PEATLAND USER MANUAL

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1. Running PEATLAND.

PEATLAND can be invoked from the command line at a Unix/Linux shell or DOS command window in Windows by typing

peatland

followed by one or more of the following command line options, separated by spaces:

option	result	default
?	lists the available command line options	
V	verbose mode, displays the progress of the model run on the shell window	
dir=directory	sets working directory for input and output files	PEATLAND home directory
par=filename	name of input parameter file to be used	params
out=filename	output file prefix, will be added to the names of the output files	

The verbose mode can come in handy to check if all parameters for the model have been defined correctly in the parameter files.

Model parameter input is done by entering parameter values in the parameter files. The parameter files consist of ASCII text files which can be edited by any ASCII text editor (do not use word processors). An extensive description is given below.

PEATLAND does not contain sophisticated parameter input windows or output plotting utilities. However, the simple command line mode allows embedding of the program in scripts (e.g. shell scripts or Perl scripts) which modify parameter files automatically and link the output to any plotting software. The author has good experience with XmGrace, which is a verstile plotting utility. Moreover, using scripts multiple model runs can easily be generated.

2. Model output files

The output files comprise a few files that are produced always, and optional output files that can be specified in the run parameter file. The filenames can be prefixed by a file name prefix to be specified on the command line. The files are simple ASCII row and column files that can be read by every plotting or math package.

All files contain the model output for a variable for each time step; the rows represent the data for each time step. In most files, the first column is always the time in days after the start of the model run (midpoint of the time step); however, check with the table below.

name	contents	optio -nal	columns
methanefluxes.dat	CH4 fluxes divided over three pathways - diffusion, ebullition, plant flux and total flux	no	1 time (days) 2 ebullition flux (mg.m ⁻² .hr ⁻¹) 3 plant flux (mg.m ⁻² .hr ⁻¹) 4 diffusive flux (mg.m ⁻² .hr ⁻¹) 5 total flux (mg.m ⁻² .hr ⁻¹)
CO2reservoirs.dat	CO ₂ fluxes from each soil organic matter reservoir	no	1 time (days) 2 flux from peat (mg.m ⁻² .hr ⁻¹) 3 flux from liquid manure (mg.m ⁻² .hr ⁻¹) 4 flux from manure solids (mg.m ⁻² .hr ⁻¹) 5 flux from root exudates (mg.m ⁻² .hr ⁻¹) 6 flux from litter and roots (mg.m ⁻² .hr ⁻¹) 7 flux from microbial biomass (mg.m ⁻² .hr ⁻¹) 8 flux from humic matter (mg.m ⁻² .hr ⁻¹) 9 flux from methane oxidation (mg.m ⁻² .hr ⁻¹) 10 flux from surface litter 11 total CO ₂ flux (mg.m ⁻² .hr ⁻¹)
CO21ayers.dat	CO ₂ fluxes from each model soil layer	no	1 time (days); 2 – 16 total CO ₂ flux from each layer starting at the top (mg.m ⁻² .hr ⁻¹) The topmost layer includes CO ₂ from CH ₄ oxidation and litter decomposition at the surface
biomass.dat	Total plant biomass (excl. microbial biomass), gross primary production, plant respiration, and net total CO ₂ flux	no	1 time (days) 2 total plant biomass including roots (kg C.m ⁻²) 3 primary production = net photosynthesis or gross photosynthesis – plant respiration (mg CO ₂ .m ⁻² .hr ⁻¹) 4 plant respiration (mg CO ₂ .m ⁻² .hr ⁻¹) 5 net CO ₂ flux (soil respiration – primary production = Net Ecosystem Exchange) (mg CO ₂ .m ⁻² .hr ⁻¹) 6 soil respiration + plant respiration = ecosystem respiration (mg CO ₂ .m ⁻² .hr ⁻¹) 7 litter mass stock (kg C.m ⁻²) 8 biomass removed by harvest and grazing (kg C.m ⁻² per timestep) 9 manure carbon added (kg C.m ⁻² per timestep) 10 LAI (m ² .m ⁻²)
peatdecmposition.	peat decomposition	no	Total peat decomposition; aerobic peat decomposition (kg C)

