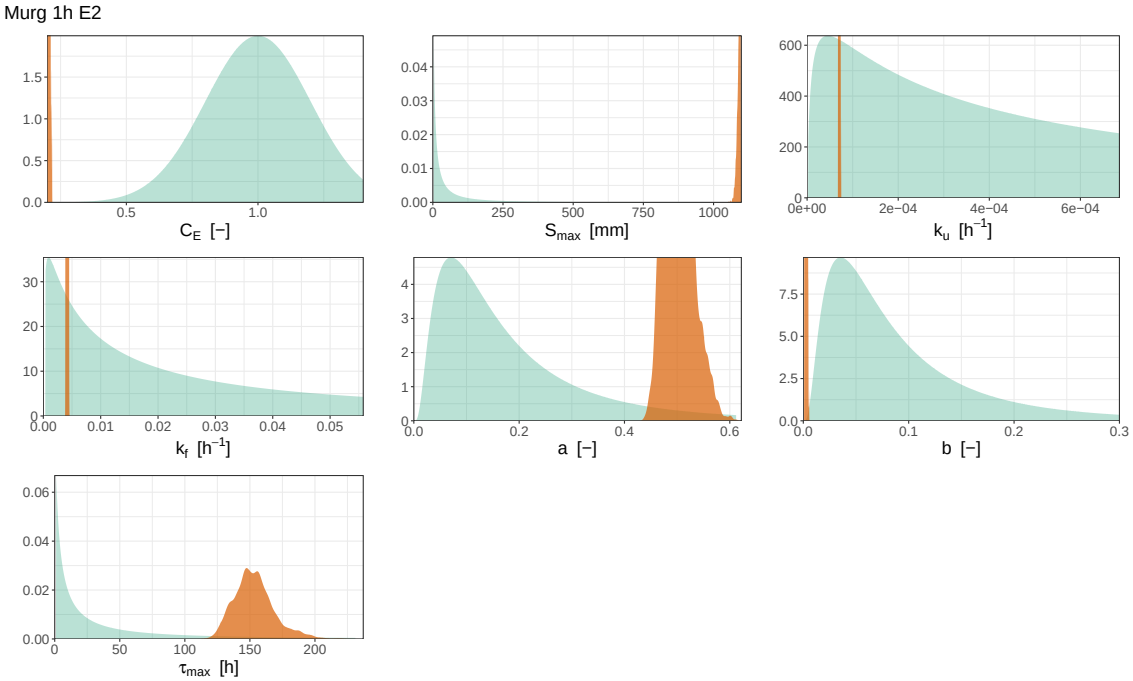

Figure S3: Marginal prior (blue) and posterior (orange) densities of hydrological and error model parameters. The combination of catchment, temporal resolution and error model is given in the top left corner.

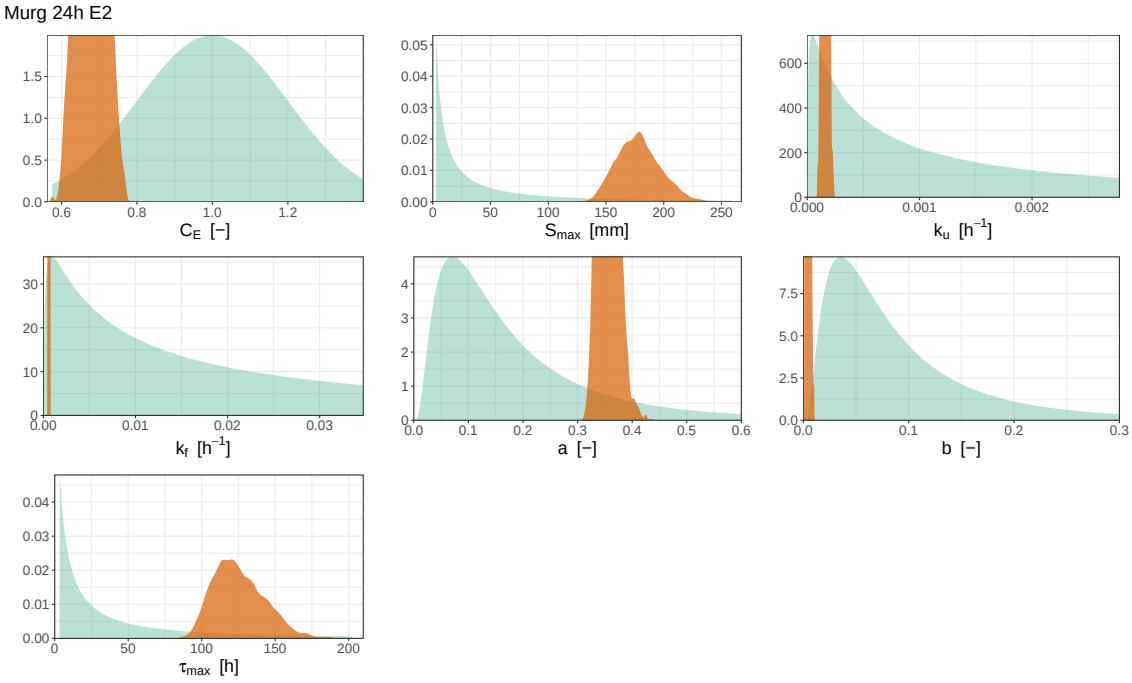

Figure S4: Marginal prior (blue) and posterior (orange) densities of hydrological and error model parameters. The combination of catchment, temporal resolution and error model is given in the top left corner.

