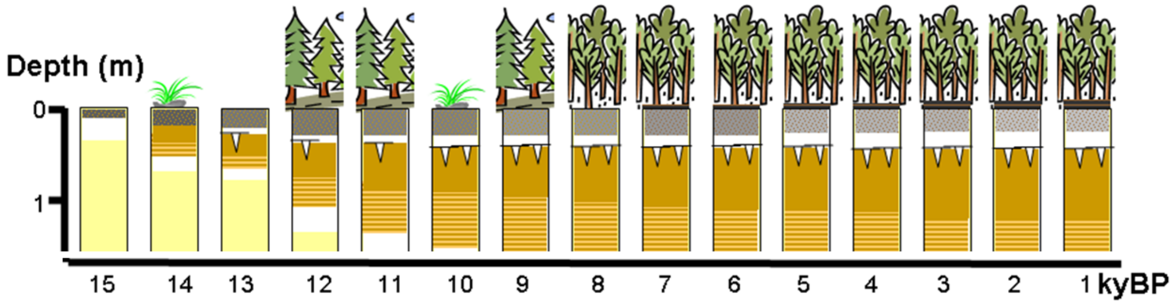
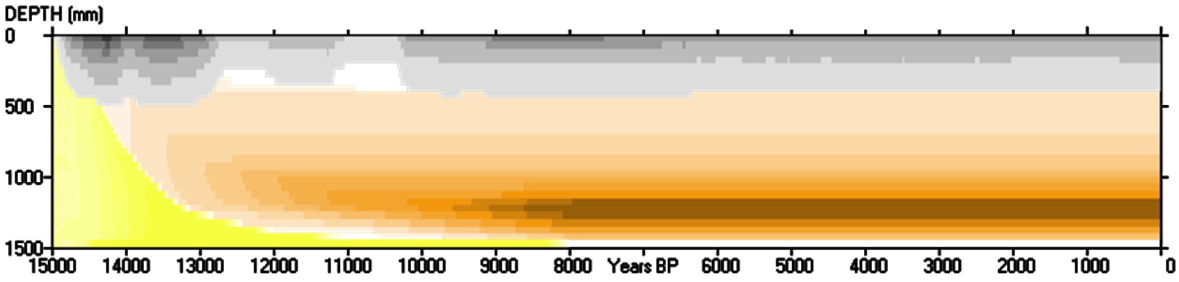
SOILGEN

A simulation model for soil development in various parent materials

USER MANUAL
for SoilGen2.24





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Part I: Using SoilGen

I.1 General

SoilGen is a simulation model for the study of pedogenesis in slightly calcareous soils such as loess. Whereas most soil genetic studies take observations in the present to reconstruct soil development in the past, this model takes an initial soil or parent material as starting point and calculates the effect of various boundary conditions over long periods on soil development. Thus, Jenny's paradigm is followed, which states that the soil we observe today is a function of the "factors of soil formation" CLORPT (CLimate, Organisms, Relief, Parent material and Time). All these factors are treated as boundaries or initial conditions whereas the soil forming processes are part of the simulation model. As such, the model can be used to (in)validate hypotheses on soil genesis at a particular location, as a process-based temporal interpolator, etcetera. The major focuses in the user interface are therefore (i) to support the definition of the initial situation and (ii) to support the description of the scenarios of the evolution of the boundary conditions over time.

Part II of this manual describes the actual processes that are implemented to model soil genesis. Processes related to water and solute flow, heat flow and soil chemistry are partly based on the concepts of LEACHM-C model (Hutson, 2003), but entirely reprogrammed in Pascal. Carbon dynamics are modeled afresh but follow the concepts of the RothC-26.3 model (Coleman and Jenkinson, 2005). Process descriptions were added on bioturbation (Finke and Hutson, 2008) and chemical weathering of primary minerals (concepts based on Van Grinsven, 1988 and Kros, 2002). The current model version, SoilGen2.24, additionally includes Al-Gibbsite chemistry, physical weathering, the clay migration process, $\Delta^{14}C$ degradation pathways, implementations of agricultural activities such as plowing and various events that can occur at the soil boundary (erosion, sedimentation, slash and burn, shallow water tables).

The initial situation is specified in 4 input files (see I.2.2):

1. A soil data input file, which essentially follows the format of a standard LEACHM-C input file for a 1 year period;
2. A file with chemical equilibrium constants (not all constants are actually used);
3. A file with process parameters needed to describe C-dynamics;
4. A file with chemical weathering parameters.

These files are plain text files and can be modified using a simple text editor. However, when defining various scenarios, the soil data input file is the most likely to be changed and the other 3 files may remain unchanged. Therefore the user interface allows to modify the soil data input file.

The boundary conditions over time are specified in 4 input files (see I.2.3):

1. A file with bioturbation time series;
2. A file with of climate and vegetation evolution;
3. A file with time series of fertilization (likely but not necessarily only during agricultural periods);
4. A file with pedogenically relevant events, such as erosion, deposition, plowing, slah&burn events and the occurrence of a shallow watertable. Additionally, if soil physical parameters (Van Genuchten parameters) are measured for (topsoil) compartments in a certain year and present in a file, this can be indicated.

