HydroBudget User Guide

Version 1.2

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Table of modifications

Version	Date of modification	Content of the modifications
V1.0	2021-02-24	Initial version of the user guide
V1.1	2021-11-05	Addition of the table of modifications Addition of the model code reference Correction of f_{inf} units Modification of the presentation of the equations ruling the HydroBudget code Change of the section 2.3 from “calibration method” to “Simulation error and objective functions” Update of the description of the application example in section 3.
V1.2	2021-12-22	Correction of eq. 28 and eq. 30 Update the reference of Dubois et al. (2021b) with the definitive DOI

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1 INTRODUCTION

HydroBudget (HB) is a spatially distributed groundwater recharge (GWR) model that computes a superficial water budget on grid cells of regional-scale watersheds with outputs aggregated into monthly time steps and with limited computational time. The model is open-source and coded in R (Dubois et al., 2021a). It was developed at UQAM by Emmanuel Dubois, Marie Larocque, Sylvain Gagné, and Guillaume Meyzonnat. HB has evolved from a previous model (named HydroBilan) that was initiated for the Quebec Groundwater Knowledge Acquisition Program (*Programme d'acquisition de connaissances des eaux souterraines - PACES*; Larocque et al., 2013, 2015a, 2015b). Its recent development was performed through a research project funded by the Quebec Ministry of the Environment (*Ministère de l'Environnement et de la Lutte contre les changements climatiques - MELCC*) (Larocque et al., 2021b). The model is currently used in several other PACES project in the Province of Quebec (Canada) and the results of its recent application over southern Quebec are presented in a submitted paper (Dubois et al., 2021b).

HydroBudget was developed as an accessible and computationally affordable model to simulate GWR over large areas (thousands of km^2) and for long time periods (decades), in cold and humid climates. The model uses commonly available meteorological data (daily precipitation and temperature, spatialized if possible) and spatially distributed data (pedology, land cover, and slopes). It is calibrated with river flows and baseflows estimated with recursive filters. The model needs reasonable computational capacity to reach relatively short computational times, e.g., 10 min for a 6 750 km^2 watershed, with 27 000 cells of 500 m x 500 m resolution, and 57 years with 15 cores and 50 Go of RAM. It is based on simplified representations of hydrological processes and is driven by eight parameters that need to be calibrated.

HydroBudget uses a degree-day snow model for snow accumulation and snowmelt, and a conceptual lumped reservoir to compute the soil water budget on a daily time step. For each grid cell and each time step, the calculation distributes precipitation as runoff (R), evapotranspiration (ET), and infiltration that can reach the saturated zone if geological conditions below the soil allow deep percolation. HB thus produces estimates of potential GWR. The daily results are compiled at a monthly time step.

When the model is used in specific projects, the model reference and the associated scientific paper should be cited (Dubois et al., 2021a, b).

2 MODELLING GROUNDWATER RECHARGE WITH HYDROBUDGET

2.1 Processes and parameters

HydroBudget is a spatially distributed GWR model that computes a superficial water budget on grid cells of regional-scale watersheds. Runoff, actual evapotranspiration (AET), and potential GWR are simulated for each grid cell (**Figure 1**), with a monthly time step, and fluxes do not transfer from a cell to another (no water routing). The model inputs are distributed daily precipitation and temperature as well as distributed data of pedology, land cover, and slope. The model script is entirely coded in R and eight parameters need to be calibrated (**Table 1**).

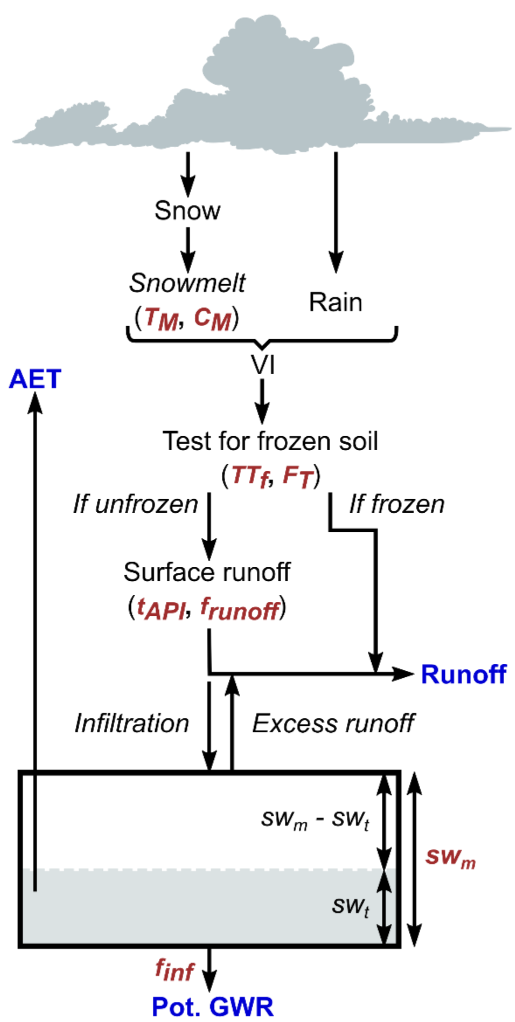

Figure 1: HydroBudget processes including the eight calibrated parameters in red (from Dubois et al., 2021b)

Table 1 : HydroBudget calibration parameters (adapted from Dubois et al., 2021b)

	Parameter		Value range
Degree-days snowmelt model	Melting temperature - T_M (°C)	Air temperature treshold for snowmelt	-2 to 2 (Massmann, 2019)
	Melting coefficient - C_M (mm/°C/d)	Melting rate of the snowpack	2 to 12 (Massmann, 2019)
Freezing soil conditions	Threshold temperature for soil frost - TT_F (°C)	Air temperature treshold for soil frost	-20 to 0 (Henry, 2007)
	Freezing time - F_T (d)	Duration of air temperature treshold to freeze the soil	5 to 30 (Henry, 2007)
Runoff	Antecedant precipitation index time - t_{API} (d)	Time constant to consider the soil in dry or wet conditions based on previous precipitation event	1 to 5 (Lal et al., 2015)
	Runoff factor - f_{runoff} (-)	Partitioning between runoff computed with the RCN method and infiltration into the soil reservoir	→1 (Neitsch et al., 2002)
Lumped soil reservoir	Maximum soil water content - sw_m (mm)	Soil reservoir storage capacity, maximum height of water stored in a 1 m soil profile	50 to 900 (Croteau et al., 2010)
	Infiltration factor - f_{inf} (d^{-1})	Fraction of soil water that produces deep percolation at each daily time step	<0.1 to 1 (Croteau et al., 2010)

The model first determines whether precipitation occurs as rain or snow using a simple air temperature threshold (0°C – not a calibration parameter but can easily be modified in the code; **Equation 1** and **Equation 2**). If precipitation occurs as snow, it accumulates until air temperature rises above a threshold melting temperature (T_M) at which snow is melted at a certain rate (C_M) using the commonly used degree-day approach (Massmann, 2019) (**Equation 3** to **Equation 5**). Snowmelt is added to rain to provide the available liquid water (vertical inflow - VI) (**Equation 6** and **Equation 7**).

