Simultaneously Determining Global Sensitivities of Model Parameters and Model Structure – Supplementary Material –

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S.1 The Raven Model with Weighted Process Options

The Raven model allows to specify multiple options for each process such as infiltration, evaporation, and baseflow. Instead of the model using one unique parametrization and output for each process it is then deriving the weighted average of outputs for the various options (Craig et al., 2020). This is defined in the main manuscript (Eq. 18) by

$$f_{\text{shared}}(\boldsymbol{x}, \boldsymbol{w}) \quad = \quad (w_{d1}D_1 + w_{d2}D_2) \cdot (w_{e1}E_1 + w_{e2}E_2 + w_{e3}E_3) + (w_{f1}F_1 + w_{f2}F_2) \tag{S1}$$

where

$$
\begin{aligned}
w_{d1} + w_{d2} &= 1 \\
w_{e1} + w_{e2} + w_{e3} &= 1 \\
w_{f1} + w_{f2} &= 1 \; .
\end{aligned}
$$

where, for example, D_1 and D_2 might be two options for one process. For example, deriving infiltration is performed once using the infiltration definition of HMETS and once derived as defined in the HBV model. The infiltration outputs D_1 and D_2 are then weighted using w_{d1} and w_{d_2} to derive the infiltration estimate Raven will use for the remainder of the simulation. The overall flowchart of the model given all hydrologic processes involved is given in the flowchart in Fig. S1. In that flowchart the processes labeled with M to Q are used here with multiple options while the processes R to W are fixed with only one option. The processes labeled with X are the ones that are also fixed at one option and this option does not contain tunable parameters. In the following we will explain briefly the process options chosen for this study that will lead to non-zero sensitivities, i.e. processes M to W. Most of these description as well as all descriptions for processes X can be found in the Raven documentation (Craig, 2020).
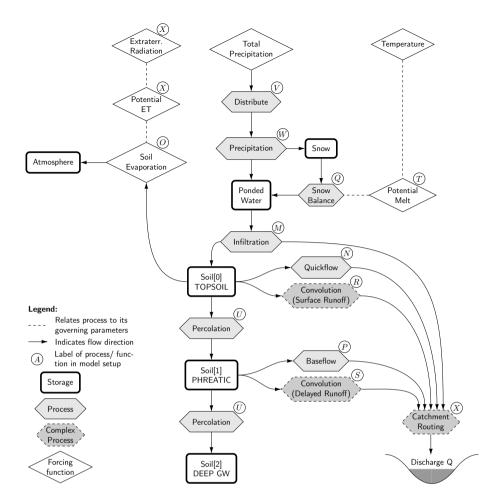
Figure S1. The model schematic of the models structure used in this study. The connection of storages (boxes with thick outlines), processes (hexagonal shapes), and forcing functions (diamond shapes) are shown. Some processes are simplified in this schematic (hexagonal shape with dashed outline). The labels used for the processes/functions in this study are indicated by the circled letters right of the processes and forcing functions. The five processes M to Q are used here with multiple options while the processes R to W are fixed with only one option. The processes labeled with X are the ones that are also fixed at one option and this option does not contain tunable parameters. Hence the sensitivity of the processes X is already prior known to be zero. The processes and options as well as the parameters active in each option are listed in Tab. C1 of the main manuscript.

S.1.1 Infiltration Process M

20 Infiltration refers to the partitioning of ponded water (the residual rainfall and/or snowmelt) between the shallow surface soil (infiltrated water) and surface water (runoff). Infiltration is typically controlled by the saturation of the soil and its hydraulic properties (e.g., hydraulic conductivity, infiltration capacity).

Infiltration always moves water from `PONDED_WATER` to `SOIL[0]` (the top soil layer), and depending upon the soil structure model specified by the `:SoilModel` command, may additionally push water to lower soil moisture stores. The remaining
25   infiltrated water is typically treated as runoff and moved to `SURFACE_WATER`.

