Supplement of

Calibration of hydrological models for ecologically relevant streamflow predictions: a trade-off between fitting well to data and estimating consistent parameter sets?

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Documentation

Rainfall-Runoff Model SMART (Soil Moisture Accounting and Routing for Transport)

Model inputs and outputs

**Figure S1** Conceptual representation of the bucket-type rainfall-runoff model SMART (after Mockler et al. 2016).

**Table S1** List and Description of the inputs of the SMART model.

| Input | Description             | Unit          |
|-------|-------------------------|---------------|
| P     | Precipitation           | mm per time step |
| EP    | Potential evapotranspiration | mm per time step |

**Table S2** List and Description of the outputs of the SMART model.

| Output | Description | Unit          |
|--------|-------------|---------------|
| Q      | Discharge   | mm per time step |
| EA     | Actual evapotranspiration | mm per time step |
Model parameters

| Parameter | Description                          | Unit  |
|-----------|--------------------------------------|-------|
| $\theta_T$ | Rainfall aerial correction factor     | –     |
| $\theta_C$ | Evaporation decay coefficient        | –     |
| $\theta_H$ | Quick runoff ratio                   | –     |
| $\theta_D$ | Drain flow ratio                     | –     |
| $\theta_S$ | Soil outflow coefficient             | –     |
| $\theta_Z$ | Effective soil depth                 | mm    |
| $\theta_{SK}$ | Surface reservoir residence time   | time step |
| $\theta_{FK}$ | Interflow reservoir residence time  | time step |
| $\theta_{GK}$ | Groundwater reservoir residence time | time step |
| $\theta_{RK}$ | Channel reservoir residence time     | time step |

Conceptual model equations

The SMART model forcings are precipitation $P$ [mm/time step] and potential evapotranspiration $E_P$ [mm/time step]. The precipitation input is first transformed into the corrected precipitation $p_C$ [mm/time step] using the aerial correction parameter $\theta_T$ [–] (Eq. S1).

$$p_C = \theta_T P$$

The ratio between corrected precipitation and potential evapotranspiration determines whether the modelling time step is under energy-limited conditions ($\gamma$ is true) or water-limited conditions ($\gamma$ is false) (Eq. S2). Then, the effective precipitation $p_E$ [mm/time step] (Eq. S3) and the precipitation contribution to the actual evapotranspiration $e_A$ [mm/time step] (Eq. S4) are determined accordingly.

$$\gamma : p_C \geq E_P$$

$$p_E = \begin{cases} 
\theta_T P - E_P, & \text{if } \gamma \\
0, & \text{otherwise}
\end{cases}$$

$$e_A = \begin{cases} 
E_P, & \text{if } \gamma \\
\theta_T P, & \text{otherwise}
\end{cases}$$

The two parameters for quick runoff ratio $\theta_H$ [–] and soil outflow coefficient $\theta_S$ [–] are adjusted according to the antecedent soil moisture conditions to become $\theta_{H'}$ [–] (Eq. S5) and $\theta_{S'}$ [–] (Eq. S6), respectively. The six soil moisture layers are of equal depths and sum up to a total field capacity defined by the parameter $\theta_Z$ [mm].

$$\theta_{H'} = \frac{\sum_{\lambda=1}^6 S_\lambda}{\theta_Z}$$

$$\theta_{S'} = \frac{\sum_{\lambda=1}^6 S_\lambda}{\theta_Z}$$

Under energy-limited conditions:
The infiltration flux $q_0$ [mm/time step] and the percolation fluxes through the soil layers $q_\lambda$ [mm/time step] are then calculated as described in Equations S7 and S8, respectively.

$$q_0 = (1 - \theta_H)p_E \quad (S7)$$

$$q_\lambda = \begin{cases} 
q_{\lambda-1} - \left( \frac{\theta}{\theta'} - S_\lambda \right), & \text{if } q_{\lambda-1} + S_\lambda > \frac{\theta}{\theta'} \\
0, & \text{otherwise} 
\end{cases} \quad (S8)$$