Degree-days snowmelt model

Determining if the temperatures generates snowfall
If $T_t \leq 0$
Then $snowfall_t = P_{TOTt}$ Equation 1
Else $snowfall_t = 0$ Equation 2

Determining if the temperature generates snowmelt, calculating snowmelt and VI.
If $T_t \leq \mathbf{T_M}$
Then $snowpack_t = snowpack_{t-1} + snowfall_t$ Equation 3
Else $snowmelt_t = \mathbf{C_M} \times (T_t - \boldsymbol{T_M}) \times snowpack_{t-1}$ Equation 4
And $snowpack_t = snowpack_{t-1} - snowmelt_t$ Equation 5
If $T_t > 0$
Then $VI_t = P_{TOTt} + snowmelt_t$ Equation 6
Else $VI_t = snowmelt_t$ Equation 7

t = the current daily time step
T_t = the air temperature (°C)
$snowfall_t$ = the snowfall in snow water equivalent (mm)
P_{TOTt} = the total precipitation (mm)
$\boldsymbol{T_M}$ = the melting temperature (°C)
$snowpack_t$ = the snowpack in snow water equivalent (mm)
$snowpack_{t-1}$ = the snowpack in snow water equivalent at the previous time step (mm)
$snowmelt_t$ = the liquid water produced by snowmelt (mm)
$\boldsymbol{C_M}$ = the melting coefficient (mm.°C^{-1}.d^{-1})
VI_t = vertical inflow (mm)

Runoff is calculated using the runoff curve number (RCN) method (USDA-NRCS, 2004; 2007). The RCN method assesses soil ability to produce runoff or infiltration for each precipitation event, based on pedology, land cover, slope, and the antecedent moisture conditions. The soil runoff capacity gradually increases when antecedent moisture conditions change from “dry” (wilting point) to “normal” (default value in the model) to “wet” (field capacity) (Hawkins et al., 2019; Ponce and Hawkins, 1996). Relative runoff capacity variations from the default value are based on algorithms developed for the local context (for Quebec: Gagné et al., 2013; Monfet, 1979) (**Equation 8** to **Equation 21**) or for a general context (Lal et al., 2019). The switch from one soil moisture stage to the next occurs when the antecedent precipitation index (API), corresponding to the sum of the VI of the previous days (5 by default in the original RCN method), reaches a threshold value for dry or wet conditions, often determined for the local context as well (Miliani et al., 2011; Monfet, 1979). Lal et al. (2015) suggested that the API varies between one and five days (the original value of the RCN method). Therefore, the time constant to compute the API (t_{API}) is a calibration parameter in HB (i.e., does not vary during a given simulation) (**Equation 8**). If t_{API} increases (or decreases), then runoff increases (or decreases). In HB, the RCN method is used on a cell-by-cell basis, similar to what is done in the Soil Water Assessment Tool (SWAT; Arnold et al., 2012; Neitsch et al., 2002). A second parameter, the runoff factor (f_{runoff}), is needed to modulate the VI partitioning between *R* and infiltration into the soil reservoir (*Inf*), and should tend toward 1 (i.e., no influence of the factor on runoff – scenario case where the runoff was calibrated separately).

Runoff Computation

Computing the antecedent soil conditions

$$API_t = \sum_{t = t - \mathbf{t_{API}}}^{t} VI_t \quad \text{Equation 8}$$

Computing the values of RCN for dry and humid soil conditions based on equations from Monfet (1979)

$$RCN_{dry} = 0.00865 \times \mathbf{f_{runoff}} \times RCN^2 + 0.0145 \times \mathbf{f_{runoff}} \times RCN + 7.39846 \quad \text{Equation 9}$$

$$RCN_{wet} = -0.00563 \times \mathbf{f_{runoff}} \times RCN^2 + 1.45535 \times \mathbf{f_{runoff}} \times RCN + 10.82878 \quad \text{Equation 10}$$

Adjusting the RCN value based on the antecedent soil conditions

If $July\ 1^{st} \leq t < September\ 1^{st}$

- If $API_t < 50$
  - Then $RCN_t = RCN_{dry}$ Equation 11
- If $API_t > 80$
  - Then $RCN_t = RCN_{wet}$ Equation 12
- Else $RCN_t = \mathbf{f_{runoff}} \times RCN$ Equation 13

If $June\ 1^{st} \leq t < July\ 1^{st}$ or $September\ 1^{st} \leq t < October\ 10^{th}$

- If $API_t < 18.5$
  - Then $RCN_t = RCN_{dry}$ Equation 14
- If $API_t > 37$
  - Then $RCN_t = RCN_{wet}$ Equation 15
- Else $RCN_t = \mathbf{f_{runoff}} \times RCN$ Equation 16

If $October\ 10^{th} \leq t < June\ 1^{st}$

- If $API_t < 11$
  - Then $RCN_t = RCN_{dry}$ Equation 17
- If $API_t > 22$
  - Then $RCN_t = RCN_{wet}$ Equation 18
- Else $RCN_t = \mathbf{f_{runoff}} \times RCN$ Equation 19

Computing runoff (with condition on the soil frost)

If $\frac{1}{\boldsymbol{F_T}} \sum_{t=t-\boldsymbol{F_T}}^{t} T_t > \boldsymbol{TT_F}$

- Then $R_t = \frac{\left[VI_t - 0.2 \times \left({1\,000}/{RCN_t} - 10\right)\right]^2}{VI_t - 0.8 \times \left({1\,000}/{RCN_t} - 10\right)}$ Equation 20
- Else $R_t = VI_t$ Equation 21

API_t = the antecedent precipitation index (mm)

$\boldsymbol{t_{API}}$ = the antecedent precipitation index time (d)

RCN = the computed value of runoff curve number for the considered pixel (-)

$\boldsymbol{f_{runoff}}$ = runoff factor (-)

RCN_{dry}= the corrected value of runoff curve number for dry soil conditions (for the Quebec environment) (-)

RCN_{wet}= the corrected value of runoff curve number for humid soil conditions (for the Quebec environment) (-)

RCN_t = the considered value of runoff curve number for the time step (-)

$\boldsymbol{F_T}$ = the freezing time (d)

$\boldsymbol{TT_F}$ = the threshold temperature for soil frost (°C)

R_t = runoff (mm)

As a simplified view of superficial conditions to freeze soil (Henry, 2007), the soil is considered frozen if air temperature has been below a given threshold (TT_F) for a given number of days (F_T). If the soil is frozen, the entire VI will directly produce runoff (*R*). If the soil is not frozen, VI can runoff, infiltrate, be evapotranspired, and eventually percolate as potential GWR (**Equation 20** and **Equation 21**).