Two additional files with boundary are possible but not mandatory:

5. A file containing partial CO2-pressure (pCO_2) of the atmosphere;
6. A file containing Δ14C values of fresh organic matter entering the soil.

Again, these files are plain text files and can be modified using a simple text editor. But they can also be created or edited via the user interface.

SoilGen is batch-sensitive, which means that if a file with the name <*SoilGenBatch.txt*> is present in the same folder as the model executable, this file is read and part of the user interface (the part described in I.2.2) is by-passed. In case also the following 4 files with boundary conditions are present and correctly formatted (see above list and section I.2.3) and site characteristics (slope, bearings, latitude) are given, only the "Run" button needs to be pressed to start model execution. You may still wish to connect a pCO_2-data file and a file with $\Delta^{14}C$ values for fresh C entering the soil (litter).

Ad 1: *bioturbINT.txt*
Ad 2: *climate.txt*
Ad 3: *fertilization.txt*
Ad 4: *events.txt*

Table 1 Example file SoilGenBatch.txt (file content in left column)

soil northfacing.txt	soil data input file
OK CAL EquilibriumConstants.txt	file with chemical equilibrium constants
OK C-Turnover.txt	file with process parameters needed to describe C-dynamics
UkkelP4 WeatheringRates.txt	file with chemical weathering parameters
15000	Model runtime (years)
11	Slope angle (degrees)
60	Upslope bearing (degrees; equivalent to Azimuth+180)
60	Downwind bearing (degrees)
51	Latitude (degrees)

Sequential runs with SoilGen are also possible. After a completed run in folder *folder*, a continuation run is possible from *folder\continuation*, which contains (a.o.) 3 files with the status of all relevant variables of the model at the end of the completed run. These files are automatically detected and read by SoilGen when the program is again started from *folder\continuation* and are called:

- *continue.rec* (a binary file)
- *continuePhysicalWeathering.txt*
- *continueVanGenuchtenMeasured.txt*

After reading these files, SoilGen produces a status report file *ContinueReport.txt* . The user then still has to specify input data for the continuation run, see I.2.3 for this.

The SoilGen executable and the above 8 to 10 (in case of a new run) input files are best copied to a folder created for the scenario to be simulated; as the model may create large numbers of files this will allow easier administration. SoilGen is written in Lazarus and can be compiled with the Free Pascal Compiler for Windows XP…8, Linux and other platforms. The standard distribution is for Windows.

I.2 User Interface

I.2.1 General

On startup, SoilGen gives a screen consisting of 3 tab sheets and 2 or 3 pull down menus (Fig. 1). The pull-down menus can be activated at any time before the model run is started. The tab sheets are used to provide names of input files and program settings.