If all soil layers reach saturation, the saturation excess flux $q_6$ [mm/time step] is divided into quick runoff as drainflow $r_{DF}$ [mm/time step] (Eq. S9) and slow runoff as interflow. The outflow from the six soil layers contributes to the three runoff pathways: interflow $r_{IF}$ [mm/time step], shallow groundwater flow $r_{SGW}$ [mm/time step], and deep groundwater flow $r_{DGW}$ [mm/time step]. First, the soil outflow contributes to the interflow runoff following a power law from the top layer to the bottom layer (Eq. S11). Then, the soil outflow contributes to the shallow groundwater runoff following an inverse law from the top layer to the bottom layer (Eq. S13). Finally, the soil outflow contributes to the deep groundwater runoff following a power law from the bottom layer to the top layer (Eq. S15). The parameter $\theta_S'$ is used in each of the three law distributions to determine the fraction of each soil layer that contributes to runoff during the modelling time step.

$$r_{DF} = \theta_{D}q_6 \quad (S9)$$

$$s_{IF\lambda} = \begin{cases} 
S_\lambda(\theta_S')^\lambda, & \text{if } \gamma \\
0, & \text{otherwise} 
\end{cases} \quad (S10)$$

$$r_{IF} = \begin{cases} 
\sum_{\lambda=1}^6 s_{IF\lambda}, & \text{if } \gamma \\
0, & \text{otherwise} 
\end{cases} \quad (S11)$$

$$s_{SGW\lambda} = \begin{cases} 
S_\lambda(\theta_S')^\lambda, & \text{if } \gamma \\
0, & \text{otherwise} 
\end{cases} \quad (S12)$$

$$r_{SGW} = \begin{cases} 
\sum_{\lambda=1}^6 s_{SGW\lambda}, & \text{if } \gamma \\
0, & \text{otherwise} 
\end{cases} \quad (S13)$$

$$s_{DGW\lambda} = \begin{cases} 
S_\lambda(\theta_S')^{7-\lambda}, & \text{if } \gamma \\
0, & \text{otherwise} 
\end{cases} \quad (S14)$$

$$r_{DGW} = \begin{cases} 
\sum_{\lambda=1}^6 s_{DGW\lambda}, & \text{if } \gamma \\
0, & \text{otherwise} 
\end{cases} \quad (S15)$$

**Under water-limited conditions:**

The water deficit $d_0$ [mm/time step] (Eq. S16) to meet the potential evapotranspiration demand is totally or partially provided by the available soil moisture evapotranspiration fluxes $e_\lambda$ [mm/time step] (Eq. S18). The variable $b_\lambda$ [–] (Eq. S20) acts as a boolean to stop the soil moisture contribution to evapotranspiration as soon as the remaining water deficit $d_\lambda$ [mm/time step] (Eq. S19) has been fully met by a given soil layer; it is initiated with a value of 1 if a deficit exists (Eq. S17). The first soil layer can fully meet the water deficit if it contains enough water, otherwise the second layer can contribute to meet the remaining water deficit with a depleted rate using the evaporation decay parameter $\theta_C$ [–] (see Eq. S19), and so forth for the next downward layer up to the bottom layer. Effectively, a lesser fraction of the available soil moisture in a layer can meet the remaining water deficit moving downwards following a power law (Eq. S19).

$$d_0 = \begin{cases} 
0, & \text{if } \gamma \\
E_P - e_A, & \text{otherwise} 
\end{cases} \quad (S16)$$
\[ b_0 = \begin{cases} 0, & \text{if } \gamma \\ 1, & \text{otherwise} \end{cases} \quad (S17) \]

\[ e_\lambda = \begin{cases} b_{\lambda-1}d_{\lambda-1}, & \text{if } S_\lambda \geq d_{\lambda-1} \\ b_{\lambda-1}S_\lambda, & \text{otherwise} \end{cases} \quad (S18) \]

\[ d_\lambda = \begin{cases} 0, & \text{if } S_\lambda \geq d_{\lambda-1} \\ \theta_C(d_{\lambda-1} - S_\lambda), & \text{otherwise} \end{cases} \quad (S19) \]

\[ b_\lambda = \begin{cases} 0, & \text{if } S_\lambda \geq d_{\lambda-1} \\ b_{\lambda-1}, & \text{otherwise} \end{cases} \quad (S20) \]