The maximum soil water content (sw_m) corresponds to the maximum height of water stored in a 1 m soil profile (i.e., 1 m multiplied by total porosity; constant through time). If the available storage in the soil reservoir is sufficient (i.e., the difference between sw_m and soil water content from the previous time step sw_{t-1}' exceeds infiltration), the portion of VI that is not mobilized through runoff (*Inf*) infiltrates into the soil reservoir (Equation 22). If the available soil storage is insufficient to accommodate the incoming infiltration, excess is added to runoff (saturation excess – *Excess R*) (Equation 23, Equation 24). Finally, the part of VI that flow at the surface (runoff) per time step (*Total R*) corresponds to the sum of *R* and the *Excess R* (Equation 25) Potential evapotranspiration (PET) is calculated using the formula of Oudin et al. (2005), based on temperature and extraterrestrial radiation, estimated based on the latitude and the Julian Day. Actual evapotranspiration (AET) is calculated as the minimum between PET and the available water in the soil reservoir (Equation 26 to Equation 29). The residual soil water is mobilized as potential GWR using an infiltration factor (f_{inf}, constant through time), which controls the maximum infiltration capacity of the soil water. The infiltration factor is the fraction of soil water that produces deep percolation at each daily time step (Equation 30, Equation 32). It is calculated as the ratio between the Darcy flux (under a unit gradient) and the parameter sw_m. For example, the conditions reported by Croteau et al. (2010), with till glacial deposits of 5.5 10^{-7} m/s hydraulic conductivity and a sw_m of 300 mm, result in a f_{inf} of 0.16 d^{-1}. Higher values of f_{inf} are used for materials with higher hydraulic conductivity while f_{inf} of 1 d^{-1} corresponds to a reservoir that can be completely drained during one time step. Water that do not infiltrate is saved for the following day (**Equation 31** and **Equation 33**).

Lumped soil reservoir

Computing infiltration as runoff excess

$Inf_t = VI_t - R_t$ Equation 22

Computing saturation excess

If $(\mathbf{sw_m} - sw'_{t-1}) \geq Inf_t$

Then $Excess\ R_t = 0$ Equation 23

Else $Excess\ R_t = Inf - (\mathbf{sw_m} - sw_{t-1}{}')$ Equation 24

$Total\ R_t = R_t + Excess\ R_t$ Equation 25

Computing the AET based on the soil water content

If $sw_{t-1}{}' + Inf_t - Excess\ R_t \geq PET_t$

Then $AET_t = PET_t$ Equation 26

$sw_t = sw'_{t-1} + Inf_t - Excess\ R_t - AET_t$ Equation 27

Else $AET_t = sw'_{t-1} + Inf_t - Excess\ R_t$ Equation 28

$sw_t = 0$ Equation 29

Computing the potential GWR based on the soil water content after the AET computation

If $sw_t > 0$

Then $GWR_t = sw_t \times \frac{sw'_{t-1} + Inf_t - Excess\ R_t}{\mathbf{sw_m}} \times \mathbf{f_{inf}}$ Equation 30

$sw_t{}' = sw_t - GWR_t$ Equation 31

Else $GWR_t = 0$ Equation 32

$sw_t{}' = 0$ Equation 33

Inf_t = infiltration to the soil reservoir (mm)

$\boldsymbol{sw_m}$ = maximum soil water content in the soil reservoir (mm)

sw_{t-1}' = soil water content at the end of the previous time step (mm)

Excess R_t = saturation excess produced by the soil reservoir (mm)

Total R_t = total runoff (mm)

PET_t = potential evapotranspiration (mm)

AET_t = actual evapotranspiration (mm)

sw_t = soil water content after the AET computation (mm)

GWR_t = potential GWR (mm)

$\boldsymbol{f_{inf}}$ = infiltration factor (d^{-1})

sw_t' = soil water content after the AET and GWR computation (mm)

Finally, the model compute the simulated monthly total runoff, AET, and GWR as the sum of the daily variables per month (**Equation 34** to **Equation 36**).

Model output per grid cell

$$R_m = \sum_{t=1}^{n} Total\ R_t$$ Equation 34

$$AET_m = \sum_{t=1}^{n} AET_t$$ Equation 35

$$GWR_m = \sum_{t=1}^{n} GWR_t$$ Equation 36

R_m = simulated monthly total runoff (mm)

n = number of days in the considered month

AET_m = simulated monthly AET (mm)

GWR_m = simulated monthly potential GWR (mm)

Although daily time steps are used for the calculation, the simulated outputs are integrated on a monthly time step. The sum of runoff and potential GWR (*Total R* + *GWR*) on the entire watershed is considered to be equal to total river flow at the watershed outlet. Potential GWR (*GWR*) is considered to be equal to baseflow.

HydroBudget calculates potential GWR, i.e., the percolating water that can reach the saturated zone if 1) the geological material below the soil horizon allows deep percolation, 2) no additional storage or losses occur in the unsaturated zone below the soil, and 3) no significant evapotranspiration occurs from groundwater (Doble and Crosbie, 2017). Actual GWR corresponds to the part of potential GWR that will reach the water table, and potential GWR is therefore a maximum.

If the local RCN application conditions are strictly applied (Monfet, 1979), superficial water bodies and wetlands would have the maximum RCN value (100), therefore producing 100% of runoff from the precipitation and keeping the soil reservoir empty (preventing AET and potential GWR). To avoid that configuration, RCN values of grid cells of water and wetlands are artificially lowered to a value of 10 to allow the majority of VI to infiltrate into a reservoir, which percolation capacity is null (no potential GWR – coded in HB R script). With this setup, high evapotranspiration (AET ≈ PET) and high excess runoff are produced, compensating for the artificially lowered primary runoff. Although wetlands do not produce potential GWR in HB, it is well known they are often connected to regional groundwater systems (e.g., Bourgault et al., 2014). Therefore, wetland representation in HB is a regional simplification that might need to be improved in future versions.