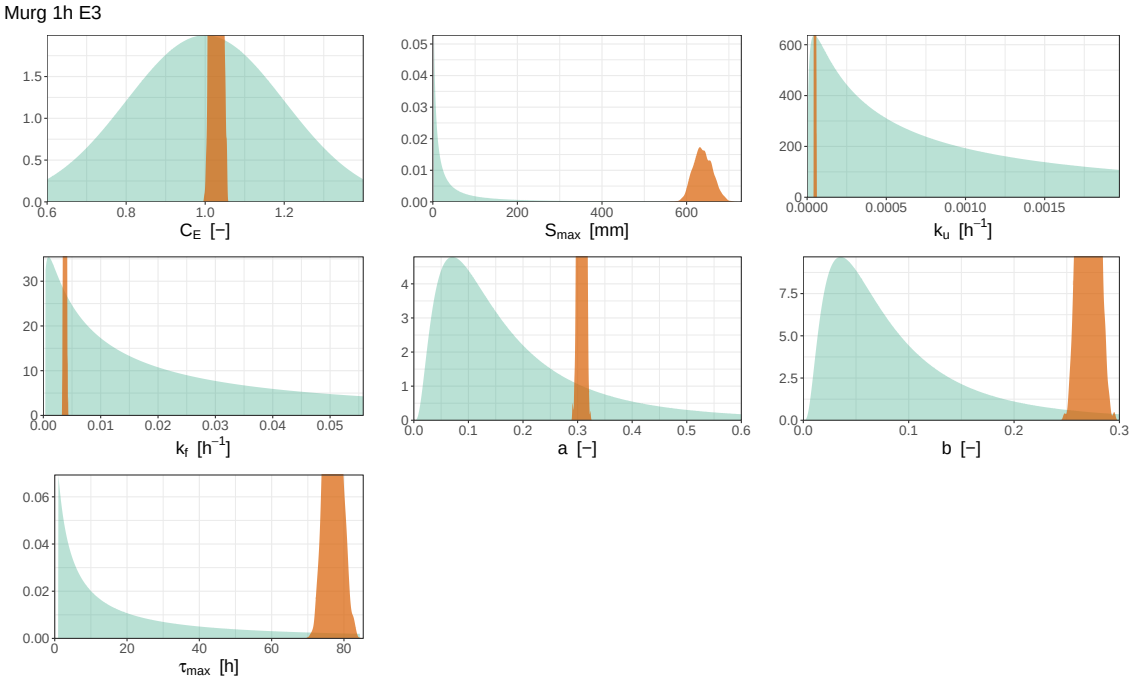

Figure S5: Marginal prior (blue) and posterior (orange) densities of hydrological and error model parameters. The combination of catchment, temporal resolution and error model is given in the top left corner.