Infiltration is limited by the availability of soil/ aquifer storage. Many of the following algorithms use the quantities of maximum soil storage (ϕ_{max} [mm]), maximum tension storage (ϕ_{tens} [mm]), and field capacity storage (ϕ_{fc} [mm]) in a layer, always calculated as:

$$\phi_{max} = Hn(1 - SF) \tag{S2}$$
$$\phi_{tens} = \phi_{max}(S_{fc} - S_{wilt})$$
$$\phi_{fc} = \phi_{max}S_{fc}$$

where H is the soil layer thickness [mm] (in this study parameter x_{29}), n is the porosity (soil property `POROSITY`), SF is the stone fraction (soil property `STONE_FRAC`), S_{fc} is the saturation at field capacity (soil parameter `FIELD_CAPACITY`), and S_{wilt} is the saturation at the wilting point (soil parameter `SAT_WILT`).

S.1.1.1   HMETS infiltration method (`INF_HMETS`) used as option M_1

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From the HMETS model (Martel et al., 2017):

$$M_1 = R \cdot \left(1 - \alpha \cdot \frac{\phi_{soil}}{\phi_{soil}^{max}}\right)$$

where R is the rainfall/snowmelt rate [mm/d], α is the unitless land use parameter `HMETS_RUNOFF_COEFF` (in this study parameter x_1), ϕ_{soil} is the topsoil layer water content, and ϕ_{max} is the maximum soil storage [mm] calculated using equation
40   S2.

S.1.1.2   VIC/ARNO method (`INF_VIC_ARNO`) used as option M_2

The VIC/ARNO model as interpreted by (Clark et al., 2008).

$$M_2 = R \cdot \left(1 - \left(1 - \frac{\phi_{soil}}{\phi_{max}}\right)^b\right)$$

where R is the rainfall/snowmelt rate [mm/d], b is the soil parameter `B_EXP` (in this study parameter x_2), ϕ_{soil} is the top soil
45   layer water content [mm], and ϕ_{max} is the maximum topsoil storage [mm] calculated using equation S2.

S.1.1.3   HBV method (`INF_HBV`) used as option M_3

The standard HBV model approach (Bergström, 1995).

$$M_3 = R \cdot \left(1 - \left(\frac{\phi_{soil}}{\phi_{max}}\right)^\beta\right)$$

where β is the soil parameter `HBV_BETA` (in this study parameter x_3), ϕ_{soil} is the soil layer water content [mm], and ϕ_{max} is
50   the maximum soil storage [mm] calculated using equation S2.

S.1.1.4 Weighted sum of all options used for infiltration process M

The combined, weighted sum of the three options is used as infiltration estimate in Raven, i.e.

$$M \quad = \quad w_1 M_1 + w_2 M_2 + w_3 M_3$$

The three weights w_i are derived from the two i.i.d. parameters r_j sampled uniform from the unit interval following the approach described in Appendix A of the main manuscript:

$$w_1 \quad = \quad 1 - (1 - r_1)^{\frac{1}{2}}$$
$$w_2 \quad = \quad (1 - w_1) r_2$$
$$w_3 \quad = \quad 1 - w_1 - w_2$$

S.1.2 Quickflow Process N

S.1.2.1 Linear storage (`BASE_LINEAR_ANALYTIC`) used as option N_1

A very common approach used in a variety of conceptual models. The baseflow rate is linearly proportional to storage (`BASE_LINEAR_STORAGE`):

$$N_1 = k \phi_{soil}$$

Where k [1/d] is the baseflow coefficient (soil parameter `BASEFLOW_COEFF` for the TOPSOIL; in this study parameter x_4), and ϕ_{soil} is the water storage [mm] in the soil or aquifer layer (Eq. S2). The alternate version `BASE_LINEAR_ANALYTIC` is used here. It simulates the same condition except using a closed-form expression for integrated flux over the time step (Δt):

$$N_1 = \phi_{soil} \cdot (1 - \exp(-k\Delta t)) / \Delta t$$

The two methods are effectively equivalent for sufficiently small time steps, but the second is preferred for large values of k. The second was used in this study.

S.1.2.2 VIC baseflow method (`BASE_VIC`) used as option N_2

From the VIC model (Wood et al., 1992) as interpreted by (Clark et al., 2008):

$$N_2 = M_{max} \left(\frac{\phi_{soil}}{\phi_{max}} \right)^n$$

where M_{max} [mm/d] is the maximum baseflow rate at saturation (soil parameter `MAX_BASEFLOW_RATE`; in this study parameter x_5), ϕ_{soil} is the water storage [mm] in the soil or aquifer layer, ϕ_{max} is the maximum soil storage capacity , and n is the user-specified soil parameter `BASEFLOW_N` (in this study parameter x_6).