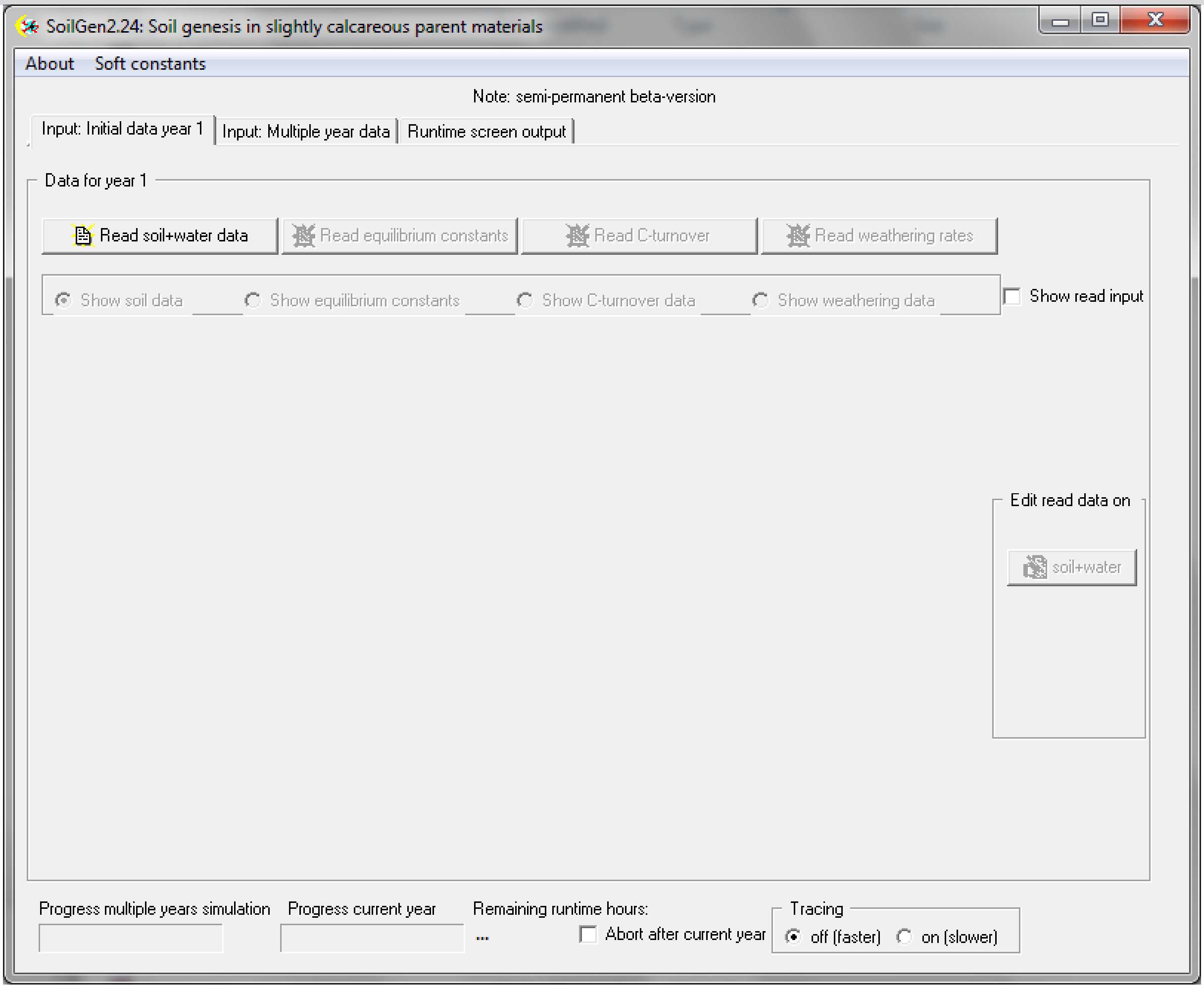


Fig. 1 Main form after starting SoilGen

Pull-down menus:

1. About: brings up a popup screen with references for model users.
2. Soft constants: brings up a popup screen in which various model parameters can be set that are normally not changed (see section I.4).
3. Memory dump: if (and only if) the model has crashed during a previous run in the same folder, the values of several variables is written to a file <dump.txt>, which can be accessed via this menu (not visible in the above figure).

Tab sheets:

1. Logically, the user starts by defining the initial soil condition and associated process parameters by activating the tab sheet *Input: Initial data year 1* (see I.2.2).
2. After the initial conditions and associated process parameters are defined successfully, the second tab sheet *Input: Multiple run data* becomes visible and can be activated. This tab sheet allows for a precise definition of the scenario in terms of scenario length, bioturbation, climate/vegetation characteristics, fertilization and pedogenetic relevant events (see I.2.3). Also, some settings relating to the output files and graphics can be chosen. The last action is the start of the simulations, which will cause the third tab sheet to become active.
3. The third tab sheet *Runtime screen output* allows monitoring the simulation progress and visualizes some selected outputs in the form of time-depth diagrams.

The lower part of the screen shows information concerning the program run.

- Program execution can be stopped in any running simulation year by checking the box *Abort this program after current simulation year* at the bottom of the form. This will cause a memory dump to be written to <dump.txt>. Note that the program cannot resume simulations after such break!
- The program will show over-all and within-year progress and will also give an indication of the remaining runtime in the lower part of the screen.
- Additionally, the option is present to trace the run program routines after an input year. This is meant for debugging purposes (to see in what part of the program is the crash occurring) and will

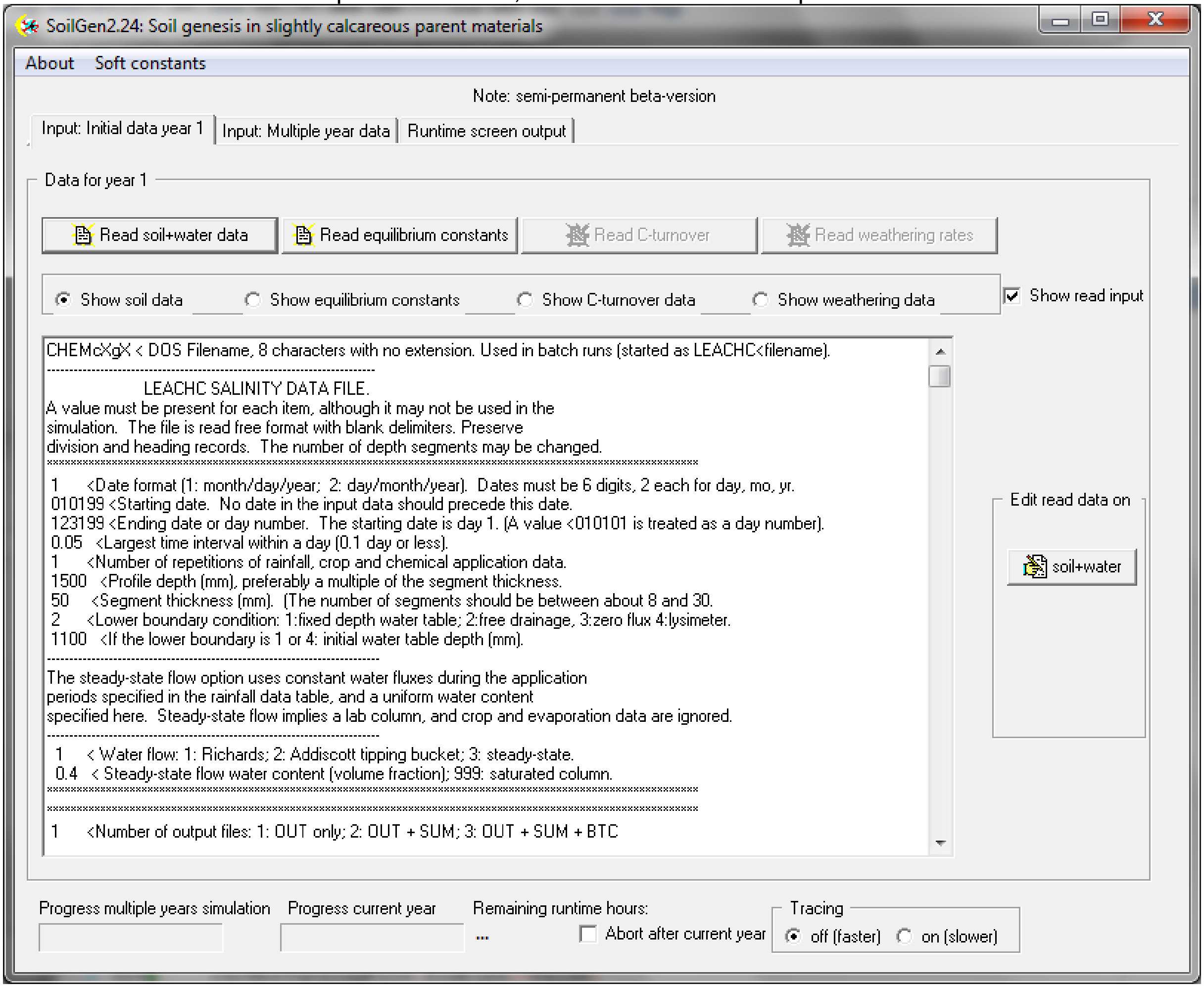
slow down program execution. This option can be switched off later during execution if desired.