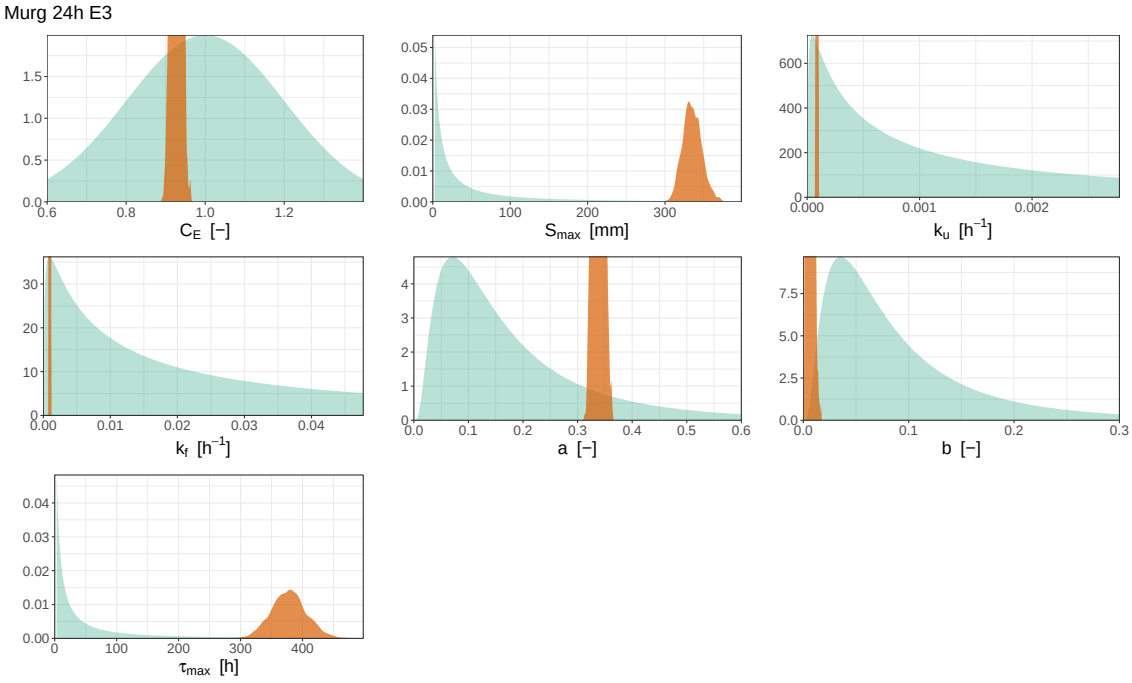

Figure S6: Marginal prior (blue) and posterior (orange) densities of hydrological and error model parameters. The combination of catchment, temporal resolution and error model is given in the top left corner.

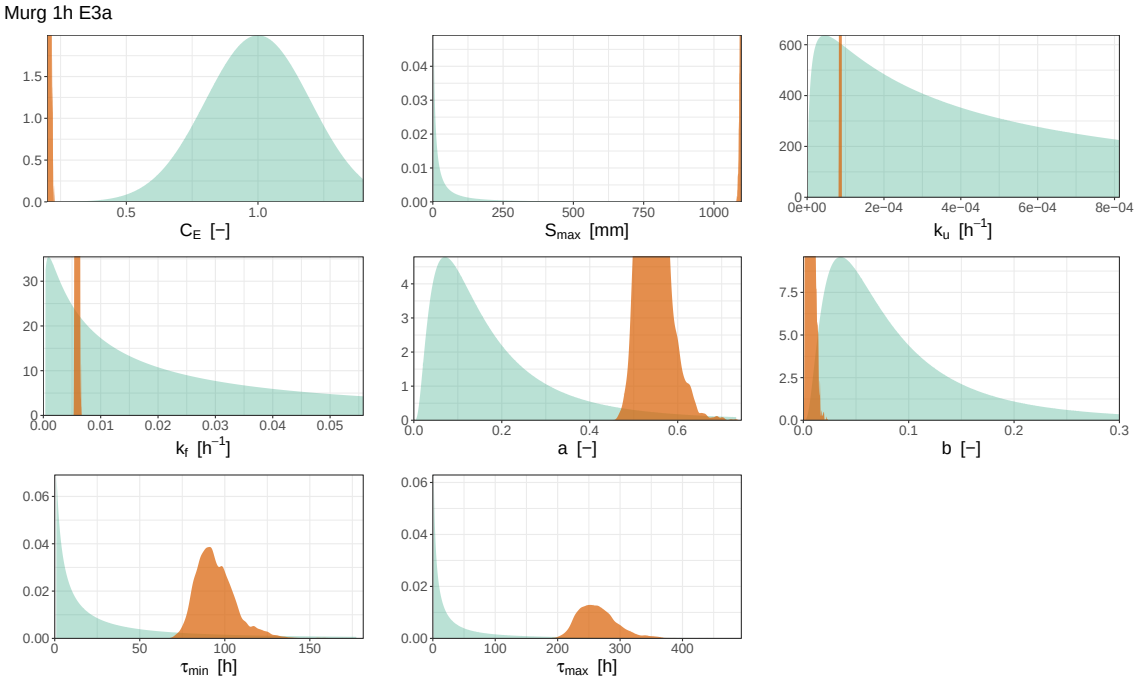

Figure S7: Marginal prior (blue) and posterior (orange) densities of hydrological and error model parameters. The combination of catchment, temporal resolution and error model is given in the top left corner.