S.1.2.3 VIC baseflow method (`BASE_TOPMODEL`) used as option N_3

From TOPMODEL (Beven and Kirkby, 1979) as interpreted by Clark et al. (2008):

$$N_3 = M_{max} \cdot \frac{\phi_{max}}{n} \cdot \frac{1}{\lambda^n} \cdot \left(\frac{\phi_{soil}}{\phi_{max}}\right)^n$$

where M_{max} [mm/d] is the maximum baseflow rate at saturation (soil parameter `MAX_BASEFLOW_RATE`; in this study parameter x_5), ϕ_{soil} is the water storage [mm] in the soil layer, ϕ_{max} is the maximum soil storage capacity, λ is the mean of the power-transformed topographic index [m] (terrain parameter `LAMBDA`; in this study parameter x_7), and n is the user-specified soil parameter `BASEFLOW_N` (in this study parameter x_6).

S.1.2.4 Weighted sum of all options used for quickflow process N

The combined, weighted sum of the three options is used as quickflow estimate in Raven, i.e.

$$N \quad = \quad w_4 N_1 + w_5 N_2 + w_6 N_3$$

The three weights w_i are derived from the two i.i.d. parameters r_j sampled uniform from the unit interval following the approach described in Appendix A of the main manuscript:

$$w_4 \quad = \quad 1 - (1 - r_3)^{\frac{1}{2}}$$
$$w_5 \quad = \quad (1 - w_4) r_4$$
$$w_6 \quad = \quad 1 - w_4 - w_5$$

S.1.3 Soil Evaporation O

Soil evaporation (really evapotranspiration) involves converting water from the soil layers to water vapour in the atmosphere via both evaporation and transpiration. The rate of evapotranspiration depends on soil moisture, plant type, stage of plant development and weather conditions such as solar radiation, wind speed, humidity and temperature.

Soil evaporation always moves water between `SOIL[m]` and `ATMOSPHERE` units. Which soil layers are subjected to evaporation depend on the soil structure model specified by the `:SoilModel` command and the particular evaporation algorithm. Soil evaporation is rate-limited by the availability of soil/aquifer storage (dependent on the soil thickness which is parameter x_{29} in this study) and by the capacity of the atmosphere to absorb water vapour.

In all notation below, PET refers to the potential evapotranspiration determined by one of the forcing function estimators for PET (see Raven manual). In all cases, this PET is modified by the soil parameter `PET_CORRECTION` (in this study parameter x_8), which only modifies PET in these algorithms.

S.1.3.1 Uncorrected evaporation algorithm (`SOILEVAP_ALL`) used as option O_1

Water is removed from soil at the maximum rate until there is no water remaining:

$$O_1 = \text{PET}$$

S.1.3.2 TOPMODEL evaporation algorithm (`SOILEVAP_TOPMODEL`) used as option O_2

Soil ET is at PET if storage exceeds the tension storage, then is linearly proportional to the soil saturation:

$$O_2 = \text{PET} \cdot \min(\frac{\phi_{soil}}{\phi_{tens}}, 1)$$

where PET is the potential evapotranspiration rate [mm/d], and ϕ_{soil} [mm] and ϕ_{tens} [mm] are defined in equation S2 (contains parameters `SAT_WILT TOPSOIL` x_9, `FIELD_CAPACITY TOPSOIL` $x_9 + x_{10}$, and thickness of `TOPSOIL` x_{29}). The HBV model uses an additional snow correction (in this study parameter x_8), such that ET is zero in non-forested areas if snow depth is non-zero.