2.2 <u>Input data</u>

2.2.1 Grid building for the study area

To simulate GWR with HB, the study area needs to be divided into a grid to compute the water budget for each grid cells. Although the simplest grid is a grid of regular square cells, a grid of various shaped cells could be used as well, thus requiring modifying the initial script of the model. The simplest way of building a grid on a study area is to compute the RCN (cf. section 2.2.3) and rasterize the spatially distributed RCN with the desired spatial resolution. In that case, the raster pixel resolution could be used as the spatial resolution of the model.

2.2.2 Climate data

HydroBudget uses spatially distributed daily total precipitation (rainfall and snowfall) and mean daily temperature. In Quebec, this data is available from the interpolated climate grid by Bergeron (2016) for the period 1691-2017, with very limited error in southern Quebec (RMSE of 3 mm/d for precipitation, 2.5°C for minimal temperature, and 1.5°C for maximal temperature). Each cell in the climate grid must be associated with each cell (RCN cells) of the study area grid to run HydroBudget (**Figure 2**).

2.2.3 Runoff Curve Number

To compute the spatialized water budget, spatialized RCN are needed at the resolution of the grid defined for the study area (cf. section 2.2.1; **Figure 2**). The RCN method is fully described in USDA (2004; 2007) and its adaptation for the province of Quebec has been described by Monfet (1979). Land use, mean slope, and “hydro-pedology” classification are needed to compute the RCN over a cell, (**Table 2**). The hydro-pedology classification describes in a qualitative way the ability of the superficial layer of soil to generate runoff or infiltration, with four levels ranging from high infiltration capacity to low infiltration capacity. Gagné et al. (2013) developed the link between the pedologic maps of Quebec and the hydro-pedology classification.

Once the RCN attribution is done, RCN values in “normal humidity conditions” are obtained (RCN). These values evolve depending on the moisture conditions, from dry (RCN_{dry}) to wet (RCN_{wet}), computed from RCN values by **Equation 9** and **Equation 10** for southern Quebec (adapted from Monfet, 1979).

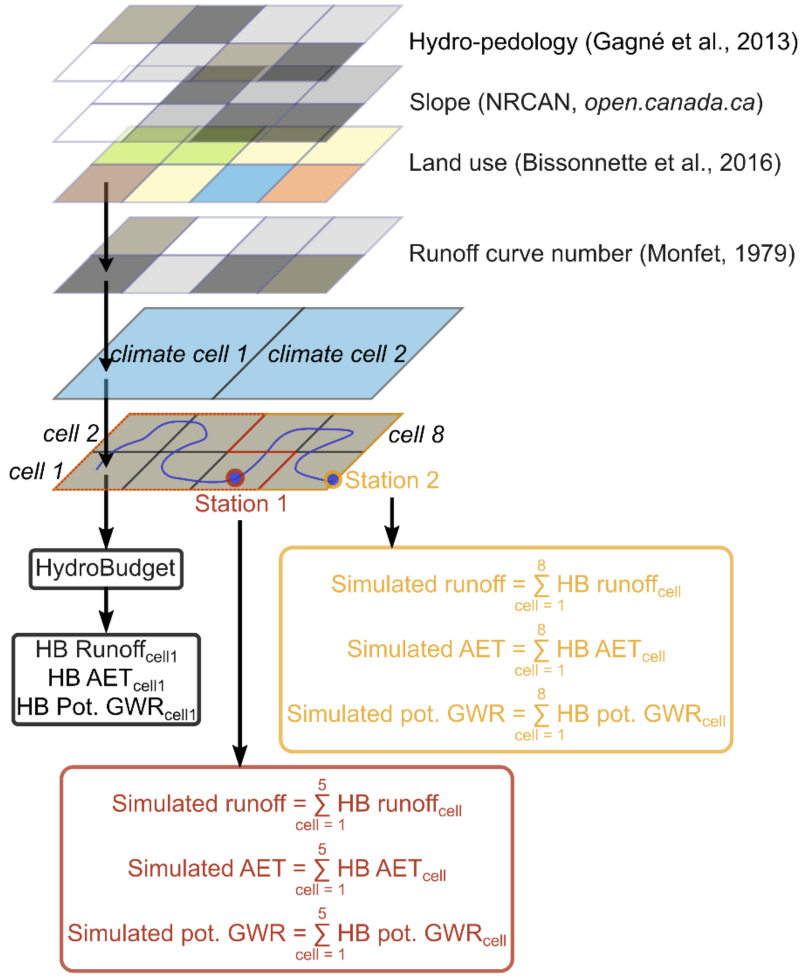

Figure 2: Composition of input data for HydroBudget in southern Quebec

The threshold values of antecedent precipitation index (API), the sum of VI of the *x* previous day (determined with the parameter t_{API} in HB), trigger the change from the “normal” RCN conditions to RCN_{dry} or RCN_{wet} are defined in Quebec by Monfet (1979) for each season (**Equation 11** to **Equation 19**). An RCN value is therefore associated for each computational iteration (RCN_t), depending on the season and the recent precipitation and used to compute the runoff of the iteration (R_t; **Equation 20**):

Although this version of the RCN method is implemented in the HB code, it could easily be modified for another locally developed version.

Table 2: Attribution of the RCN value for Quebec adapted from Monfet (1979)

Land use	Slope	Hydro-pedology classification*	RCN II value
Agriculture	slope < 3%	A	61.5
	slope < 3%	B	72
	slope < 3%	C	79
	slope < 3%	D	81.5
	3% < slope < 8%	A	64
	3% < slope < 8%	B	75.5
	3% < slope < 8%	C	83.5
	3% < slope < 8%	D	87.5
	slope > 8%	A	69.5
	slope > 8%	B	79.5
	slope > 8%	C	86.5
	slope > 8%	D	90
Forest	slope < 3%	A	23.5
	slope < 3%	B	54
	slope < 3%	C	67.5
	slope < 3%	D	75.5
	3% < slope < 8%	A	33
	3% < slope < 8%	B	59
	3% < slope < 8%	C	72.5
	3% < slope < 8%	D	79
	slope > 8%	A	44
	slope > 8%	B	65.5
	slope > 8%	C	77.5
	slope > 8%	D	82.5
Urban	-	A	66
		B	78.5
		C	85
		D	88
Wetland	-	-	100
Water	-	-	100

**The hydro-pedology classification ranges from A (high infiltration capacity) to D (very poor infiltration capacity)*

2.3 Simulation error and objective functions

For a given watershed, computation of the HB simulation error and of the objective functions is based on the following hypotheses: 1) surface watersheds match hydrogeological watersheds, 2) the rivers drain unconfined aquifers, and 3) the watershed response time is shorter than one month, thus compensating for the absence of water routing. Under these conditions, for any given watershed, monthly potential GWR should be similar to monthly river baseflow at the outlet, and the sum of monthly runoff and monthly potential GWR should be equal to the total flow at the outlet (although monthly flows are considered, daily time steps are used in the calculations).

