Supplementary material A : Estimating soil surface temperature from external conditions

The CMIP6 climate scenarios used in this work provide access to air temperature and precipitation projections for the next century. However, permaFoam is a solver dedicated to water and heat transfer within the soil, and boundary conditions at the soil surface must be provided. The soil surface is separated from the air by a vegetation layer (in Kulingdakan, mainly lichens and mosses), which is covered by a snow layer in winter. In order to carry out numerical simulations to quantify climate change impact on the Kulingdakan soil thermal and hydrological regime, a dedicated procedure has to be set up to estimate soil surface temperature from external conditions. The methodology should be based on the variables for which in-situ measurements are available:

- A measurement campaign made in Kulingdakan between August 2003 and September 2005 providing daily measurements of soil temperature at different depths : top of the moss layer, top of the organic soil horizon (duff), top of the mineral horizon and at 10cm and 20cm depths within the mineral soil horizon.

- Measurements from the Tura weather station between 1999 and 2014: daily snow depth, air temperature (including min/max), and precipitation (undifferentiated rain or snow). The town of Tura is located five kilometres away from the Kulingdakan watershed. The air temperature measured at Tura was compared with the temperature at the top of the moss layer during the summer months (June to August), when there is no snow separating the moss layer from the ambient air. The two signals variations are similar, with an average difference of 1.9°C in the order of magnitude of a difference between open place / sub-canopy temperature measurement (Zellweger et al., 2019, Haesen et al., 2021). Therefore, the meteorological data from the Tura weather station are used as approximation of the meteorological conditions in the Kulingdakan watershed.

The proposed empirical transfer function, based on parametrical calibrations, is not directly transferable to other study sites. The methodology is solely aiming at translate the range of possible future climatic conditions into soil surface signals in the slopes of the Kulingdakan watershed, in order to build proper surface boundary conditions for performing the targeted cryohydrogeological simulations. Model output compared to available data and climate projections can be found in Figures 3 and 4. The soil surface temperature estimator produced a signal with an average error limited to 1.4°C and 1.6°C for North- and South aspected slopes respectively (L^1 norm).

In the following, we describe the details of this methodology, organised in two steps : a model for the evolution of the snow cover and and an estimator of the soil surface temperature.

Estimation of snowpack evolution

As empirical models of snowpack evolution, temperature index models allows to simulate snowpack dynamics using only a limited number of variables. A more detailed and physically based snow model would require the use of additional variables beyond air temperature and precipitation only, and is therefore beyond the scope of this work. Since only air temperature and precipitation data are available for simulating the snow pack of the Kulingdakan watershed, we use such a temperature index model. Besides, only snow depths observations are avalaible in this area, not Snow Water Equivalent that is the main output of a temperature index model. Thus for enabling the training of the temperature index model, we estimated SWE from snow depths measurements, we use a data assimilation approach.

Here, we base our approach on the formulation of Hock (2003), and express the variation of snow water equivalent mass per day ΔSWE [$mm.day^{-1}$] as a result of melt *M* [$mm.day^{-1}$] and accumulation through snow precipitation *P* [$mm.day^{-1}$] – Equation (A.1).

$$\Delta SWE = P - M \quad \text{(A.1)}$$

The accumulation term is estimated by snow precipitation, which is considered to be the precipitation recorded by weather station when air temperature is below 0°C. The melt term is zero when air temperature is below 0°C and positive when the air temperature is strictly above 0°C. It is estimated using a degree-day factor DDF and air temperature, with $M=DDF*T_{air}$. The DDF need to be calibrated to represent the observed melt during the thaw season. In the case of Kulingdakan, a high value of DDF is found to be optimal (15 $mm.day^{-1}.K^{-1}$) due to the abrupt thaw event at the end of the snow season, when the entire snow cover is usually melted within two weeks. Evaporation, sublimation or wind transport effects during the winter season are neglected. Due to the continental climate, strong diurnal temperature variations can be observed at the Tura station, and thaw events may be reported even when daily mean temperature is negative. Since extremum temperatures reached each day are available in the weather data, we include them in the modelisation by considering that the air temperature varies during the day from T_{min} to T_{max} as a piecewise linear function of time (linear between T_{min} and T_{mean}, and between T_{mean} and T_{max}), while respecting the daily mean temperature. Taking this temperature variation into account, Equation (A.1) is modified so that both melting and accumulation can occur on the same day, leading to Equation (A.2). Precipitation is assumed to be equally distributed throughout the day but is considered as snow only when T(t) > 0°C.

$$\Delta SWE = \int_{t=0}^{t=24h} \left(P(t) - M(t) \right) dt \tag{A.2}$$

In order to calibrate this empirical model to the Tura weather station data, the Snow Water Equivalent (SWE) must be estimated from the available snow depth measurements. For this purpose, we use the Multiple Snow Data Assimilation System (MuSA) of Alonso-Gonzalez et al. (2022). MuSA is an ensemble based data assimilation toolbox, designed to fuse observation with the mechanistic model the Flexible Snow Model (FSM2; Essery, 2015). The simulations are fed by ERA5 land global reanalysis data (Hersbach et al., 2020) perturbing the precipitation and the temperature in order to fit the output snow depth to local data. The objective SWE is obtained from the posterior mean of the ensembles (Figure 3a).