name	contents	optio -nal	columns
carbonbalance.dat	all carbon balance elements in moles C	no	All entries in mol C per timestep 1 primary production 2 carbon inputs from manure and livestock excretion 3-9 Changes in each soil carbon reservoir (see CO2reservoirs.dat) 10 total CO2-C emission from aerobic decomposition 11 total CO2-C emission from anaerobic decomposition 12 CO2-C from above-ground litter decomposition 13 total CH4-C emission 14 CO2-C from CH4 oxidation 15 CO2-C from plant respiration 16 (not yet implemented) storage change (anaerobic) CO2 in soil water 17 storage change CH4 in soil water 18 (not yet implemented) CO2 - and CH4-change export by groundwater flow 19 harvest + grazing 20 storage change above-ground biomass 21 storage change litter layer 23 total outgoing C (sum of 10, 11, 12, 13, 14, 19) - 15 not included, is not included in primary production 24 total incoming C (sum of 1 and 2) 25 total storage change (sum of 3-9, 17, 20, 21, 22) 26: Balance (sum of 23 - 25)
temperature.dat	soil temperature at each model soil layer	yes	soil temperature at each model soil layer, starting at the top, °C
moisture.dat	relative moistue / air content (saturation) of the pore volume at each model soil layer	yes	soil pore volume saturation with air, for each layer, starting at the top, dimensionless values 0-1
methane.dat	soil methane concentration for each model layer	yes	methane concentration for each model soil layer starting at the top, millimol.m ⁻³ in soil pore volume, including bubbles
roots.dat	root mass per layer	yes	root mass for each model soil layer starting at the top, (kg C.m ⁻²)
labileSOM.dat	sum of labile organic matter reservoirs per layer	yes	sum of liquid manure, solid manure, root exudates, litter and roots, microbial biomass per layer starting at the top(kg C.m ⁻²)
ice.dat	ice mass per soil layer	yes	ice mass per layer starting at the top(kg.m ⁻²)
peat.dat	peat carbon per layer	yes	peat carbon per layer starting at the top(kg C.m ⁻²)
liquid_manure.dat	liquid manure carbon per layer	yes	liquid manure carbon per layer starting at the top (kg C.m ⁻²)

name	contents	optio -nal	columns
solid_manure.dat	solid manure carbon per layer	yes	solid manure carbon per layer starting at the top (kg C.m ⁻²)
rhizodep.dat	rhizodeposition carbon per layer	yes	rhizodeposition carbon per layer starting at the top (kg C.m ⁻²)
litter_roots.dat	litter and roots carbon per layer	yes	litter and roots carbon per layer starting at the top (kg C.m ⁻²)
microbes.dat	microbial biomass carbon per layer	yes	microbial biomass carbon per layer starting at the top (kg C.m ⁻²)
humus.dat	humus carbon per layer	yes	humus carbon per layer starting at the top (kg C.m ⁻²)

3. Model parameter input.

The parameter files are ASCII text files and can be edited with any text editor. Eventually the parameter files can be modified using shell or Perl scripts, allowing the generation of a large number of model runs in batch mode.

The input parameters of the model consist of three main files, which are mandatory - the model cannot run without these. The default parameter file **defaults** contains all the parameters the model minimally needs to run, together with their default values. Parameters for a specific run must be specified in an extra run parameter file, with the default name **params**. Parameters specified in this file, always override the default values specified in defaults - that means that the model will use the value specified in **params** instead of that in **defaults**. A different name for this parameter file can be specified on the command line. The third file is a file with a soil profile description. The name of this file must be specified in the run parameter file.

Furthermore there are a number of input files for soil physical parameters which depend on the way in which certain soil physical aspects are used - either specified externally in a file or calculated from a simple model. E.g. the soil surface temperature can be specified for each time step, or calculated by the soil temperature module of Peatland.

file	function	man-	filename		
		datory	default	remarks	
default parameter file	contains all the parameters for the model and their default values. User modification is generally not necessary	yes	defaults	do not change the name of this file	
run parameter file	contains the parameters for the specific model run, paramater values defined here override the default values, be sure that everything that has be changed for a specific model run is included here!	yes	params	alternative names can be specified on the command line	

file	function	man-	filename
soil file	contains the soil profile parameters.	datory	has to be specified in parameter file
groundwater table data	contains grondwater table for each time step	no	has to be specified in parameter file
soil moisture data	contains soil moisture data (theta) for each depth step and time step	no	has to be specified in parameter file
soil surface temperatures	contains the soil surface temperature for each time step	no	has to be specified in parameter file
soil temperatures	contains the soil temperature for each depth and time step	no	has to be specified in parameter file
harvest	harvest dates and fraction of biomass harvested	no	has to be specified in parameter file
snow depth	contains the thickness of the snow layer at each time step	no	has to be specified in parameter file

3.1. Structure of the parameter files.

The definition of a parameter value in the parameter files is done by specifying the name of the parameter, followed by an = sign, the value of the parameter, and a semicolon, e.g:

```
NrOfSteps = 100;
```

This line defines the number of time steps the model has to run as 100 steps.