**Under water-limited and energy-limited conditions:**

At each time step, whether under water-limited or energy-limited conditions, the soil layer states \( S_\lambda \, [\text{mm}] \) are updated given their inward and outward fluxes during the time step as described in Eq. S21.

\[ \frac{dS_\lambda}{dt} = q_{\lambda-1} - s_{\text{IF}} - s_{\text{SGW}} - s_{\text{DGW}} - e_\lambda \quad (S21) \]

The routing for the five runoff pathways is conceptualised as five linear reservoirs which are characterised by three residence time parameters \( \theta_{SK} \, [\text{time step}] \), \( \theta_{FK} \, [\text{time step}] \), and \( \theta_{GK} \, [\text{time step}] \) (see Equations S22–S26). The five runoff pathways contribute to a final linear reservoir for channel routing which is characterised by the residence time parameter \( \theta_{RK} \, [\text{time step}] \) to compute the catchment total flow \( Q \, [\text{mm/time step}] \) (Eq. S27).

\[ q_{\text{OF}} = \frac{S_{\text{OF}}}{\theta_{SK}} \quad (S22) \]

\[ q_{\text{DF}} = \frac{S_{\text{DF}}}{\theta_{SK}} \quad (S23) \]

\[ q_{\text{IF}} = \frac{S_{\text{IF}}}{\theta_{FK}} \quad (S24) \]

\[ q_{\text{SGW}} = \frac{S_{\text{SGW}}}{\theta_{GK}} \quad (S25) \]

\[ q_{\text{DGW}} = \frac{S_{\text{DGW}}}{\theta_{GK}} \quad (S26) \]

\[ Q = \frac{S_{R}}{\theta_{RK}} \quad (S27) \]

Finally, the reservoir states [mm] are updated given their inward and outward fluxes during the time step as described in Equations S28–S33.

\[ \frac{dS_{\text{OF}}}{dt} = (p_E - q_0) - q_{\text{OF}} \quad (S28) \]

\[ \frac{dS_{\text{DF}}}{dt} = r_{\text{DF}} - q_{\text{DF}} \quad (S29) \]

\[ \frac{dS_{\text{IF}}}{dt} = (q_6 - r_{\text{DF}}) + r_{\text{IF}} - q_{\text{IF}} \quad (S30) \]

\[ \frac{dS_{\text{SGW}}}{dt} = r_{\text{SGW}} - q_{\text{SGW}} \quad (S31) \]
Procedural model

The procedural implementation of the SMART conceptual model equations is open-source (Hallouin et al., 2019). It is available in a pure Python version, and a Python version boosted with a C++ extension. This procedural model works with any 2.7.x, 3.5.x, or 3.6.x version of Python. The procedural model numerically solves the model conceptual equations using the Explicit Euler approach, and the procedural model executes the conceptual model equations in the order shown in the above section, i.e., using an operator splitting technique.

\[
\frac{dS_{DGW}}{dt} = r_{DGW} - q_{DGW} \tag{S32}
\]

\[
\frac{dS_{RK}}{dt} = q_{OF} + q_{DF} + q_{IF} + q_{SGW} + q_{DGW} - Q \tag{S33}
\]
References

Hallouin, T., Mockler, E., and Bruen, M.: SMARTpy: Conceptual Rainfall-Runoff Model (Version 0.2.0), doi:10.5281/zenodo.2564042, 2019.

Mockler, E. M., O’Loughlin, F. E., and Bruen, M.: Understanding hydrological flow paths in conceptual catchment models using uncertainty and sensitivity analysis, Computers & Geosciences, 90, 66–77, doi:10.1016/j.cageo.2015.08.015, 2016.