S.1.3.3 Weighted sum of all options used for soil evaporation process O

The combined, weighted sum of the two options is used as soil evaporation estimate in Raven, i.e.

$$O \quad = \quad w_7 O_1 + w_8 O_2$$

The two weights w_i are derived from one parameter r_j sampled uniform from the unit interval following the approach described in Appendix A of the main manuscript:

$$w_7 \quad = \quad r_5$$
$$w_8 \quad = \quad 1 - w_7$$

S.1.4 Baseflow Process P

S.1.4.1 Linear storage (`BASE_LINEAR_ANALYTIC`) used as option P_1

The same linear storage computation as described in Sec. S.1.2.1 is used here. The only difference is the baseflow coefficient k [1/d] that is now the soil parameter `BASEFLOW_COEFF` for the PHREATIC soil layer (in this study parameter x_{11}).

$$P_1 = \phi_{soil} \cdot (1 - \exp(-k\Delta t))/\Delta t$$

S.1.4.2 Non-linear storage (`BASE_POWER_LAW`) used as option P_2

The non-linear storage is a very common approach used in a variety of conceptual models, including HBV (Bergström, 1995). The baseflow rate is non-linearly proportional to storage:

$$P_2 = k\phi_{soil}^n$$

Where k [1/d] is the baseflow coefficient (soil parameter `BASEFLOW_COEFF` here for the PHREATIC soil layer; parameter x_{11}), and ϕ_{soil} is the water storage [mm] in the soil or aquifer layer, and n is the user-specified soil parameter `BASEFLOW_N` (in this study parameter x_{12}).

S.1.4.3 Weighted sum of all options used for baseflow process P

The combined, weighted sum of the two options is used as baseflow estimate in Raven, i.e.

$$P \quad = \quad w_9 P_1 + w_{10} P_2$$

The two weights w_i are derived from one parameter r_j sampled uniform from the unit interval following the approach described in Appendix A of the main manuscript:

$$w_9 \quad = \quad r_6$$
$$w_{10} \quad = \quad 1 - w_9$$

S.1.5 Snow Balance Process Q

Snow balance algorithms are used to simulate the strongly coupled mass and energy balance equations controlling melting and refreezing of snow pack and the liquid phase in the snow pores.

Most snow balance algorithms consists of multiple coupled equations, and there are also many 'to' and 'from' compartments, depending on which algorithm is selected. 'From' compartments include SNOW (as SWE), SNOW_LIQ and SNOW_DEPTH. 'To' compartments include SNOW, ATMOSPHERE, SNOW_LIQ, SNOW_DEPTH and SURFACE_WATER. Snow balance is rate-limited by the storage in 'from' and 'to' compartments.

Most of the snowmelt algorithms that explicitly simulate liquid water content within the snowpack use the global parameter SNOW_SWI to determine the maximum possible liquid water storage of the snowpack:

$$\phi_{max}^{sl} = SWE \cdot SWI$$

where ϕ_{max}^{sl} [mm] is the maximum liquid water storage of the snowpack, SWE is the snow water equivalent of the snowpack [mm], and SWI is the global parameter SNOW_SWI, which defaults to 0.05 if not specified.

S.1.5.1 HMETS snow balance (SNOBAL_HMETS) used as option Q_1

A snowmelt model documented in Martel et al. (2017). This is a simple single layer snowmelt model with degree day freezing, which tracks liquid water content in the snowpack in addition to SWE. The refreeze rate (constrained by water availability) is given by:

$$Q_1 = K_f \cdot (T_{rf} - T_{di})^f$$

where K_f is the land use property REFREEZE_FACTOR (in this study parameter x_{18}), $T_r f$ is the degree day refreeze factor (land use property DD_REFREEZE_TEMP; parameter x_{16}), and f is the land use parameter REFREEZE_EXPONENT (parameter x_{17}). The water retention capacity (upper limit of liquid water content in snow) varies over the course of the year based upon cumulative snowmelt:

$$\mathrm{SWI} = \max\left(\mathrm{SWI}_{min}, \mathrm{SWI}_{max} \cdot (1 - \alpha \cdot M_{cumul})\right)$$

160   where SWI_{min} and SWI_{max} are the land use parameters `SNOW_SWI_MIN` (parameter x_{13}) and `SNOW_SWI_MAX` (parameter $x_{13} + x_{14}$), α is the land use parameter `SWI_REDUCT_COEFF` (parameter x_{15}), and M_{cumul} is the cumulative melt since the last period of zero snow depth.