Comments can be added, and are preceded by a % sign:

Everything after a sign up to the next end of line will be ignored by the program.

Parameters can be defined more than once, but only the first definition will be effective. So

will set the number of time steps to 100.

Different types of parameters may be entered:

```
NrOfSteps = 100; number of time steps
```

This is a single value parameter.

```
% SOM decomposition constants for each reservoir Kdecay = [0.02 100 4 365 4 365 0.005];
```

This is an array parameter, consisting of 7 values. Note the rectangular parenthesis.

This is a matrix parameter; note the rectangular parenthesis and the semicolons separating the rows of the matrix.

```
SoilProfile = "guisveld"
% Definition of the soil profile parameter file to be used
```

This is a string parameter, used mainly for output and input file specifications

3.2. Description of the parameters

Not all parameters need revision for each model run. Many parameters, in particular physical constants, are not specific to a site or model run. These parameters are defined in the **defaults** file and can be left alone. Run-specific parameters, e.g. a soil profile descrition and decay constants, need to be specified in either the run specific parameter file or the soil profile description file. A few parameters may function as tuning parameters, which may be used to optimize the model performance with respect to a specific site. These will be entered also in the run specific parameter file.

Name	Example	Units	Description	Module
SoilProfile	"ilperveld"		Filename containing soil data (see next table)	model configuration
NrLayers	15		number of model layers of soil profile	model configuration
LayerThickness	0.1	m	layer thickness	model configuration
TStepHeat	0.01	day	time step temperature model	model configuration
DStepHeat	0.1	m	minimum depth step temperature model	model configuration
MaxDepthHeat	5	m	maximum depth temperature model, range 5-15 m	model configuration
Timestep	1	day	timestep model input and output; this is also the timestep of anerobic decomposition model; value 1-10	model configuration
NrOfSteps	5000		number of timesteps; unlimited; add at least 10 years model spinup	model configuration
StartDay	1		Julian day number (day of the year) of starting day	model configuration

Name	Example	Units	Description	Module
StartYear	2000		Starting year, to calculate leap years	model configuration
StartDate	"01/01/2000"	date	Date string with format DD/MM/YYYY, indicating the start date of the model run. It has to be defined if harvest is specified in a harvest file with harvest dates. Its definition overrides StartYear and StartDay.	model configuration
EndDate	"01/01/2020"	date	Date string with format DD/MM/YYYY, indicating the start date of the model run. It has to be defined if harvest is specified in a harvest file with harvest dates. Its definition overrides StartYear, StartDay andNrOfSteps.	
ThermModel	0		Sets the type of thermal model: 0 for complete numerical simulation of thermal diffusivity including permafrost and soil freezing and observed temperatures at the soil surface 1 for analytical solution of heat diffusion using uniform diffusivity with depth and sinusoidal surface temperature 2 for constant temperature	model configuration
DensOrg	1200	kg.m ⁻³	density organic matter in peat kg	soil physical constant
DensMin	2650	kg.m ⁻³	density of mineral matter	soil physical constant
DensWater	1000	kg.m ⁻³	density of water at 0° C	soil physical constant
DensIce	917	kg.m ⁻³	density of ice at 0° C	soil physical constant
Rgas	8.31446	J.K ⁻¹ .mol ⁻¹	Gas constant	soil physical constant
MethaneDiff		m ² .day ⁻¹	diffusivity of methane in air	soil physical constant
MethaneDiffWater		1.7280E-4	diffusivity of methane in water	soil physical constant
DissimAssimRatio	2.3		Dissimilation/Assimilation ratio aerobic decomposition; range 1.0 - 2.3 (dissimilation = decomposition in mol C, assimilation = newly formed microbial biomass)	aerobic decomposition
ResistFrac	0.1		Fraction of decomposed organic material that is transferred to resistant humus fraction	aerobic decomposition
Cfrac	[0.55, 0.38 0.38 0.38 0.38 0.38 0.55]		Carbon fraction (kg/kg) each SOM reservoir	aerobic decomposition
Kdecay	[0.02 100 4 365 4 365 0.005]	Kg C year-1	SOM decomposition constants for each reservoir	aerobic decomposition
AerobicQ10	[3.5 2.0 2.0 2.0 3.0 2.0 4.0]		Q10 values of aerobic decomposition separately for each reservoir	aerobic decomposition
T_ref	10	°C	Reference temperature for Q10 calculation	aerobic decomposition