In the current version of HB, baseflows are estimated from the river flow time series following Ladson et al. (2013) proposition for a standard approach of the Lyne and Hollick filter (Lyne and Hollick, 1979), using a stochastic calibration and 30 passes of the filter. Total flows and baseflows are divided by the area of the given watershed to provide flow values in mm/month and thus facilitate the comparison of calibration results between watersheds of very different sizes.

For a GWR simulation, model performance is assessed with the Kling–Gupta Efficiency (KGE, Gupta et al., 2009) calculated for monthly measured river flows and simulated river flow (KGE_{qtot}), as well as monthly baseflow and monthly potential GWR (KGE_{qbase}). In the script, each river flow time series is divided into a calibration period (first two thirds) and a validation period (last third), therefore allowing to compute the objective functions per period per gauging station. In the case of a group of gauging station, $(KGE_{qtot})_{ws}$ corresponds to the mean of the individual KGE_{qtot} per station ($(KGE_{qtot})_{station}$) and the $(KGE_{qbase})_{ws}$ to the mean of the individual KGE_{qbase} per station ($(KGE_{qtot})_{station}$) (**Equation 37** and **Equation 38**). The average KGE of the simulation (KGE_{mean}) is computed as the weighted average of $(KGE_{qtot})_{ws}$ and $(KGE_{qbase})_{ws}$ (**Equation 39**). The weights *x* and *y* attributed to each objective function in KGE_{mean} can be set to arbitrary values, depending on the study's objectives. For example, for the model developed to simulate GWR over southern Quebec, the set (x = 0.4; y = 0.6) was chosen to maximize the quality of the reproduction of the baseflows, considered as the proxy for GWR (KGE_{qbase}), without dropping the benefits of the multi-objective optimization (Dubois et al., 2021b).

An example of calibration procedure of the HB model based on these objective functions can be found in Dubois et al. (2021b). It was developed to optimize the eight HB parameters on several river watersheds, based on a simultaneous calibration on all the available gauging stations and based on the automatic calibration procedure of the R package *caRamel* (Monteil et al., 2020).

$$(KGE_{qtot})_{ws} = \frac{1}{N_{ws}} \sum_{station=1}^{N_{ws}} (KGE_{qtot})_{station}$$ Equation 37

$$\left(KGE_{qbase}\right)_{ws} = \frac{1}{N} \sum_{station=1}^{N_{ws}} (KGE_{qbase})_{station}$$ Equation 38

$$KGE_{mean} = x \times \left(KGE_{qtot}\right)_{ws} + y \times \left(KGE_{qbase}\right)_{ws}$$ Equation 39

$(KGE_{qtot})_{ws}$ the KGE obtained for the total flow over a river watershed (group of gauging stations)
$(KGE_{qtot})_{station}$ the KGE obtained for the total flow for a gauging station
N_{ws} the number of gauging stations per watershed
$(KGE_{qbase})_{ws}$ the KGE obtained for the potential GWR over a river watershed (group of gauging stations)
$(KGE_{qbase})_{station}$ the KGE obtained for the potential GWR for a gauging station
KGE_{mean} the average KGE for the simuation
x and y the weights attributed to each objective function

2.4 Similarities with other models

In water budget models, GWR is computed as the residual of the water budget (Scanlon et al., 2002), therefore they are all based on similar processes (**Table 3**). They use precipitation as input and sometimes estimate interception, snow accumulation and snowmelt. The RCN method (USDA-NRCS, 2004; 2007) is a widely-used empirical method to compute runoff. It is used in HELP (Schroeder et al. 1994), SWAT (Neitsch et al., 2002), SWB (Westenbroek et al., 2010) and in the water balance GIS tool (Portoghese et al., 2005). WetSpass (Batelaan and De Smedt, 2007) and WGHM (Döll et al., 2003) use similar empirical methods, based on runoff coefficients to compute runoff as a ratio of precipitation. In HB, a freezing soil condition is used to produce 100% of runoff from the available water if the soil is frozen. This approach is not included in the models listed in **Table 3**, but WGHM accounts for freezing soil in permafrost and glacier areas (Döll et al., 2003). In all the models, the remaining water (precipitation minus runoff) is routed to the soil where evapotranspiration is removed based on potential evapotranspiration formulas or based on specific land cover for WetSpass and WGHM (using crop and vegetation coefficients). The soil modelling widely varies depending on model complexity and modeling objectives. For example, HELP considers a 2 m layered soil column (unsaturated zone) generating subsurface runoff and infiltration for each soil layer, and the excess water reaching the base of the soil column is considered as GWR (Croteau et al., 2010). Similarly, the water balance GIS tool uses soil hydraulic conductivity to partition infiltration water into sub-surface runoff or potential GWR (Portoghese et al., 2005). The SWB model uses the Thornthwaite soil moisture retention equations to estimate if the soil moisture retention is exceeded and potential GWR is generated (Dripps and Bradbury, 2007). WGHM considers GWR as a portion of superficial runoff using an infiltration factor (Döll and Fiedler, 2008) while WetSpass computes GWR as the residual water of the water budget.

While being very similar to other water budget models, HB uses a simplified soil representation and the most accessible data as input and computes potential GWR, similarly to SWB and the water balance GIS tool (**Table 3**). HELP, WetSpass and WGHM produce actual GWR although only WetSpass takes into account the feedback of the water table depth on the GWR. The potential GWR calculated in HB is mostly sensitive to the runoff factor (f_{runoff}) and the infiltration factor (f_{inf}) equivalent to that found for SWB and WetSpass to a certain extent. The simulation of GWR with HELP, SWB, and WetSpass seem sensitive to unsaturated zone parameters as well, as the unsaturated zone processes in these models are relatively detailed.