I.2.2 Data file import and settings for year 1

The initial settings for soil properties and process parameters are done by specifying 4 files:

1. a soil data input file (essentially a LEACHM-C input file with a few additions but backwards compatible ; it should still be a valid input file for LEACHM-2003) (see Appendix at p.35);
2. a file with chemical equilibrium constants (see Appendix at p.38);
3. a file with process parameters needed to describe C-dynamics (see Appendix at p.39);
4. A file with chemical weathering parameters (see Appendix at p.40).

Each of these files is read after pressing the associated button and selecting the file with a dialog box. The file is tested on its completeness and adequate format, and if applicable an error message appears. Only after an input file is accepted, the button for the next input file becomes active. When the box “Show read input” is checked, each one of the read input files can be consulted.



```
CHEMcXgX < DOS Filename, 8 characters with no extension. Used in batch runs (started as LEACHC<filename).
------------------------------------------------------------------------
                    LEACHC SALINITY DATA FILE.
A value must be present for each item, although it may not be used in the
simulation.  The file is read free format with blank delimiters. Preserve
division and heading records.  The number of depth segments may be changed.
**********************************************************************************************************
 1      <Date format (1: month/day/year;  2: day/month/year).  Dates must be 6 digits, 2 each for day, mo, yr.
 010199 <Starting date.  No date in the input data should precede this date.
 123199 <Ending date or day number.  The starting date is day 1. (A value <010101 is treated as a day number).
 0.05   <Largest time interval within a day (0.1 day or less).
 1      <Number of repetitions of rainfall, crop and chemical application data.
 1500   <Profile depth (mm), preferably a multiple of the segment thickness.
 50     <Segment thickness (mm).  (The number of segments should be between about 8 and 30.
 2      <Lower boundary condition: 1:fixed depth water table; 2:free drainage, 3:zero flux 4:lysimeter.
 1100   <If the lower boundary is 1 or 4: initial water table depth (mm).
------------------------------------------------------------------------
The steady-state flow option uses constant water fluxes during the application
periods specified in the rainfall data table, and a uniform water content
specified here.  Steady-state flow implies a lab column, and crop and evaporation data are ignored.
------------------------------------------------------------------------
  1     < Water flow: 1: Richards; 2: Addiscott tipping bucket; 3: steady-state.
  0.4   < Steady-state flow water content (volume fraction); 999: saturated column.
**********************************************************************************************************
**********************************************************************************************************
 1      <Number of output files: 1: OUT only; 2: OUT + SUM; 3: OUT + SUM + BTC
```

Fig. 2 Main form after importing the soil data file

The soil data file is the most complex data file, and therefore it can be edited from the user interface by pressing the button “*soil+water*”. Then a new form (Fig. 3) opens which allows the user to edit three categories of soil data:

1. **General data**;

These data comprise

- the *profile depth* and the *segment thickness*. The profile depth is always an integer multiplicity of the segment thickness. In case one of both is changed by the user, automatically new soil segments are created. These still have to be filled with data. A large number of soil segments considerably increases the runtime.
- the *dispersivity*; The dispersivity is used to solve the Richards equation for unsaturated water flow. The value should be between 0.5* and 2* the segment thickness, as these values will result in negligible numerical dispersion. Dispersivity values near 0.5* segment thickness are

advised after a comparative analysis.