Name	Example	Units	Description	Module
KLitter	0.5	Kg C year-1	Decomposition constant for standing dead biomass and above-ground litter	aerobic decomposition
pFpoints	[2.7 4.2; 1.0 0.2]	Above row: matric potential (m³/m³, water volume per soil volume)	Determines environmental correction factor for dryness. Defines a linear decrease of the aerobic decomposition constant (Kdecay) between the pF values in the upper row of pFpoints. The range of the correction factor is given in the lower row of pFpoints.	aerobic decomposition
HalfSatPoint	0.1		Environmental correction factor of the aerobic decomposition constant for poor aeration of the soil by high water saturation. The correction depends linearly on water filled pore space. The factor equals 0.0 at completely water filled pore space, 0.5 at the value given by HalfSatPoint, and 1.0 at 2 x HalfSatPoint.	aerobic decomposition
RootAeration	0.0 – 1.0		Root mass dependent correction of the poor aeration factor, for improved aeration by root growth. If 0, this is switched off.	aerobic decomposition
PrimingCorrection	0.0 or > 0.0		Environmental factor for the priming effect exerted by root exudates on the decomposition rate of slow C reservoirs; value > 0; if 0, this is switched off. The priming effect increases Kdecay. The actual value in the model depends on the root mass in each layer, the growth rate of vegetation and given minimal and maximum primary production, and eventually time of the year (see SpringCorrection)	aerobic decomposition
AnaerobicCO2	1 or 0		Switch for allowing anaerobic decomposition (nitrate, Fe, sulfate reduction etc) resulting in anaerobic CO ₂ production, if 0 not accounted for	anaerobic CO2
KAnaerobic	[0.005 0.01 0.01 0.01 0.01 0.01 0.0001]	Kg C . year-1	Anaerobic decomposition constants, for all SOM reservoirs	anaerobic CO2
Q10Anaerobic	3.5		Q10 of anaerobic decomposition (not reservoir dependent, so one value; reference temperature is equal to reference temperature for CH ₄ production)	anaerobic CO2
AnaerobicDARatio	30.0		Anaerobic Dissimilation/Assimililation ratio; typical range 19 - 49	anaerobic CO2
ProductionModel	4		Production model: 0 for simple sinusoidal function over the year; 1 for production dependent on temperature of upper soil layer 2 for production data read from file, variable NPPFile has to be defined (in kgC.m ⁻² .day ⁻¹) 3 for photosynthesis model based on Haxeltine & Prentice, global radiation data supplied in PARFile (in Joule.cm ⁻² .day ⁻¹), which is recalculated to PAR (Photosynthetic Active Radiation) by the model 4 for photosynthesis model, cloud cover data supplied in PARFile (fractions 0 - 1), PAR calculated, based on Latitude (should be defined) 5 for photosynthesis model for tundra, Shaver et al, J. Ecology 2007 (not depending on CO2 concentration) PAR data supplied in PARFile (as with Productionmodel 3) 6 for photosynthesis model for tundra, Shaver et al, J. Ecology 2007 (cloud cover data supplied in PARFile)	Organic production

Name	Example	Units	Description	Module
PARunits	0	PAR in umol m ⁻² s ⁻¹ , or shortwave radiation Joule.cm ⁻² .day ⁻¹ or cloud cover fraction	Units in which PAR (Photosynthetic Active Radiation) is given in PARfile (see below) for ProductionModel 3 or 4. 0: PAR in umol m ⁻² s ⁻¹ 1: Shortwave radiation energy as often given by weather stations - Joule.cm ⁻² .day ⁻¹ ; is be converted to PAR 2: cloud cover fraction, from which PAR is estimated	
NPPFile	"filename" (string)	Kg C m ⁻² per timestep	external file with gross photosynthesis for production model 2	Organic production
PARFile	"filename"	See PARunits	Photosynthetic Active Radiation or Global shortwave radiation per day, or cloudcover fraxtion per day – see PARunits	Organic production
Latitude	52.0	degrees	site latitude for calculation of incoming radiatin from cloud cover data (ProductionModel model 4 and 6).	Organic production
Phenology	[1 10.0 150 2.0 1 0.9 30 240]		Phenology parameters for production model 3 to 6; 1 type of phenology (0 for evergreen, 1 for summergreen) 2 the base for calculating the heat sum (growing degree days) 3 the heat sum when maximum LAI (leaf area index) is reached 4 the maximum LAI 5 C3 or C4 photosynthesis (1 or 2) 6 the fraction of leafy biomass that is littered in autumn, and at the same time determines the minimum winter LAI by multiplication with the maximum LAI 7 the day number of the earliest start of the growing season 8 the day of the year that autumn / leaf senescence starts	Organic production
GreenBiomassRatio	0.5 – 1.0		Ratio of photosyntesizing biomass to total biomass for ProductionModel 3, high for grasslands, lower for woody vegetation	
KBeer	0.5		Beer's law constant for light extinction in the vegetation canopy for photosynthesis models, values around 0.5	Organic production
LAICarbonFraction	0.1	kg C.m ⁻²	relates LAI to kg C.m ⁻² of vegetation (kg C.m ⁻² per unit of LAI)	Organic production
PhotoPar	[0.5 0.05 16.0 0.03]	See description	Parameters for photosynthesis model 5 and 6 for tundra, Shaver et al, J. Ecology 2007 1 Plant respiration at zero degrees per m ⁻² leaf area (μmol.m ⁻² .s ⁻¹), range 0.4-1.5 2 Temperature sensitivity factor plant respiration range 0.03 – 0.07 (°C ⁻¹) 3 light-saturated photosynthetic rate per unit leaf area (μmol.m ⁻² .s ⁻¹) range 6-20 4 initial slope of the light response curve (μmol CO ₂ μmol ⁻¹ photons) range 0.05 - 0.12	Organic production
AmbientCO2	415	ppmv	Ambient CO ₂ concentration (ProductionModel 3,4)	Organic production
CO2File	"" or "filename"		File with variable CO ₂ values, for each simulation year one value + 1 extra value, for ProductionModel 34; if an empty string, a constant value defined by AmbientCO ₂ is used.	Organic production