S.1.5.2   Simple melt (`SNOBAL_SIMPLE_MELT`) used as option Q_2

The melt rate (in [mm/d]) is simply calculated by applying the potential melt rate to the snowpack until it is gone.

165
$$Q_2 = \begin{cases} M_{potmelt}, & \text{if } S \geq 0 \\ 0, & \text{if } S < 0 \end{cases}$$

where $M_{potmelt}$ [mm/d] is calculated using the method described in section S.1.6.2, i.e. $M_{potmelt} = T_1$. Note that the simple melt process option Q_2 for simulating the snow balance does not include any tunable parameter x.

S.1.5.3   HBV snow balance (`SNOBAL_HBV`) used as option Q_3

The HBV snow balance (Bergström, 1995) represents both melt and liquid water storage in the pore space of the snow. The melt
170   rate is determined by the potential melt rate algorithm (`POTMELT_HBV` for true HBV emulation), while refreeze is calculated using:

$$Q_3 = M_{refreeze} = K_a \cdot \max(T_f - T, 0)$$

where K_a is the land use parameter `REFREEZE_FACTOR` [mm/d/°C] (in this study parameter x_{18}). Meltwater fills the snow pore space first with the maximum fillable pore space determined by the global parameter `SNOW_SWI` (in this study pa-
175   rameter x_{19}) and is then allowed to overflow. All overflow percolates into `SOIL[0]` by default, but may be redirected to `PONDED_WATER` using the `:Redirect` command if desired.

S.1.5.4   Weighted sum of all options used for snow balance process Q

The combined, weighted sum of the three options is used as snow balance estimate in Raven, i.e.

$$Q \quad = \quad w_{11}Q_1 + w_{12}Q_2 + w_{13}Q_3$$

180   The three weights w_i are derived from the two i.i.d. parameters r_j sampled uniform from the unit interval following the approach described in Appendix A of the main manuscript:

$$w_{11} \quad = \quad 1 - (1 - r_7)^{\frac{1}{2}}$$
$$w_{12} \quad = \quad (1 - w_{11})r_8$$
$$w_{13} \quad = \quad 1 - w_{11} - w_{12}$$

S.1.6 Processes with Single Options With Tunable Parameters

For the following processes only one option has been used during this study for simplicity. Each option is hence theoretically weighted with 1.0 in every model run.

S.1.6.1 Convolution Processes for Surface and Delayed Runoff (R and S)

Since convolution methods store the time history of inputs to convolution storage of a duration consistent with the longest time delay in the convolution, it is not suggested to use convolution with a time constant in days with an hourly time step. Typically the order of the time delay should be on the order of the model time step.

The below convolution methods are available. All of them perform a discrete version of the following convolution:

$$R_1 = S_1 = \int_0^\infty UH(\tau)I(t-\tau)d\tau$$

where $I(t)$ is the input flux history (in mm/d) to the convolution storage unit and $UH(t)$ is the transfer function; the area under the transfer function is always equal to one to ensure mass balance. For the convolution of the surface and delayed runoff two different transfer functions have been used.

Gamma transfer function 1 (`CONVOL_GAMMA`) used as option R_1

For the convolution of the surface runoff R the following transfer function is used

$$UH(t) = \frac{1}{t}\frac{(\beta t)^a}{\Gamma(a)}\exp(-\beta t)$$

where a and β are the land use parameters `GAMMA_SHAPE` and `GAMMA_SCALE` (in this study parameters x_{20} and x_{21}, respectively).

Gamma transfer function 2 (`CONVOL_GAMMA2`) used as option S_1

For the convolution of the delayed runoff S the following transfer function is used

$$UH(t) = \frac{1}{t}\frac{(\beta t)^a}{\Gamma(a)}\exp(-\beta t)$$

where a and β are the land use parameters `GAMMA_SHAPE2` and `GAMMA_SCALE2` (in this study parameters x_{22} and x_{23}, respectively).