Considering the evolution of the snow pack over the 12 winters for which data are available (Fig. 3a), the used temperature index model well predicts the extent of the snow period, while the maximum snow water equivalent obtained in the snow pack is predicted with an accuracy of 24% in the L2 error norm (respectively 22% for the L1 norm, 5% minimum error, 37% maximum error). The projection of the snowpack dynamics to the year 2100 (Fig. 3b) shows that the increase in temperature leads to a shortening of the snow season (1 month shorter in SSP5-8.5), while the increase in precipitation leads to a higher accumulation rate in the winter hearth, leading to an increase in maximum SWE of up to 26% (+41mm, SSP5-8.5).

Estimation of soil surface temperature

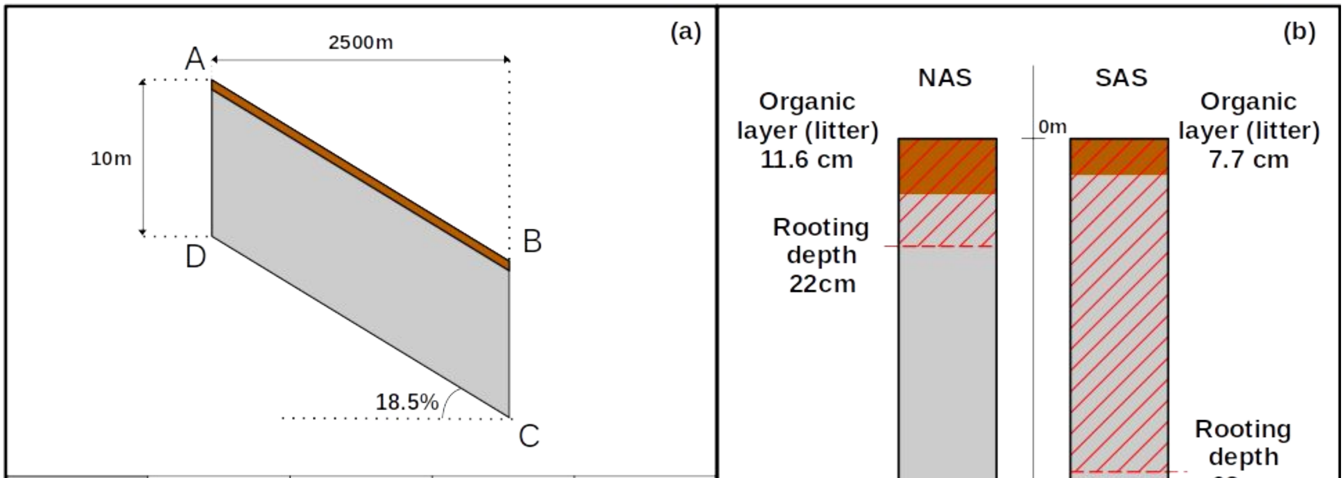
In order to estimate soil surface temperature, an empirical method based on multiple regression is implemented. The soil surface temperature is estimated by two different approaches, depending on whether snow covers the moss layer during winter (hereafter referred to as the “cold season”), or during the rest of the year (referred to as the “warm season”).

During the warm season, the soil surface is only separated from the ambient air by the moss layer. Moreover, liquid precipitation enhances the heat transfer from external air and soil surface temperature variations follow external air variations with a significantly shorter response time than in the presence of snow. Therefore, for the warm season, we use a direct estimator of soil surface temperature in the form of first-order multiple regression based on air temperature and precipitation.

During the cold season, both the snow layer and the moss layer isolate the soil surface, and conduction effects with slower time response occur, when heat fluxes are affected by snow thickness. In order to mimic this behavior while maintaining a simple, empirical and data-based approach, we used a multiple regression which is based on the time derivative of soil surface temperature as a function of SWE and temperature difference with the air temperature. We used a first order regression for each variable, since higher order tests did not produce any better soil surface temperature estimation. The cold season and warm season models are activated below or above the 0°C air temperature threshold. In order to ensure the smoothness of the signal, an interpolation between the two models was used when temperature is close to 0°C (±0.5°C). Figure 4 presents the comparison between measurements and the estimates obtained by the described empirical procedure for the two years of soil temperature data acquisition.