Name	Example	Units	Description	Module
ShootsFactor	0.5		mass fraction of primary production that is allocated to shoots; the remainder (1.0 – ShootsFactor) is allocated to roots. For agricultural crops ShootsFactor is generally >0.5, for natural vegetation <0.5.	Organic production
RespFac	[0.015 0.01]		fraction of primary production that is respired by plants (plant respiration); first value is growth respiration, second maintenance respiration. Production model 1 and 2: used to calculate plant respiration Production model 3 - 6 do not use RespFac.	Organic production
ProdTFunc	[5 25]	°C	temperature dependent production for production model 1 1st number is minimum temperature, 2nd optimum temperature	Organic production
SatCorr	0.0		correction of production for saturation of topsoil, depresses production at high saturation, switched off when 0	Organic production
SpringCorrection	0.0		Correction (0-1) for stronger exudation in spring; influences priming and exudate production, if 0, spring correction is disabled. The correction is a factor of 1+SpringCorrection.	Organic production
MaxProd	0.01	kgC.m ⁻² .day ⁻¹	Maximum primary productivity for Production model 0 and 1	Organic production
MinProd	0.0	kgC.m ⁻² .day ⁻¹	Minimum primary productivity for Production model 0 and 1	Organic production
MaxRootDepth	0.5	m	Maximum root depth	Organic production
NoRootsBelowGWT	0 or 1		Set presence or absence of root growth below the water table (presence or absence of telmatophytes). If 1, no roots will grow below groundwater table; for wetlands, set this always to 0.	Organic production
RootLambda	5.0		Parameter for exponential root distribution function; larger values result in steeper decrease of root mass with depth	Organic production
RootSenescence	0.003		Root senescence factor = proportion of root mass that dies and is transferred to the litter/roots soil carbon reservoir during each time step	Organic production
InitRoots	0.5	kg C.m ⁻²	Initial root mass in all layers	Organic production
ExudateFactor	0.1	kg C.m ⁻²	Mass fraction of of below-ground production that is allocated to root exudates	Organic production
BioMass	0.5	kg C.m ⁻²	Initial above ground biomass. NB: this is excluding the root mass, which is specified in InitRoots	Organic production
LitterLayer	0.2	kg C.m ⁻²	Organic matter stored in above ground litter layer and dead biomass	Organic production
LitterConversion	0.001		Conversion factor of daily conversion of above ground to below ground litter in the top layer at reference temperature T_ref; the factor is temperature adjusted such that at 0 degrees the conversion factor is also 0	Organic production
BioMassSenescence	0.001	day ⁻¹	Proportion of biomass that dies off at each day as fraction of above-ground biomass. This is regardless of season.	Organic production