S.1.6.2 Potential Melt T

Potential snow melt can be estimated using a number a methods in the Raven model. To set the appropriate process in the model the RVI must include the `:PotentialMeltMethod` keyword along with the appropriate value for the method selected. The method selected here is:

Potential Melt HMETS method (`POTMELT_HMETS`) used as option T_1

A revised degree day model from the HMETS model (Martel et al., 2017), which uses a degree day factor which varies with cumulative snowmelt. The degree day model is given as

$$T_1 = M_a \cdot (T - T_f)$$

where T is the daily average temperature. T_f is the melt temperature (zero by default, but can be set with the land use parameter `DD_MELT_TEMP`; in this study parameter x_{26}), and M_a [mm/d/°C] is the degree day melt factor, calculated as a function of cumulative melt:

$$M_a = \min\left(M_a^{max}, M_a^{min} \cdot (1 + \alpha \cdot M_{cumul})\right)$$

where the following land use parameters are used: the minimum melt rate M_a^{min} [mm/d/°C] (`MIN_MELT_FACTOR`; in this study parameter x_{24}), the maximum melt rate M_a^{max} [mm/d/°C] (`MAX_MELT_FACTOR`; in this study parameter $x_{24} + x_{25}$), and α [1/mm] is the parameter `DD_AGGRADATION` (in this study parameter x_{27}).

S.1.6.3   Percolation Process U

Percolation refers to the net downward flow of water from one soil/ aquifer unit to another. This process is physically driven by a moisture gradient, but this is often simplified in conceptual percolation models.

Percolation moves water between `SOIL[m]` or `AQUIFER` units, depending upon the soil structure model specified by the `:SoilModel` command. The user typically has to specify both the 'from' and 'to' storage compartments. Percolation is rate-limited by the availability of soil/aquifer storage and by the capacity of the receptor 'to' compartment.

Linear Percolation (`PERC_LINEAR`) used as option U_1

Percolation is proportional to soil water content:

$$U_1 = k\phi_{soil}$$

where k [1/d] is the soil parameter `PERC_COEFF` (in this study parameter x_{28} for TOPSOIL and x_{35} for PHREATIC soil layer) and ϕ_{soil} [mm] is defined in equation S2. All parameters refer to that of the 'from' soil compartment.

S.1.6.4   Rain-Snow Partitioning Process V

If only total precipitation is specified at a gauge station or grid cell, then this total precipitation is partitioned into rain and snow. All of the provided algorithms in Raven calculate the snow fraction α_s, and rain and snow are determined from:

$$
\begin{aligned}
R &= (1 - \alpha_s)P \\
S &= \alpha P
\end{aligned}
$$

where R [mm/d], S [mm/d], and P are rainfall, snowfall, and total precipitation rates, respectively.

Linear approach (`RAINSNOW_HBV`) used as option V_1

In these approaches, a linear transition between all snow and all rain is determined from the average daily temperature, T_{ave}:

$$\alpha_s = 0.5 + \frac{T_{trans} - T_{ave}}{\Delta T}$$

in the range from $T_{trans} - \Delta T/2$ to $T_{trans} + \Delta T/2$, where T_{trans} is the rain/snow transition temperature (global parameter `RAINSNOW_TEMP`, [°C]; in this study parameter x_{31}) and ΔT is the global parameter `RAINSNOW_DELTA` [°C] (in this study parameter x_{32}). If T_{ave} is outside of this temperature range, the precipitation is either all snow ($\alpha_s = 1$) or all rain ($\alpha_s = 0$), accordingly. This snow fraction is applied for the entire day.

S.1.6.5 Precipitation Correction Process W

Measured total precipitation, snow precipitation, or rain precipitation may be corrected on a gauge-by-gauge basis by using gauge-dependent rainfall and snowfall corrections to correct for observation bias. This is handled using the `:RainCorrection` and `:SnowCorrection` commands given for each gauge. The parameters used in this study are x_{33} and x_{34}, respectively.

S.1.7 Processes with Single Options Without Tunable Parameters

The following processes have been fixed at single options that do not contain tunable parameters. They have been added for completeness and have been labeled as process X_1 which is known a priori to have a sensitivity of zero since no parameter will be perturbed during the analysis. We refer to the Raven documentation (Craig, 2020) for details on those options. The options are SW_RAD_DEFAULT for Extraterrestrial Shortwave Generation, PET_OUDIN for potential evapotranspiration, ROUTE_DUMP for in-catchment routing, and in-channel routing is switched off (ROUTE_NONE) since only lumped catchments are analyzed here.

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