- the *molecular diffusion*; The molecular diffusion is used to solve the convection-dispersion equation for solute transport.
- the *Largest time interval within a day* controls to a limited extent the runtime.
- The 3 *Particle densities* are used to calculate porosity.

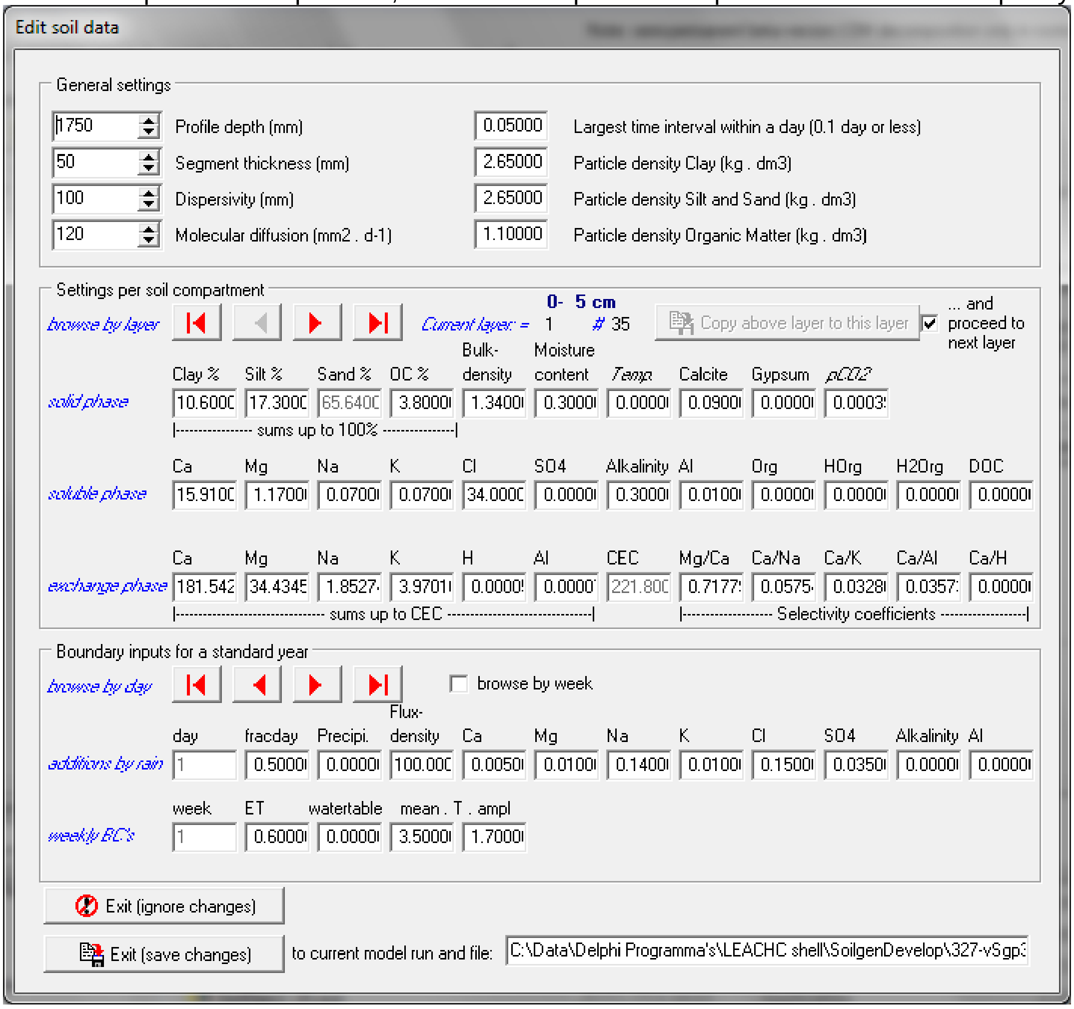
2. **Soil properties that vary by soil segment** (soil segments, or compartments, are layers of equal thickness defined in the general settings);

A number of soil compartment browser buttons can be used to select the appropriate compartment data. Some of the soil parameters cannot be edited, which means that they are calculated (Sand% and CEC) by SoilGen.
The parameter values can be changed by typing in the appropriate box. A hint will be displayed containing the dimensions. In case a homogeneous profile is to be created, the values of a compartment can be copied to the compartment below.

3. **Soil boundary conditions that vary with time within 1 standard simulation year**. Note that the values of this standard year may be scaled in any simulated year using the climate change scenarios (discussed in I.2.3).

Also here, the temporal data can be browsed (either by week or by day). Basically, there are 2 groups of temporal data:

- the precipitation-related data that are input by day;
- the potential evaporation, water table depth and temperature data that are input by week.