Name	Example	Units	Description	Module
Harvest	[180 0.75; 240 0.75]	See description	Harvest dates as day of the year (1st column) and fraction of biomass harvested (2nd column, kg C.m ⁻²). This represents harvest on fixed dates each year; if harvest dates vary per year, these need to be specified with a <i>HarvestFile</i>	Organic production
HarvestFile	"Harvest.txt"	See description	Ascii textfile with harvest data: year, month, day, fraction harvested. Separated by spaces, for each date a new line. If defined, harvest dates may vary from year to year. The variable Harvest, which assumes the same harvest dates every year, is ignored.	
HarvestLitter	0.05	fraction	Fraction of harvest that remains as litter on the soil and is added to the litter carbon pool	
Manure	[80 0.01; 200 0.01]	See description	Manure application dates (column 1) and quantity (column 2) in kg C.m ⁻² per model time step	Organic production
ManureFluidFrac	0.75		Fluid fraction of manure	Organic production
ManureLayers	[0.7 1.0; 0.3 0]	See description	Partitioning fractions of manure among layers; first column: fluids; second column: solids; first row is top layer, 2 nd row 2 nd layer etc.; the colums have to sum to 1	Organic production
Grazing	[0 130 0.0001 0.00005; 250 365 0.0001 0.00005]		Parts of the year in which grazing occurs, each row is a range of days (day of the year) followed by the amount of biomass removed (kg C.m ⁻² .day ⁻¹) and the amount of excretion (kg C.m ⁻² .day ⁻¹)	Organic production
GrowFuncConst	1.0		Proportionality constant for use of different production models for plant transport in methane model (plant transport depends partly on plant growth rate)	Methane model
MethaneReservoirs	[0.0001 1.0 1.0 1.0 0.5 0.0 0.0]		This parameter excludes or (partly) includes which reservoirs are being used for calculation of methane production. A 1.0 includes a reservoir, 0.0 excludes it. Included reservoirs should be generally labile reservoirs (manure, exudates), although a fraction of less labile reservoirs (e.g. peat) can be included by a fraction.	Methane model
MethaneR0	0.4	milliMol. hr ⁻	Methane production rate factor for fresh organic C	Methane model
CO2CH4ratio	0.5		Molar ratio between CH_4 and CO_2 production, based on mode of methane formation; for acetate splitting this is 0.5, for CO_2 reduction 0.0, may also be a number between 0.0 and 0.5 if both modes occur; the smaller the value, the larger amount of CH_4 is produced over CO_2	Methane model
MethanepHCorr	0.05		Correction factor of methane production for pH. For every pH unit lower or higher than neutral, MethanepHCorr*R0 is substracted from / added to R0	Methane model
MethaneQ10	5.0		Q10 value for temperature sensitivity of methane production; range 1.7 - 16 ref (Walther & Heimann 2000)	Methane model
MethaneOxQ10	1.4		Q10 value for temperature correction of methane oxidation; range 1.4 - 2.1, ref. in Walther & Heimann 2000	Methane model

Name	Example	Units	Description	Module
MethaneTRef	10.0	°C	Reference temperature for temperature sensitivity methane production and oxidation; if negative, the average of the input temperature time series is used.	Methane model
MethaneVmax	50.0	μMol.hr ⁻¹	V _{max} of Michaelis-Menten equation for methane oxidation, range 5-50	Methane model
MethaneKm = 5	5.0	μMol	K _m in Michaelis-Menten equation for methane oxidation; range 1-5	Methane model
MethaneMaxConc	500.0	MilliMol.m ⁻³	Maximum methane concentration in pore water (millimol/m3 in soil pore volume); above this value bubbles are formed	Methane model
MethaneERateC	1.0	hr ⁻¹	Ebullition rate constant; a value of 1.0 means all methane above the ebullition treshold is added to ebullition	Methane model
MethanePRateC	0.01	hr ⁻¹	Rate constant for plant transport of methane; value should not be higher than 0.1!	Methane model
MethanePlantOx	0.9		Fraction of methane that is oxidized during transport in plants	Methane model
MethanePType	15		Vegetation type factor for gas transport by plants range: 0-15	Methane model
MethaneAir	1.8	ppmv	Methane concentration in the air above the soil	Methane model
PartialAnaerobe	0.0		This allows methane production in anaerobic microsites above the water table, depending on soil saturation. This may occur in dense clayey soils (e.g. Wagner et al 2017 nature Scientific Reports) It determines the slope of the relation of partial anaerobe soil fraction above the water table to soil saturation, value >1; if ≤1, no partial anarobe fraction is assumed to be present and no methane pruduction above the water table is modelled. The relation between saturation and anaerobic fraction is linear; the value of PartialAnaerobe determines the steepness of the relation: anarobic fraction = 1 − PartialAnarobe * saturated fraction.	Methane model
AnaerobeLagFactor	0.0	days	The time lag for development of sufficiently anaerobic conditions for methanogenesis after rapid saturation of a layer by rapid water table rise.	Methane model
InitMethane	[1 1 40 80 100 150 300 400 450 500 500 500 500 500 500]	millimol.m-3	Initial methane concentration profile (in soil pore volume, including bubbles)	Methane model
GwFile	"" or "filename"	m below surface (negative values are below surface)	If this is not an empty string, a water table time series will be read from the file indicated by the string. If an empty string, the water table will be modelled, either as a simple sinusoidal variation over the year, or a model based on input of times series of evaporation and precipitation. The choice of modelled watertable based on precipitation/evaporation is based on the definition of <i>PrecipFile</i> (see below)	Water / ice
SoilMoisture	"" or "filename"	m³/m³ per timestep and layer	File of size number of time time steps x number of layers with soil moisture data (string with valid file name) as alternative to calculation of soil moisture (string empty)	