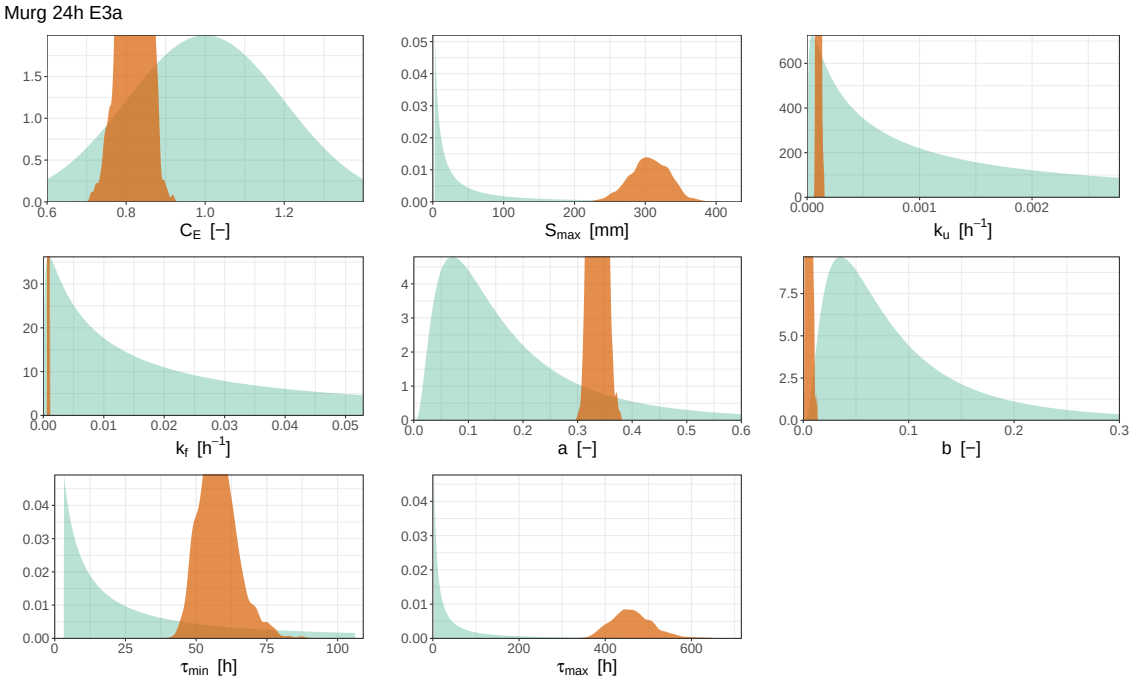

Figure S8: Marginal prior (blue) and posterior (orange) densities of hydrological and error model parameters. The combination of catchment, temporal resolution and error model is given in the top left corner.

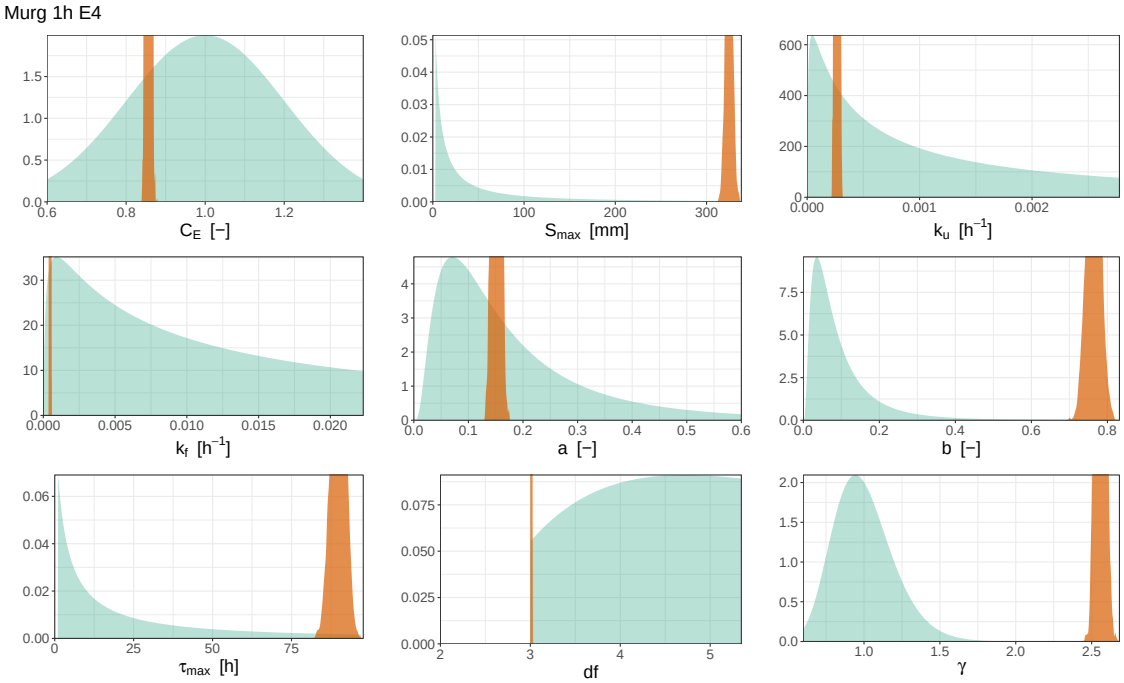

Figure S9: Marginal prior (blue) and posterior (orange) densities of hydrological and error model parameters. The combination of catchment, temporal resolution and error model is given in the top left corner.