Using only two full years of data makes difficult the statistical assessment of the empirical estimation accuracy. However, the soil surface temperature obtained with the present model consistently follows the dynamics observed in the field, while the extremum temperature remains in a similar range for both north aspected slope ([-18.0;13.0] for field measurements, [-18.6;12.5] for model output) and south aspected slope ([-15.9;14.5] for field measurements, [-17.9;12.5] for model output).

Supplementary material B : Calculation set up & detail



Section	AB	AD	BC	CD
Name	Top	UpSlope	DownSlope	Bottom
Thermal BC	Temperature signal	Zero gradient	Zero gradient	Geothermal fluxes
Hydric BC	Liquid precipitation flux	No flux	Static pressure	No flux

Figure S1: (a) Schematic diagram of the numerical domain geometry and main variables boundary conditions. (b) Representation of the first soil column meter for north aspected slope (NAS) and south aspected slope (SAS).

The calculation setup follows that used in previous work (Orgogozo et al., 2019) and is described below. The procedure consists of eight calculations, corresponding to the four SSP scenarios applied to the two slopes of the Kulingdakan watershed. The calculation are performed between 2014 and 2100 based on climate scenario and estimated soil surface temperature (see Supplementary material A. and Figures 3 and 4). An additional 30 years of calculations were carried out with a repetition of the final conditions corresponding to the year 2100 in order to assess the thermohydric equilibrium state of the first metres of soil after the simulated climate change sequence. Calculation have been made using the OpenFOAM version v2212 and permaFoam solver at the version of January 2023.

Geometry and mesh information

The geometry used to represent a slope of Kulingdakan watershed is a 2D parallelogram, covering 2.5km in x-direction and 10 metres of thickness (z-direction), with an inclination of 18.5%. Mesh is constructed using uniform mesh size regarding x direction and non uniform cell thickness with a geometrical growth, with a finer mesh close to the soil surface where steep fronts occur. The mesh used for climate scenarios is 2048x256 cells mesh, with cell length of 1.22m and thickness ranging from 2.53mm close to the surface to 16.5 cm at the bottom of the domain.

This mesh has been chosen following a convergence study constituted by three refinement levels : 1024x128, 2048x256 and 4096x512. Current conditions, constructed as a mean year of years between 1999 and 2014, are used for mesh convergence study. The criteria for assessing numerical convergence is active layer thickness evolution. This preliminary study showed that the 1024x128 cells mesh produces unrealistic active layer thickness estimation (e.g. 12cm for north aspected slope). The 4096x512 mesh, on the other hand, results in a small difference on active layer thickness compared to the 2048x256 case (for north aspected slope : 65cm and 64cm respectively ; for south aspected slope, 98cm and 100cm), while involving computational cost to heavy to be carried out on centennial scale, in this case requiring approximately four times more CPU hours compared to using the 2048x256 case.

Thermohydraulic properties

The domain is represented by a porous media constituted by either a organic or mineral soil matrix, filled with water (whether on liquid or solid state) and air. The thermal properties used for the simulation are described in Table S1, while hydraulic properties are listed in Table S2, they are the same as those used in Orgogozo et al., 2019. Note that organic layer thickness is of 11.6cm on North aspected slope, and 7.7cm on South aspected slope.

	Organic matrix	Mineral matrix	Liquid water	Ice	Air
Heat capacity [$J.m^{-3}.K^{-1}$]	2.51 x 10^6	1.92 x 10^6	4.18 x 10^6	1.90 x 10^6	1.23 x 10^3
Thermal conductivity [$J.m^{-1}.s^{-1}.K^{-1}$]	0.25	2.9	0.6	2.14	0.026
Latent heat of fusion ice/liquid water [$J.m^{-3}$]	-	-	3.34 x 10^8		-

Table S1 : Thermal properties used to represent soil in permaFoam simulations conducted in this work.

	Organic soil	Mineral soil
Maximum water volume fraction [-]	0.766	0.412
Saturated hydraulic conductivity [$m.s^{-1}$]	9.26 x 10^{-7}	4.63 x 10^{-7}

Table S2 : Hydraulic properties used to represent soil in permaFoam simulations conducted in this work.