Table 3: Main characteristics of a selection of groundwater recharge water budget models

Model	References (not exhaustive)	Main input data (not exhaustive)	Model structure	Sensitive parameters listed in references
HydroBudget	Dubois et al., 2021b; Larocque et al., 2013, 2015a, 2015b	Spatially-distributed total precipitation and temperature time series, hydrologic soil groups, slopes, land cover	Computes runoff with RCN; infiltration = precipitation - runoff; AET from soil reservoir; potential GWR = portion of the soil reservoir water	Runoff factor, infiltration factor, soil freezing temperature, time constant to switch from wet to dry soil conditions, and the soil water content capacity
HELP	Allen et al., 2004; Carrier et al., 2013; Croteau et al., 2010; Guay et al., 2013; Jyrkama and Sykes, 2007; Kurylyk and MacQuarrie, 2013; Lefebvre et al., 2015; Rivard et al., 2013; Schroeder et al. 1994; Scibek and Allen, 2006; Talbot-Poutin et al., 2013	Spatially-distributed total precipitation and temperature time series, solar radiation, annual average wind velocity, relative humidity, growth season length, unsaturated soil parameters (total porosity, field capacity, wilting point, unsaturated hydraulic conductivity, and thickness of each soil layer of the unsaturated zone)	Computes runoff with RCN; infiltration = precipitation - runoff; subsurface runoff based on each soil layer, GWR = water reaching the base of the soil layers	Soil parameters including unsaturated hydraulic conductivity and root depths
SWB	Dripps and Bradbury, 2007; Nielsen and Westenbroek, 2019; Westenbroek et al., 2010	Daily total precipitation and temperature, interception rates, root depths, hydrologic soil groups, land cover, slopes, soil moisture capacity, surface flow directions, initial soil moistures, and initial snow cover	Computes runoff with RCN; superficial water routing; infiltration = precipitation - interception - runoff; AET from soil reservoir; potential GWR = excess water from the Thornthwaite soil moisture equation	RCN, crop coefficients, maximum potential infiltration rates, and root depths

Model	References (not exhaustive)	Main input data (not exhaustive)	Model structure	Sensitive parameters listed in references
water balance GIS tool	Portoghese et al., 2005	Spatially-distributed interannual monthly rainfall and PET, vegetation cover and monthly crop coefficients, soil-moisture contents, soil thickness and hydrologic soil groups, land cover (including the percentage of pervious/ impervious surfaces), slopes	Computes runoff with RCN; infiltration = precipitation - runoff; AET = PET corrected with crop coefficients and available soil moisture; computation of sub-surface runoff based on the soil texture, potential GWR = residual water of the water budget	n.a.
WetSpass	Abdollahi et al., 2017; Batelaan and De Smedt, 2007; Zomlot et al., 2015	Soil texture, groundwater depth, slope, rainfall, potential evapotranspiration, number of rainy days, wind, temperature, and land cover with the detail of vegetated cover, bare soil, open water, and impervious surface on each grid cell	Computes runoff as a fraction of precipitation; Infiltration = precipitation - interception - runoff; AET = PET corrected with crop coefficients; GWR = residual water of the water budget	Runoff coefficients, soil moisture coefficients, and interception parameters
WGHM	Döll and Fiedler, 2008; Döll et al., 2003	Spatially-distributed precipitation and temperature, number of wet days per month, cloudiness, daily sunshine hours, land use, superficial drainage	Computes AET as the minimum of PET and the available soil water; runoff is a function of the difference precipitation - AET and of the soil moisture; superficial water routing; GWR = percentage of runoff	n.a.

3 EXAMPLE FOR THE PETITE DU CHENE RIVER (QUEBEC)

An application example can be taken on the Petite du Chêne River watershed (460 km^2), a St. Lawrence tributary located in southern Quebec (**Figure 3**). Two gauging stations monitored river flows mainly from 1993 to 2007 (gap of 6 days in 2005) for the station 23701 and from 2007 to 2017 for the station 23702. Interpolated climate data are available from 1961 to 2017 and distributed on 10x10 km grid (post-processed from Bergeron, 2016). The application example will simulate the water budget on the watershed for the entire 1961-2017 period.

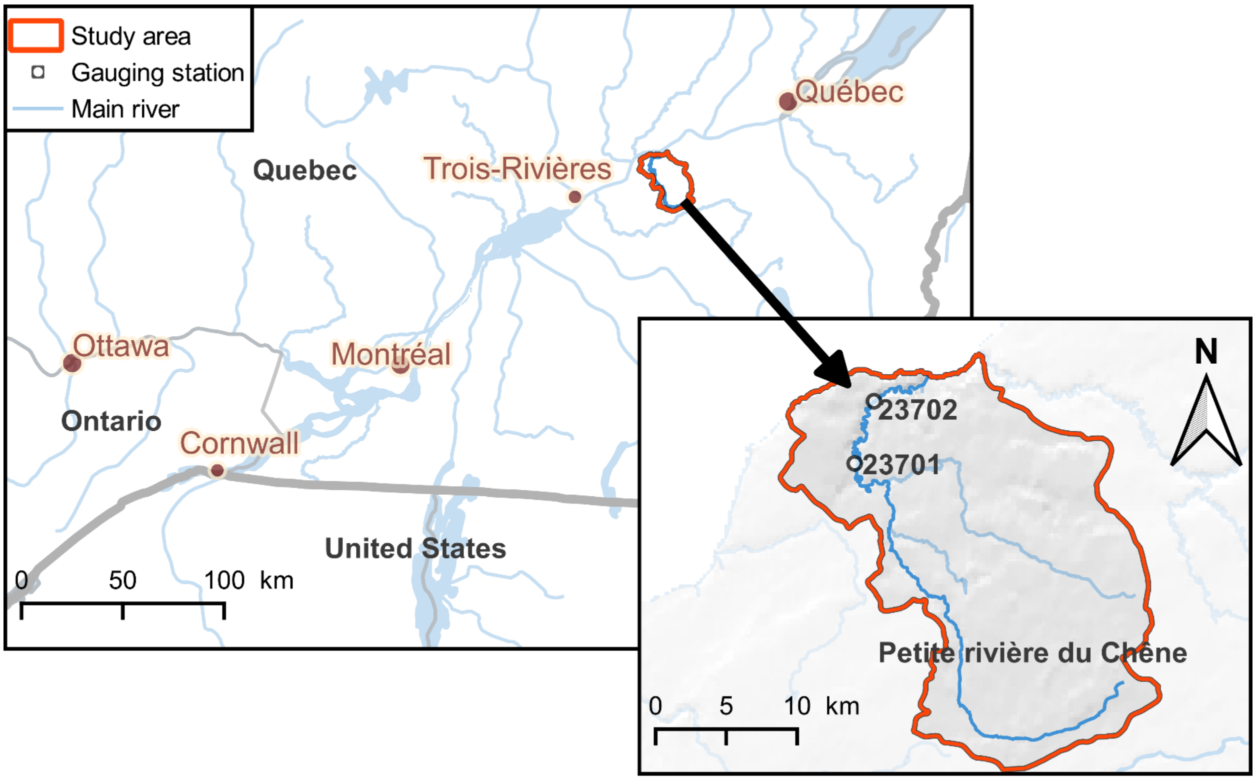

Figure 3: Location of the Petite du Chêne River watershed

3.1 Folder HydroBudget

The model scripts, the input data, the river flows time series, and the shape files (GIS) for the area are located in the HydroBudget folder:

- **The folder 01-input** contains the input data:
  - **alpha_lyne_hollick.csv**: statistically calibrated α following Ladson et al. (2013) procedure for the Lyne and Hollick (1979) baseflow computation for the two gauging stations (the baseflow computation itself is included in HB script). The file contains two attributes:
    - station: name of the gauging station
    - alpha: value of the calibrated alpha parameter
  - **input_climate.csv**: daily total precipitation (mm/d) and average daily temperature (°C) of the Quebec climate interpolated grid (Bergeron, 2016) from 1961/01/01 to 2017/12/31. The file contains six attributes:
    - climate_cell: ID of the 10 km x 10 km climate cell
    - day: day of the date
    - month: month of the date
    - year: year of the date
    - t_mean: average temperature of the day (°C)
    - p_tot: total precipitation of the day (mm/d)
    - lat: latitude of the climate cell (°)
  - **input_rcn.csv**: RCN values on a 500 m x 500 m grid. A RCN value is given for each grid cell of the watershed with the corresponding climate cell and the coordinates of the center of each RCN cell in NAD83 Quebec Lambert (EPSG: 32198):
    - climate_cell: ID of the 10 km x 10 km climate cell
    - cell_ID: ID of the 500 m x 500 m RCN cell
    - RCNII: value of the RCN computed for the RCN cell
    - X_L93: x coordinate of the center of the RCN cell
    - Y_L93: y coordinate of the center of the RCN cell

- **input_rcn_gauging.csv**: table with the list of RCN cells located in each gauging station watershed. The table is composed of two attributes:
  - cell_ID: ID of the 500 m x 500 m RCN cell
  - gauging_stat: gauging station associated to that cell

    Note: Since the watersheds of the two gauging stations can be overlaying, RCN cells can be associated with the two gauging stations; in that case, the RCN cell ID appears twice in the table, once with each gauging station
- **observed_flow.csv**: measured river flow (mm/d) of the 2 gauging stations for the entire time period covered by the climate data with:
  - year: year of the date
  - month: month of the date
  - day: day of the date
  - 23701: measured river flow at the 23701 station (mm/d)
  - 23702: measured river flow at the 23702 station (mm/d)

    Note: unavailable data (including if flow measurements do not exist for a given period) are marked with a "NA" (Not Available).

Note: all the csv files are "data.table" formatted for R

- **The folder 02-scripts_HB** contains two R scripts:
  - **01-river_flow_data_processing.R**: R script used to process the observed river flow rates. It will automatically fill the gaps in the daily time series (up to 5 missing days) and select a subset of the longest period of river flow observations within the simulation period for each station; extract the list of the gauging stations with observations during the simulation period; compute the Lyne and Hollick baseflow using the calibrated α for the gauging stations; and resample river flows and baseflows with a monthly time step.

- **02-HB_function.R**: R script containing the HydroBudget function (HB). The function will run HB in parallel on all the grid cells of the watershed following Figure 1 processes. After defining all the variables in the function (sections 1.1 to 1.4), a first parallel loop runs the degree-day model and compute Oudin PET on each climate cell for the chosen simulation period (section 1.5 of the script). A second parallel loop runs HB water partitioning on each RCN cell (section 1.6 of the script). To start and finish the parallel loops, the code needs to be changed if the model is run on a computer without a Windows environment (change package "doParallel" for Windows to package "doMC"). The options for the non-Windows environment are muted by default. The monthly spatialized and averaged water budget is saved in the working directory. As well, the function automatically analyzes the results for each available gauging station based on the comparison of the simulated monthtly total flow (runoff + excess runoff + potential GWR) and potential GWR to the monthly river flow and baseflow (section 1.7). For each station the code considers a calibration period (first 2/3 of the observation period) and a validation period (last 1/3 of the observation period). The last section (1.8) exports rasters of the interannual simulated runoff, AET, and potential GWR with the resolution of the RCN grid and in NAD83 Quebec Lambert coordinates (EPSG: 32198) into the working directory. In case the RCN method needs to be adapted to another version of the method, changes need to be done in the subsections 3.6.1.3 to 3.6.1.5 of the parallel loop of the model.

- **The folder 03-GIS_petite_du_chene** contains shapefiles and rasters (GIS) in NAD83 Quebec Lambert (EPSG: 32198) with**:**

Note: all coordinates are in NAD83 Quebec Lambert (EPSG: 32198)

Note: all the files associated to a shapefile are in a compressed ZIP file

- **L_watercourse_NRCAN_petite_riv_du_chene_NAD83.zip** (lines): Petite du Chene River watercourse extracted and simplified (one attribute with the name of the river) from https://www.nrcan.gc.ca/science-and-data/science-and-research/earth-sciences/geography/topographic-information/geobase-surface-water-program-geeau/national-hydrographic-network/21361
- **P_gauging_stations_petite_riv_du_chene_NAD83.zip** (points): location of the gauging station with 3 attributes:
  - station_id: name of the gauging station
  - x_NAD83: x coordinate of the station
  - y_NAD83: y coordinate of the station
- **R_RCN_NAD83.tif** (raster): raster of the RCN values for the RCN cells
- **S_climate_grid_petite_riv_du_chene_NAD83.zip** (polygons): 10 km x 10 km climate cells for the Petite du Chene River watershed (one attribute with the climate cell ID)
- **S_gauging_station_watersheds_NAD83.zip** (polygons): watersheds of the gauging stations (one attribute with the name of the gauging station) from https://www.cehq.gouv.qc.ca/hydrometrie/index.htm
- **S_grid_gauging_petite_riv_du_chene_NAD83.zip** (polygons): the grid for the gauging stations with 3 attributes:
  - cell_id: ID of the 500 m x 500 RCN cell
  - gauging_st: gauging station
  - clim_cell: ID of the 10 km x 10 km climate cell

    Note: Since the watersheds of the two gauging stations can be overlaying, RCN cells can be associated with each of them; in that case, the cell_id appears twice in the attribute table, once with each gauging station
- **S_grid_petite_riv_du_chene_NAD83.zip** (polygons): grid for the river watershed with 2 attributes:
  - cell_id: ID of the 500 m x 500 RCN cell
  - clim_cell: ID of the 10 km x 10 km climate cell
- **S_watershed_petite_riv_du_chene_simul_NAD83.zip** (polygon): watershed of the Petite du Chene River (one attribute corresponding to the ID given to the watershed in Dubois et al. (2021b))