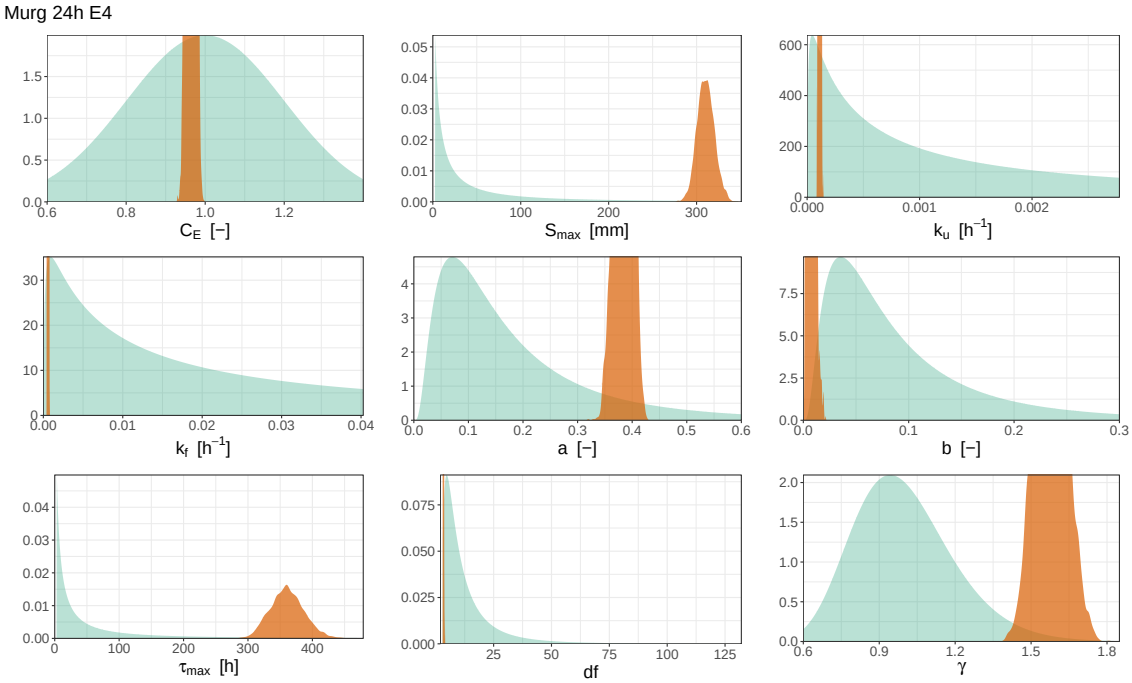

Figure S10: Marginal prior (blue) and posterior (orange) densities of hydrological and error model parameters. The combination of catchment, temporal resolution and error model is given in the top left corner.

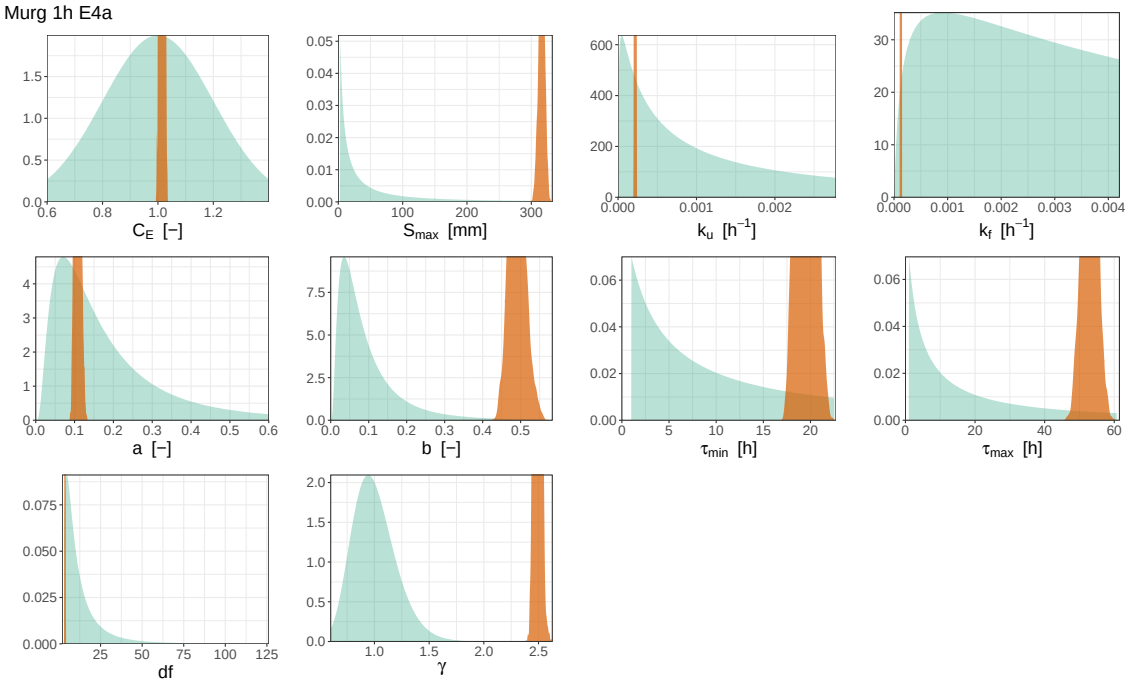

Figure S11: Marginal prior (blue) and posterior (orange) densities of hydrological and error model parameters. The combination of catchment, temporal resolution and error model is given in the top left corner.