Edit soil data

General settings

1750 Profile depth (mm)
50 Segment thickness (mm)
100 Dispersivity (mm)
120 Molecular diffusion (mm2 . d-1)
0.05000 Largest time interval within a day (0.1 day or less)
2.65000 Particle density Clay (kg . dm3)
2.65000 Particle density Silt and Sand (kg . dm3)
1.10000 Particle density Organic Matter (kg . dm3)

Settings per soil compartment

browse by layer

0- 5 cm
Current layer: = 1 # 35

Copy above layer to this layer ☑ ... and proceed to next layer

	Clay %	Silt %	Sand %	OC %	Bulk-density	Moisture content	*Temp*	Calcite	Gypsum	*pCO2*
solid phase	10.600	17.300	65.640	3.8000	1.3400	0.3000	0.0000	0.0900	0.0000	0.0003

|--------------- sums up to 100% ---------------|

	Ca	Mg	Na	K	Cl	SO4	Alkalinity	Al	Org	HOrg	H2Org	DOC
soluble phase	15.910	1.1700	0.0700	0.0700	34.000	0.0000	0.3000	0.0100	0.0000	0.0000	0.0000	0.0000

	Ca	Mg	Na	K	H	Al	CEC	Mg/Ca	Ca/Na	Ca/K	Ca/Al	Ca/H
exchange phase	181.542	34.434	1.8527	3.9701	0.0000	0.0000	221.80	0.7177	0.0575	0.0328	0.0357	0.0000

|------------------------------ sums up to CEC ------------------------------| |------------------ Selectivity coefficients ------------------|

Boundary inputs for a standard year

browse by day ☐ browse by week

	day	fracday	Precipi.	Flux-density	Ca	Mg	Na	K	Cl	SO4	Alkalinity	Al
additions by rain	1	0.5000	0.0000	100.00	0.0050	0.0100	0.1400	0.0100	0.1500	0.0350	0.0000	0.0000

	week	ET	watertable	mean . T	ampl
weekly BC's	1	0.6000	0.0000	3.5000	1.7000

Exit (ignore changes)

Exit (save changes) to current model run and file: C:\Data\Delphi Programma's\LEACHC shell\SoilgenDevelop\327-vSgp

Fig. 3 Form for editing the imported soil data

After modifications are done, the user can either ignore (undo) these changes or save the changes (both internally in the program and to a specified file name).

I.2.3 Multi-annual scenario import and settings

After the input for year 1 is done, the second tab sheet can be accessed. The left part of this sheet is devoted to the input of multi-annual scenario data, the right part can be used to define output settings (see I.2.4). The scenarios are set by 5 major activities (Fig. 4), that should occur in order listed below:

1. Definition of the simulation period.

A number between 1 and 15000 years can be chosen, assuming that that the end of the simulation period is always the current year (considered: 0 BP).

2. Definition of the bioturbation in the simulation period.

If a bioturbation scenario file with the name <*BioturbINT.txt*> is found, the user can choose to use or to ignore this file. If the file is ignored or not present, the user can press the button *define or import Bioturbation time series* to construct a bioturbation scenario (see below). Bioturbation data are interpolated between non-specified years.

3. **Definition of the climate change** over the simulation period.

If a climate scenario file with the name <*Climate.txt*> is found, the user can choose to use or to ignore this file. If the file is ignored or not present, the user can press the button *define or import Climate time series* to construct a scenario (see below). Climatic data are interpolated between non-specified years. Additionally, a file containing time series of atmospheric CO_2-levels (pCO_2, in bar) can be imported to impose changes in these levels. pCO_2-data are interpolated between non-specified years. If this file is not imported, constant pCO_2-values will be assumed (0.0003 bar).

4. **Definition of the fertilization** over the simulation period.