Boundary conditions, Sink term and initial conditions

To build the SSP scenarios, a representative year for meteorological forcings under current climatic condition is built from weather data measured between 1999 and 2014. A multi-annual average is obtained for year-round evolution of precipitation and air temperature along seasons by averaging these data for each days of the available measurement years. The air temperature and precipitations annual trends provided by SSP scenarios are then applied to this virtual, averaged year representative of current climatic conditions in order to build the atmospheric conditions up to year 2100.

The top boundary conditions for soil surface temperature is constructed from the atmospheric forcings as described in the “Material and Methods” section and in the Supplementary material A.

Water fluxes at top boundary conditions are directly taken as the liquid precipitations (considered liquid when $T_{air} > 0°C$), with a switching boundary conditions for dealing with water saturated soil surface (Orgogozo et al., 2019). All other variable are submitted to a zero gradient boundary conditions.

For upslope side of the domain, a zero gradient boundary conditions is applied to all the variables, except for the water pressure described with the noRainFlux conditions, which imposes a zero flux (Orgogozo et al., 2023).

For downslope side of the domain, a zero gradient boundary conditions is applied to all the variables, except for the water pressure described with static pressure head.

At the bottom of the domain, geothermal flux is imposed for thermal equation ($0.018 W.m^{-2}$) as mentioned in section 2.3 of the main text. Water pressure is described by a noRainFlux boundary condition (no water flux), while the boundary conditions for other variables are zero gradient.

As seen in Equation (1), water which is uptaken by roots is represented by a sink term in Richards equation. This volumetric term is calculated from a potential evapotranspiration (PET) rate distributed over the root layer thickness. The PET is calculated using Hamon formula based on air temperature (Hamon, 1963) which has already been used in studies of forested boreal areas (Frolking, 1997). As mentioned earlier root layer thickness is of 22cm on North aspected slope (10 cm into the mineral horizon) and 68cm on South aspected slope (60cm into the mineral horizon).

The initial conditions are obtained by a spin-up procedure. The first guess corresponds to the state of the active layers extracted from previous calculations under early 21st century conditions for the same site (2003-2012, see Orgogozo et al.,2019). In the absence of observation of the moisture in depth, an initial value of 0.335 is chosen, resulting from the annual mean of the water content averaged on the north and south slope active layers obtained in these previous calculations. This state is then used as the seed for a spin-up performed by cycling simulations considering the representative year for meteorological forcings under current climatic condition until convergence, i.e. until 10 years. The convergence criterion is defined by evaluating the change in active layer thickness from one year to the next. At the end of the ten-year spin-up, a variation of less than 0.2% on both slopes is achieved. Beyond the depth of the active layer, the soil water content remains practically equal to the value chosen at initialization due to very slow water flow under permanently frozen conditions.

Supplementary material C

The tables in the section of the Supplementary Material compile the main variables change between present conditions and 2100 for the four climate scenarios considered in this paper (SSP1-2.6, SSP2-4.5, SSP3-7.0, SSP5-8.5) for north aspected slope (Table S3) and south aspected slope (Table S4)

Variables (NAS)	Annual value in present climate	Change from present values in projections to 2100			
		SSP1-2.6	**SSP2-4.5**	**SSP3-7.0**	**SSP5-8.5**
Air temperature	-8.2°C	+1.6°C	+3.0°C	+5.6°C	+6.9°C
Yearly precipitations	408mm	+56mm / +14%	+49mm / +12%	+111mm / +27%	+115mm / +28%
Maximum snow water equivalent	108mm	+7mm / +6%	+13mm / +12%	+27mm / +25%	+29mm / +27%
Snow season extent	202days	-6days	-8days	-14days	-17days
Soil surface temperature	-3.3°C	+1.4°C	+2.3°C	+4.3°C	+5.2°C
Soil temperature (10cm depth)	-4.1°C	+0.9°C	+1.4°C	+2.9°C	+3.4°C
Soil temperature (1m depth)	-5.12°C	+0.6°C	+1.0°C	+2.2°C	+2.6°C
Soil temperature (5m depth)	-5.06°C	+0.6°C	+1.0°C	+2.2°C	+2.5°C
Soil temperature (10m depth)	-4.9°C	+0.6°C	+1.0°C	+2.0°C	+2.5°C
Active layer thickness	64cm	+7.8cm +12%	+11.9cm +19%	+23.9cm +37%	+28.2cm +44%
Total water content (averaged over root layer)	0.510	$+1.7\text{x}10^{-4}$ +0.0%	$-1.2\text{x}10^{-2}$ -2.3%	$-1.7\text{x}10^{-2}$ -3.3%	$-2.4\text{x}10^{-2}$ -4.7%
Liquid water content (averaged over root layer)	0.197	$+1.2\text{x}10^{-2}$ +6.3%	$+1.4\text{x}10^{-2}$ +7%	$+2.8\text{x}10^{-2}$ +14.1%	$+3.3\text{x}10^{-2}$ +16.5%
Ice water content (averaged over root layer)	0.313	$-1.2\text{x}10^{-3}$ -3.9%	$-2.6\text{x}10^{-2}$ -8.1%	$-4.5\text{x}10^{-2}$ -14.3%	$-5.6\text{x}10^{-2}$ -18%
Total water content (averaged over 0-2m)	0.365	$+3.2\text{x}10^{-3}$ +0.9%	$+3.0\text{x}10^{-3}$ +0.8%	$+6.7\text{x}10^{-3}$ +1.8%	$+6.3\text{x}10^{-3}$ +1.7%
Liquid water content (averaged over 0-2m)	0.074	$+1.1\text{x}10^{-2}$ +14.7%	$+1.8\text{x}10^{-2}$ +23.8%	$+3.6\text{x}10^{-2}$ +49.3%	$+4.4\text{x}10^{-2}$ +60.1%
Ice water content (averaged over 0-2m)	0.291	$-7.7\text{x}10^{-3}$ -2.7%	$-1.5\text{x}10^{-2}$ -5.0%	$-3.0\text{x}10^{-2}$ -10.2%	$-3.8\text{x}10^{-2}$ -13.1%
Actual evapotranspiration	350mm	+40mm / +11%	+52mm / +15%	+98mm /+28%	+100mm / +29%