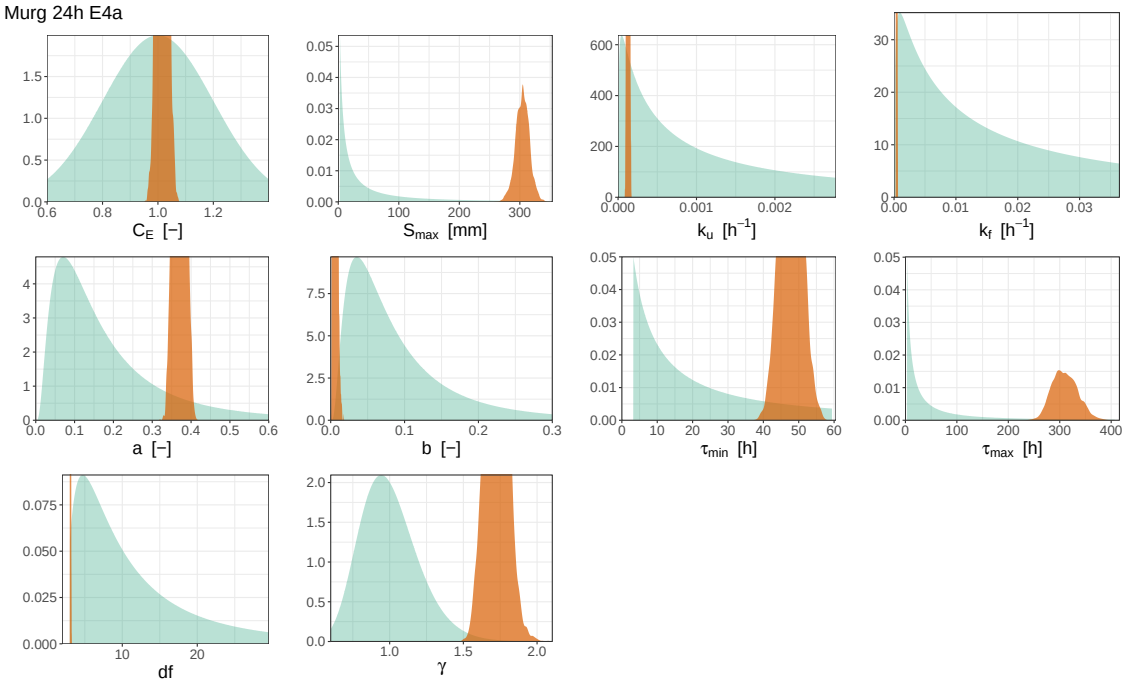

Figure S12: Marginal prior (blue) and posterior (orange) densities of hydrological and error model parameters. The combination of catchment, temporal resolution and error model is given in the top left corner.