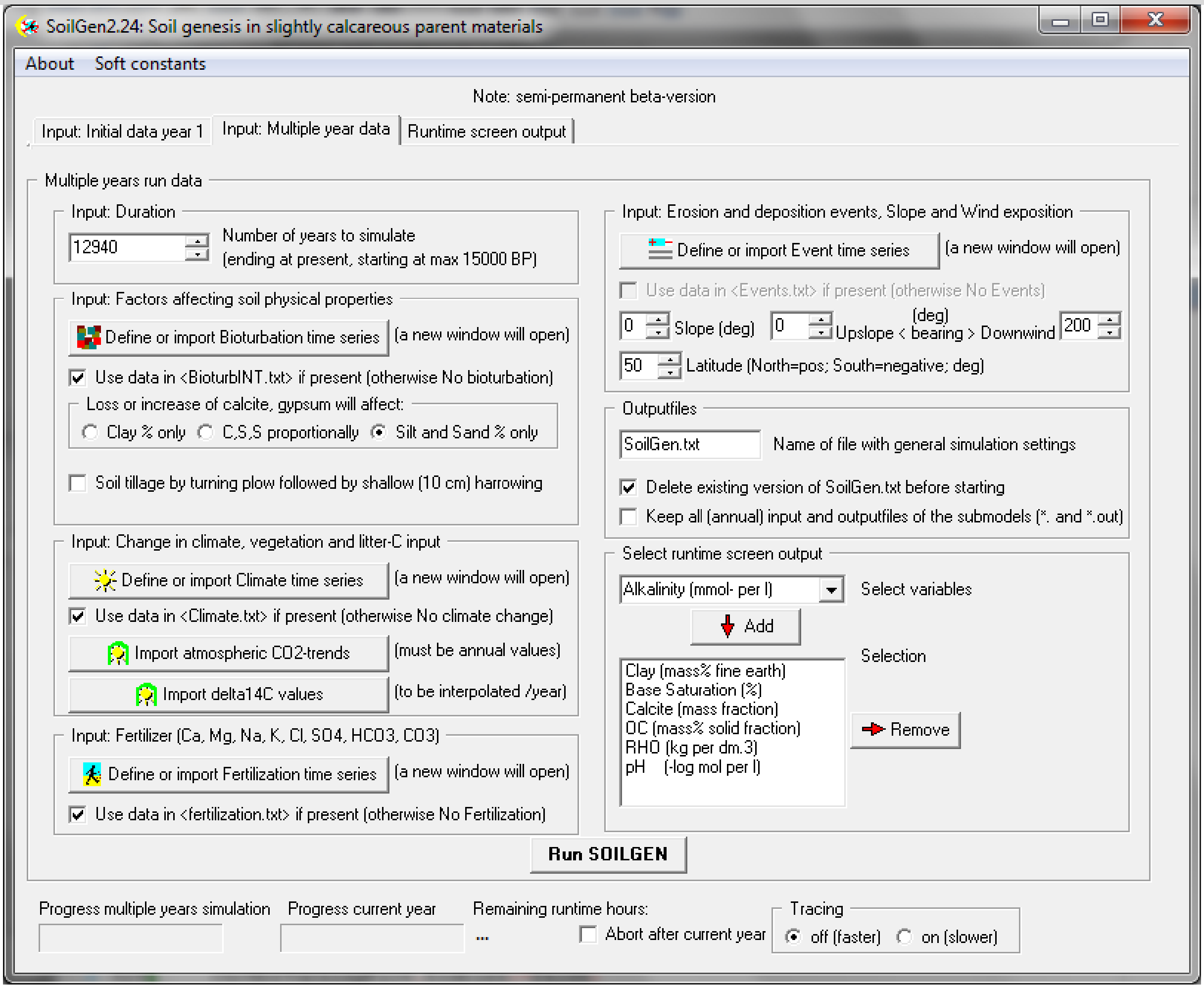
If a fertilization scenario file with the name <*Fertilization.txt*> is found, the user can choose to use or to ignore this file. If the file is ignored or not present, the user can press the button *define or import Fertilization time series* to construct a scenario (see below). Note that SoilGen will apply fertilization even when the land use is not *agriculture* (defined in Climate scenario), and will not apply fertilization in years between those defined in the scenario.

5. **Definition of events** over the simulation period.

If an events file with the name <*Events.txt*> is found, the user can choose to use or ignore this file. If the file is ignored or not present, the user can press the button *define or import Events* to construct a scenario (see below). Note that SoilGen will not apply events in years between those defined in the scenario.

Besides bioturbation, also the dissolution/precipitation of calcite and gypsum, clay migration and physical weathering can affect soil physical properties in a soil compartment via soil texture and bulk density. These processes must be activated via the main screen:

1. A choice must be made on how changes in calcite and gypsum affect the grain size distribution. For instance, it is usually assumed that calcite in loess is not in the clay fraction.
2. The soil mixing by plowing and harrowing (only when land use=agriculture) is by default determined by harrowing. Checking the box makes SoilGen emulate a turning plow followed by shallow harrowing. Mixing depths are set in the soil data input file and can be annually changed via the Events.txt file (see elsewhere).



12940 Number of years to simulate (ending at present, starting at max 15000 BP)

☑ Use data in <BioturbINT.txt> if present (otherwise No bioturbation)

Loss or increase of calcite, gypsum will affect: ○ Clay % only ○ C,S,S proportionally ● Silt and Sand % only

☐ Soil tillage by turning plow followed by shallow (10 cm) harrowing

☑ Use data in <Climate.txt> if present (otherwise No climate change)

☑ Use data in <fertilization.txt> if present (otherwise No Fertilization)

☐ Use data in <Events.txt> if present (otherwise No Events)

0 Slope (deg) 0 Upslope < (deg) bearing > Downwind 200

50 Latitude (North=pos; South=negative; deg)

SoilGen.txt Name of file with general simulation settings

☑ Delete existing version of SoilGen.txt before starting

☐ Keep all (annual) input and outputfiles of the submodels (*. and *.out)

Alkalinity (mmol- per l) Select variables

Selection:
Clay (mass% fine earth)
Base Saturation (%)
Calcite (mass fraction)
OC (mass% solid fraction)
RHO (kg per dm.3)
pH (-log mol per l)

☐ Abort after current year

Tracing ● off (faster) ○ on (slower)