- **00-demonstration_HB.Rproj:** R project that opens the R scripts 01-HydroBudget.R (if it does not, manually load the script in the R project)

- **01-HydroBudget.R**: R script that runs HB on the Petite du Chêne River with a single set of parameters. It contains the references to the inputs data located in the folder 01-input previously detailed and the references to the scripts located in 02-scripts_HB. It creates a folder for the results, simulates the water budget on the watershed, saves the results for the entire watershed (spatially distributed, averaged on the watershed, and averaged for each gauging station), computes the objective functions for the 2 gauging stations per period ($(KGE_{qtot})_{station}$, $(KGE_{qbase})_{station}$, and KGE_{mean} for both calibration and validation periods), and saves a summary of the simulation in a separate csv file;

3.2 Run HydroBudget with the 01-HydroBudget.R script

The script is divided in 4 sections:

- Section **1-Load the packages**

  All the packages need to be loaded before running the model. Please install them if it is the first use of the model. The package "doMC" replaces the package "doParallel" if the model is used on a computer with an exploitation system different than Windows. If doMC is used, adjustments need to be done in the HB function for the parallel computing options (script 02-scripts_HB/ 02-HB_function.R; sections 1.5.1 and 1.6.1)

- Section **2-Load the input data for the simulation and enter the parameters values**

  This section is detailed in several subsections. The first step (2.1) consists of defining the path to the demonstration folder, from which the code will create a folder "YYYY_MM_DD_HH_mm_simulation_HydroBudget" to store all the results. Then the input data are loaded (2.2), and the user assigns values to the model parameters (2.3). Parameter values from Dubois et al. (2021b) are pre-assigned. The simulation period and the spatial resolution (not used in the actual computation in the model) are defined in 2.4 (values pre-assigned for the example). A subset of the river flow measurements is made for the years of the simulation period. The parallel computing options are given in 2.5.

- Section **3- Process the river flow observations and load the HB function**

  The first part of this section refers to the script 02-scripts_HB/01-river_flow_data_processing.R, used to process the river flow observations for the simulation.

  The second part of this section automatically loads the R function called “HB” in the local environment based on the script 02-scripts_HB/02-HB_function.R.

- Section **4-Simulation with HB**

  This section runs the HB function loaded in section 3 with the inputs defined in section 2 and the river flow observation processed in the beginning of section 3. It saves the results in the folder created in subsection 2.1:

  - 01_bilan_spat_month.csv: the spatialized simulated water budget by RCN cell for all the RCN cells of the Petite du Chêne River with monthly time step with:
    - year: considered year
    - month: considered month
    - VI: vertical inflow of the month (mm/month)
    - t_mean: average temperature of the month (°C)
    - runoff: simulated runoff (mm/month)
    - pet: Oudin PET (mm/month)
    - aet: simulated AET (mm/month)
    - gwr: simulated potential GWR (mm/month)
    - runoff_2: simulated excess runoff (mm/month)
    - delta_reservoir: monthly budget of the soil reservoir (mm/month)
    - rcn_cell: ID of the 500 m x 500 m RCN cell
  - 02_bilan_unspat_month.csv: averaged simulated water budget on the Petite du Chêne River with monthly time step (not spatialized) with:

- year: considered year
- month: considered month
- VI: vertical inflow of the month (mm/month)
- t_mean: average temperature of the month (°C)
- runoff: simulated runoff (mm/month)
- pet: Oudin PET (mm/month)
- aet: simulated AET (mm/month)
- gwr: simulated potential GWR (mm/month)
- runoff_2: simulated excess runoff (mm/month)
- delta_reservoir: monthly budget of the soil reservoir (mm/month)

o 03_bilan_unspat_month_23701.csv and 03_bilan_unspat_month_23702.csv: averaged water budget per gauging station (not spatialized) with the observed flow and baseflows with:

- year: considered year
- month: considered month
- q: observed river flow (mm/month)
- qbase: baseflow computed with Lyne and Hollick (mm/month)
- VI: vertical inflow of the month (mm/month)
- t_mean: average temperature of the month (°C)
- runoff: simulated runoff (mm/month)
- pet: Oudin PET (mm/month)
- aet: simulated AET (mm/month)
- gwr: simulated potential GWR (mm/month)
- runoff_2: te simulated excess runoff (mm/month)
- delta_reservoir: te monthly budget of the soil reservoir (mm/month)

Note: If one of the station does not have observation data during the simulation period, then the associated file with the simulated water budget is not created.

- 04-simulation_metadata.csv: summary of the simulation with:
  - gauging_stat: considered gauging station
  - cal_beg: first year of the calibration period
  - Cal_end: last year of the calibration period
  - val_beg: first year of the validation period
  - val_end: last year of the validation period
  - T_snow: temperature threshold for precipitation to occur as rain or snow (°C)
  - T_m: melting temperature (T_M – °C)
  - C_m: melting coefficient (C_M – mm/°C/d)
  - TT_F: threshold temperature for soil frost (TT_F - °C)
  - F_T: freezing time (F_T – d)
  - t_API: antecedent precipitation index time (t_{API} – d)
  - f_runoff: runoff factor (f_{runoff} – –)
  - sw_m: te maximum soil water content (sw_m – mm)
  - f_inf: infiltration factor (f_{inf} – d-1)
  - KGE_qtot_cal: $(KGE_{qtot})_{station}$ in calibration period
  - KGE_qbase_cal: $(KGE_{qbase})_{station}$ in calibration period
  - KGE_qtot_val: $(KGE_{qtot})_{station}$ in validation period
  - KGE_qbase_val: $(KGE_{qbase})_{station}$ in validation period
  - qtot_sim: interannual simulated total flow (mm/yr)
  - aet_sim: interannual simulated AET (mm/yr)
  - gwr_sim: interannual simulated potential GWR (mm/yr)
  - time: date and time when the water budget was saved
  - KGE_mean_cal: KGE_{mean} in calibration period
  - KGE_mean_val: KGE_{mean} in validation period
- 05_interannual_runoff_NAD83.tif,06_interannual_aet_NAD83.tif, 07_interannual_gwr_NAD83.tif: rasters of the corresponding variable with interannual values over the simulation period in NAD83 Quebec Lambert (EPSG: 32198)

  Note: total runoff is the sum of runoff and runoff_2 and total flow is the sum of runoff, runoff_2, and gwr

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