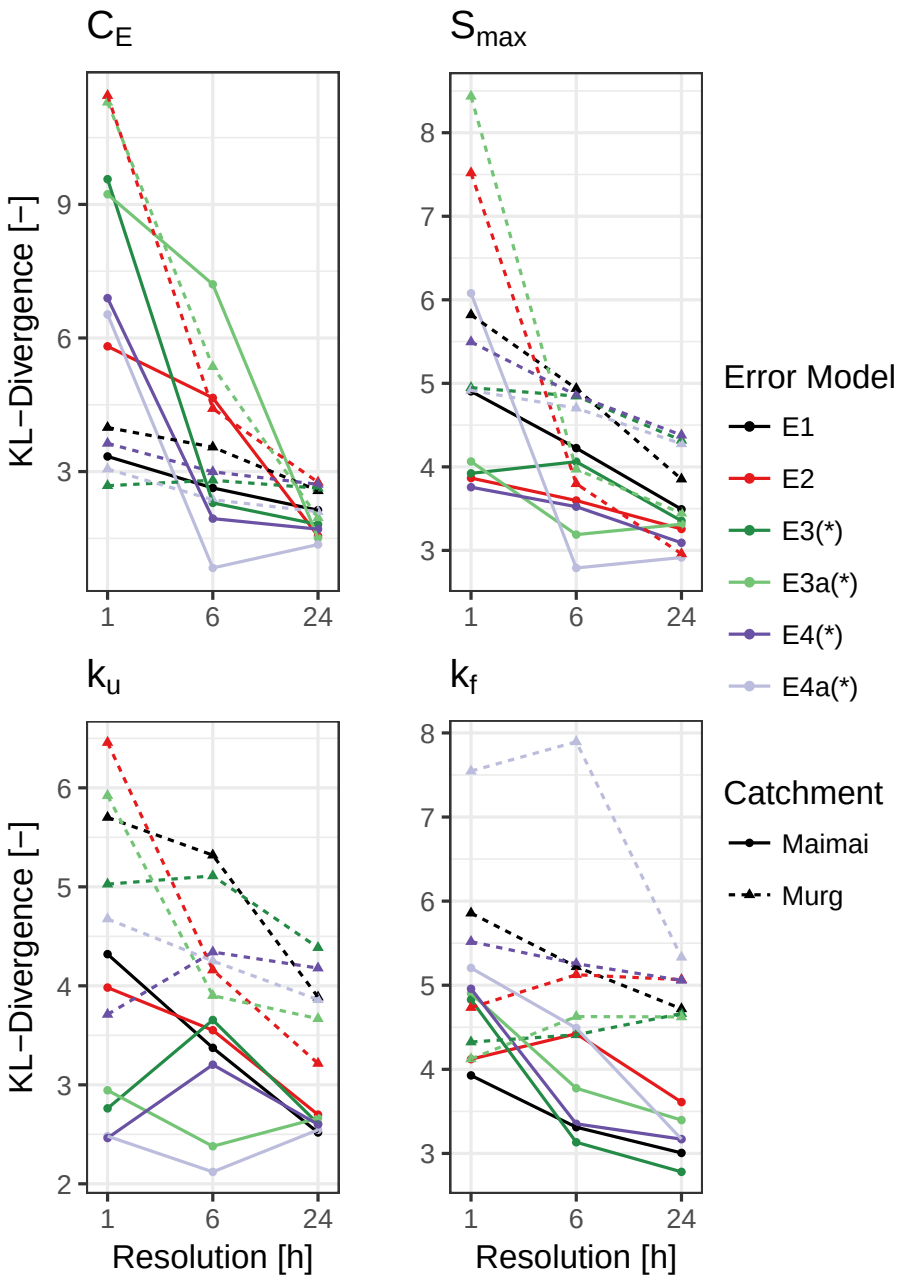

Figure S13: Kullback-Leibler divergence of the marginal prior and posterior distributions of the hydrological parameters, calculated with the nearest-neighbour method based on a prior and posterior sample size of 10000 each.