Table S3: Summary of values obtained for current conditions and the four climate projections for 2100 used in this study for north aspected slope.

Variables (SAS)	Annual value in present climate	Change from present values in projections to 2100			
		SSP1-2.6	SSP2-4.5	SSP3-7.0	SSP5-8.5
Air temperature	-8.2°C	+1.6°C	+3.0°C	+5.6°C	+6.9°C
Yearly precipitations	408mm	+56mm/+14%	+49mm / +12%	+111mm / +27%	+115mm / +28%
Maximum snow water equivalent	108mm	+7mm / +6%	+13mm / +12%	+27mm / +25%	+29mm / +27%
Snow season extent	202days	-6days	-8days	-14days	-17days
Soil surface temperature	-2.6°C	+1.5°C	+2.3°C	+4.4°C	+5.2°C
Soil temperature (10cm depth)	-3.1°C	+1.1°C	+1.7°C	+3.4°C	+4.0°C
Soil temperature (1m depth)	-4.15°C	+1.0°C	+1.5°C	+2.9°C	+3.3°C
Soil temperature (5m depth)	-4.11°C	+0.9°C	+1.5°C	+2.4°C	+2.7°C
Soil temperature (10m depth)	-4.0°C	+0.9°C	+1.5°C	+2.3°C	+2.5°C
Active layer thickness	99cm	+13cm +13%	+20.0cm +20%	+36.3cm +37%	+45.2cm +46%
Total water content (averaged over root layer)	0.375	$-1.6x10^{-2}$ -4.3%	$-2.1x10^{-2}$ -5.6%	$-3.2x10^{-2}$ -8.5%	$-3.7x10^{-2}$ -9.7%
Liquid water content (averaged over root layer)	0.153	$+1.1x10^{-3}$ +0.7%	$+3.5x10^{-3}$ +2.3%	$+1.2x10^{-2}$ +8.0%	$+1.5x10^{-2}$ +9.8%
Ice water content (averaged over root layer)	0.222	$-1.7x10^{-2}$ -7.7%	$-2.4x10^{-2}$ -11.0%	$-4.4x10^{-2}$ -19.9%	$-5.1x10^{-2}$ -23.1%
Total water content (averaged over 0-2m)	0.343	$-1.8x10^{-2}$ -5.4%	$-1.7x10^{-2}$ -5.0%	$-3.4x10^{-2}$ -9.8%	$-3.7x10^{-2}$ -10.8%
Liquid water content (averaged over 0-2m)	0.090	$+6.6x10^{-3}$ +7.3%	$+1.5x10^{-2}$ +16.2%	$+3.4x10^{-2}$ +37.7%	$+4.6x10^{-2}$ +50.7%
Ice water content (averaged over 0-2m)	0.253	$-2.5x10^{-2}$ -9.9%	$-3.2x10^{-2}$ -12.6%	$-6.8x10^{-2}$ -26.8%	$-8.3x10^{-2}$ -32.7%
Actual evapotranspiration	364mm	+18mm/+5%	+34mm/+9%	+76mm/+21%	+94mm/+26%

Table S4: Summary of values obtained for current conditions and the four climate projections for 2100 used in this study for south aspected slope.