Name	Example	Units	Description	Module
EvapFile	"" or "filename"	mm per timestep	Evaporation data file, evaporation in millimeter, for water table model	Water / ice
PrecipFile	"" or "filename"	mm/timestep	Precipitation data file, precipitation in mm, for water table model. If this variable is an non-empty string, the water table is modelled based on precipitation/evaporation.	Water / ice
DrainageFile	"" or "filename"	m below surface	File with water level data of ditch or or other drainage channel at some distance of modelled site; water level with respect to site level (optional, empty string if not present). Alternative is fixed drainage level defined by <i>DrainLevel</i>	Water / ice
DrainLevel	-1.0	m	Fixed reference level of water in the drains/river channel with respect to top of soil surface (m)	Water / ice
RunOnFile	"" or "filename"	mm/timestep	File with run-on / runoff data for water table calculation (optional, empty string if not present)	Water / ice
DayMinGW	220	Day of the year	Day of lowest groundwater table for simple sinusoidal water table	Water / ice
AmplitudeGW	0.2	m	Amplitude of water table for simple sinusoidal water table	Water / ice
MinGW	-0.5	m	Lowest water table level at this day (m below surface). For modelled water table using the water table model this is the minimum watertable for the entire simulation period. Negative values indicate water table below surface	Water / ice
EvapCorrection	0.02		Correction factor to reduce evaporation if water table is below surface, for water table model	Water / ice
RunoffThreshold	0.1	m	Threshold above which a ponded water layer produces runoff; for modelled water table	Water / ice
OpenWaterFactor	1.0		Evaporation correction factor for open water evaporation for water table model	Water / ice
CropFactor	1.0		Makkink Crop factor to correct evaporation for vegetation properties for water table model	Water / ice
DrainageDist	10	m	Distance to nearest drainage channel (m) for calculation of groundwater flow	Water / ice
Ksat	0.01	m.day ⁻¹	Saturated hydraulic conductivity for subsoil	Water / ice
Tdata	"" or "filename"	°C	Data file with surface temperature time series; if an empty string, a sinusoidal temperature time series will be used. Otherwise a numerically solved heat transport model will be used based on the heat diffusion equation and soil properties.	Temperature model
T_average	10.5	°C	Average yearly temperature for simple sinusoidal temperature model	Temperature model
Γ_amplitude	12.0	°C	Amplitude of soil surface temperature for sinosoidal temperare model	Temperature model
ThermDiff	0.0136	m ² .s ⁻¹	Fixed thermal diffusivity for sinosoidal temperare model. For the numerically solved model, the diffusivity is estimated from soil parameters and actual water/ice content.	Temperature model

Name	Example	Units	Description	Module
T_init	[0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0 1.1 1.2 1.3 1.4 1.5; 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10	m,°C	Intitial temperature of each layer; 2 row vector, top layer is depth below surface; second row is temperature	Temperature model
MaxSnowdepth	0.0	m	Maximum snow depth (meters)	Temperature model
DayMaxSnowdepth	60	Day of the year	Day number of maximum snow depth - NB: is supposed to lie in the first half of the year, so < 182	Temperature model
SnowMeltrate	0.01	m/°C	Rate of snowmelt, meter per °C above zero per day	Temperature model
VegTScalingFactor	0.7		Scaling factor for air to soil surface temperature; equal to one if actual soil surface temperature is input; outherwise a value between 0.6 and 1.0	Temperature model
HCOrg	2.496E+06	J.m ⁻³ .K ⁻¹	volumetric heat capacity organic matter	Temperature model
HCMiner	2.385E+06	J.m ⁻³ .K ⁻¹	volumetric heat capacity mineral matter	Temperature model
HCAir	1.212E+03	J.m ⁻³ .K ⁻¹	volumetric heat capacity air (saturated with water vapour)	Temperature model
HCWater	0.000E+00	J.m ⁻³ .K ⁻¹	volumetric heat capacity water	Temperature model
HCIce	1.926E+06	J.m ⁻³ .K ⁻¹	volumetric heat capacity ice	Temperature model
CondOrg	0.25	J.m ⁻¹ .s ⁻¹ .K ⁻¹	thermal conductivity organic matter	Temperature model
CondMiner	2.5		thermal conductivity mineral matter (range 2.5 – 8.0; 2.5 is for clay, 8.8 for pure sand which is the conductivity for quartz)	Temperature model
CondQuartz	8	J.m ⁻¹ .s ⁻¹ .K ⁻¹	thermal conductivity quartz (for sand fraction)	Temperature model
CondAir	0.025	J.m ⁻¹ .s ⁻¹ .K ⁻¹	thermal conductivity air	Temperature model
CondWater	0.56	J.m ⁻¹ .s ⁻¹ .K ⁻¹	thermal conductivity water	Temperature model
CondIce	2.21	J.m ⁻¹ .s ⁻¹ .K ⁻¹	thermal conductivity ice	Temperature model
CondSnow	0.35	J.m ⁻¹ .s ⁻¹ .K ⁻¹	thermal conductivity snowpack (density ~ 350 kg m ⁻³ , see Williams & Smith 1991, p. 110) – varies strongly with density and stucture	Temperature model
LatentHeat	[-0.0125, 1.955, 333.5]	J kg ⁻¹	parameters for approximation of temperature- dependent latent heat of fusion of ice (334000 J kg ⁻¹ at 0°C)	Temperature model