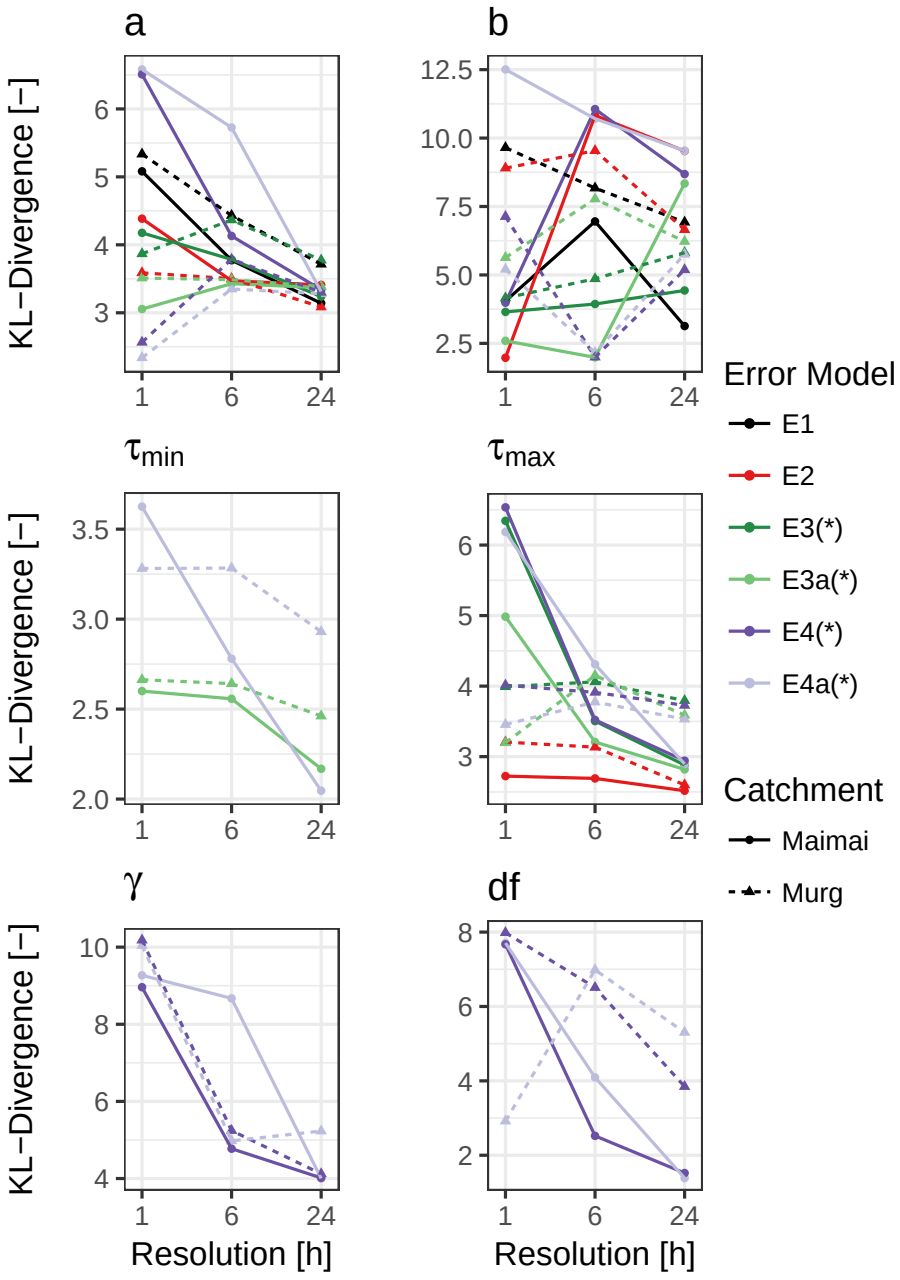

Figure S14: Kullback-Leibler divergence of the marginal prior and posterior distributions of the error model parameters, calculated with the nearest-neighbour method based on a prior and posterior sample size of 10000 each.

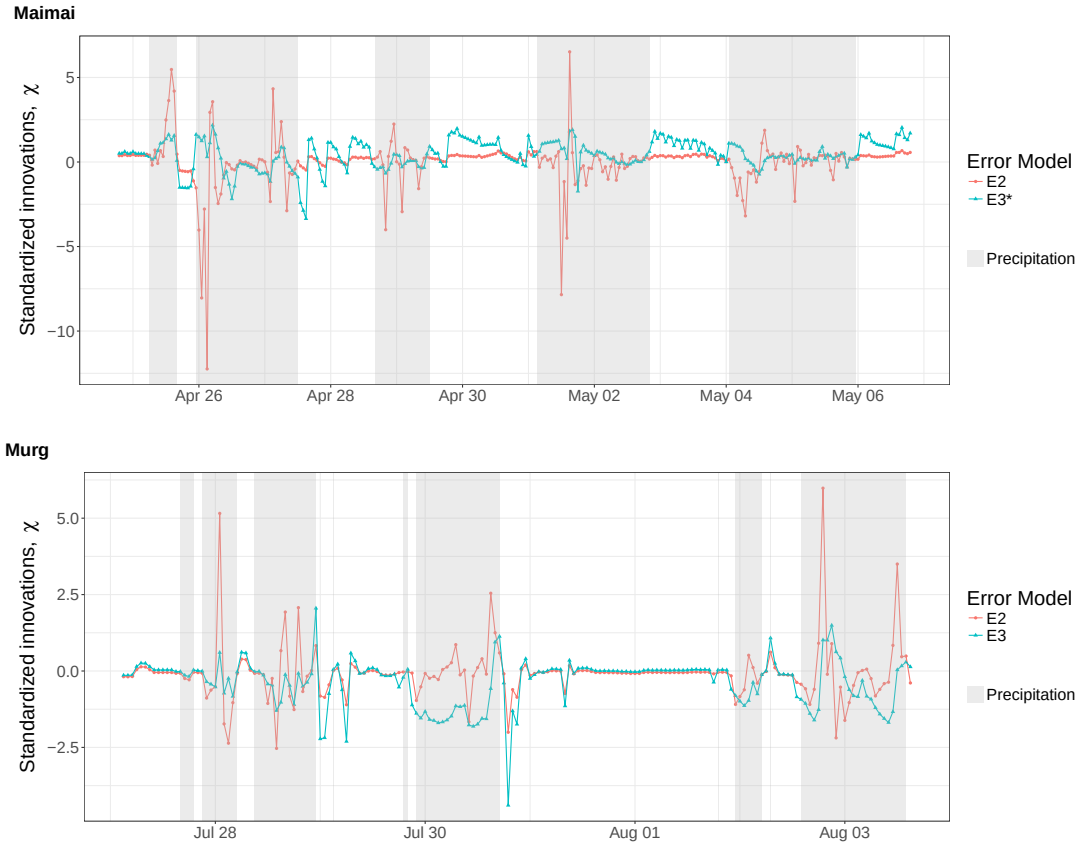

Figure S15: Standardized innovations, χ (Eq. S1), based on the parameter values at the maximum posterior density obtained with error models E2 and E3(*) for hourly data resolution in the Maimai and the Murg catchment. * : smoothing $P_{\text{err}}(t)$ with a moving average window of size 5 h before applying Eq. (11).

where $\Delta t = t_i - t_{i-1}$. χ is the decorrelated and standardized version of η (compare to Eq. (4) and should correspond to white noise if all the underlying assumptions are fulfilled. Note that η, and therefore also χ, can only be calculated for a given set of parameters, $\boldsymbol{\theta}$ and $\boldsymbol{\psi}$. Figure S15 shows a specific period of the time series of χ based on the parameter set with the maximum posterior density for error models E2 and E3 (E3*) in the Murg (Maimai) catchment.