Name	Example	Units	Description	Module
ProfileOutput	[1 2 3 4 5 6 7 8 11 12 13 14 15 16 17]	Unus	Generates output files for vertical profiles of state variables 1: temperature profile 2: aeration 3: methane profile 4: root mass 5: labile SOM reservoirs (2-6) summed 6: ice in kg.m3 soil 7: water table 8: npp 9: totalSOM all SOM reservoirs (1-7) summed	Output
			11, 12, 13, 14, 15, 16, 17: SOM reservoir 1, 2, 3, 4, 5, 6, 7; peat; dissolved organic matter manure; manure solids; root exudates; litter and roots; microbial biomass; humus	

3.3. Description of the parameters in the soil description parameter file (SoilProfile).

Name	Example	Units	Description
NrHorizons	3		Number of soil horizons in the profile description
Horizons	[0.1 0.4 1.5]	m	Horizon base depths with respect to surface for each horizon
CNRatio	[14.5 15.8 25.0]		C/N ratios for each horizon; the decomposition of peat can be made dependent on these. Currently not used in the model; will be used later for environmental correction of organic matter decomposition
DBD	[465.3 482.0 330.5]	kg.m ⁻³	Dry bulk density for each horizon
PercOrg	[45.09 35.26 47.91]		Weight percentage of organic matter for each horizon
Layer_pH	[5.82 5.35 5.93]	pН	pH for each horizon
SandFraction	[0.05 0.05 0.05]		Weight fraction of mineral fraction consisting of sand for each horizon; this is used for thermal conuctivity calculation
ClayFraction	[0.5 0.5 0.5]		Weight fraction of clay in mineral fraction; will be used for calculating organic matter stabilization of humic fraction (not yet implemented)
Layer_pF	[0.772 0.766 0.757 0.744 0.729 0.714 0.320; 0.835 0.831 0.830 0.830 0.797 0.770 0.320; 0.835 0.831 0.830 0.830 0.797 0.770 0.320]	m ³ .m ⁻³	pF Curves for each layer; each row represents the soil moisture at the matric potentials indicated in pFVal . Alternatively the pF curves can be defined using the parameters of the Van Genuchten equation. In that case the rows of Layer_pF contain the Van genuchten parameters θ_r , θ_s , α , 1 and n.
pFVal	[0.0 0.4 1.0 1.5 1.8 2.0 4.2]	log cm H ₂ O	Soil moisture potentials at which the moisture values in Layer_pF are defined if the curves are not defined by Van Genuchten parameters.

Name	Example	Units	Description
InitRes	[0.69 0.0 0.0 0.0 0.01 0.0 0.3; 0.92 0.0 0.0 0.0 0.0 0.0 0.08; 0.93 0.0 0.0 0.0 0.0 0.0 0.07]		Initial fractions of soil organic stored in each horizon and SOM reservoir; rows correspond to horizons, columns to to reservoirs. All rows should sum to 1.0
FreezingCurve	[1.5 1.5 1.5]		Unfrozen water content curve at below-zero temperatures, for calculating soil freezing in conditions of deep seasonal frost or permafrost. Relation: $f = f_{inf} + 1/(b-T)^a$, where a is a constant given in FreezingCurve for each horizon. b is determined by $theta_{sat}$ (water content at saturation and $theta_{wilt}$ (water content at wilting point) a has values between 1.5 and 2 (the larger values for sand, the smaller for clay and organics)