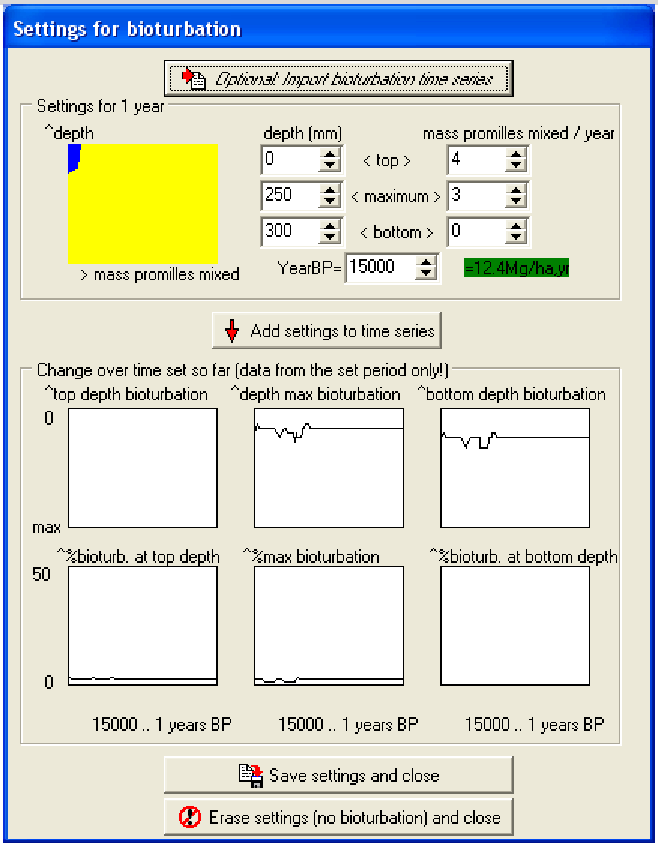
Fig. 4 Tab sheet for input of multi-annual (scenario) data

Defining a Bioturbation scenario

The form in Fig. 5 is used to entry, import or modify a bioturbation scenario. Bioturbation is defined in any year Before Present by 6 parameters: the depths of the shallowest, maximal and deepest bioturbation, and for each of these 3 depth the mass fraction (per 0.1%) that is being mixed by bioturbation in this year. Using the bulk densities input in the soil data file, the total mass being bioturbated is calculated while the above 6 parameters are being changed.

The 6 parameters are set for a series of specific simulation years, year 1 being the first year of the simulations in the more distant past. Non-specified years will be linearly interpolated. The 6 graphs visualize the recorded values over time.

The form can be exited by 2 buttons. Either the settings are saved to a file called <*BioturbINT.txt*>, or the settings are not saved and an existing version of *BioturbINT.txt* will be deleted.



depth (mm)		mass promilles mixed / year
0	< top >	4
250	< maximum >	3
300	< bottom >	0

YearBP= 15000 =12.4Mg/ha.yr

Fig. 5 Appearance of the bioturbation form after importing an existing scenario

Defining a Climate scenario

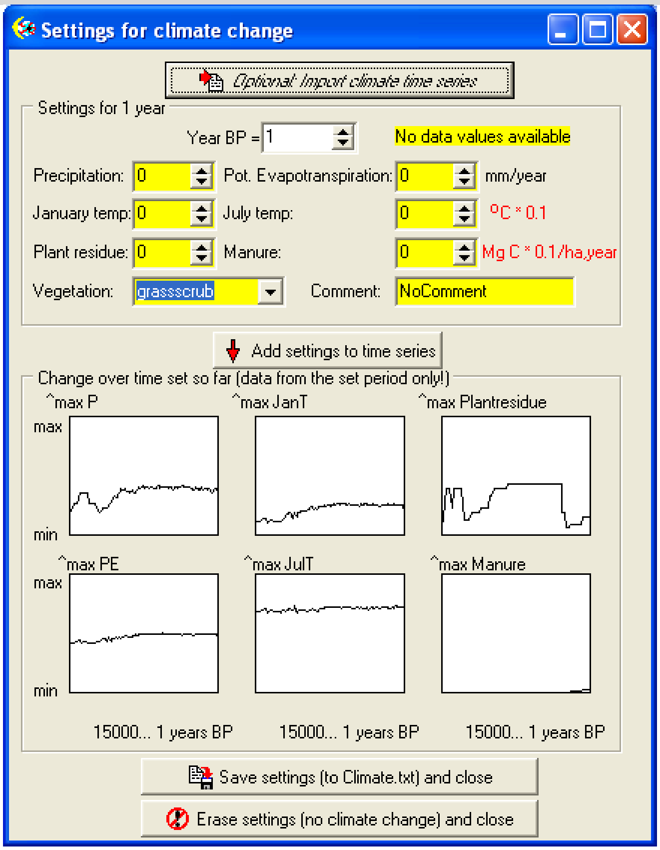
The form in Fig. 6 is used to entry, import or modify a climate change scenario. Climate is defined in any year by the following parameters:

1. the *annual precipitation* in mm;
2. the annual *potential evapotranspiration* in mm;
3. the average temperature in January (in ^{o}C, but set in multitudes of 0.1 degrees Centigrade);
4. the average temperature in July (in ^{o}C, but set in multitudes of 0.1 degrees Centigrade);
5. the net plant residue, being the annual sum of the root litter and leaf litter input in and on the soil (in Mg C . ha^{-1}, but set in multitudes of 100 kg . ha^{-1});
6. the manure input (also in Mg C . ha^{-1}, but set in multitudes of 100 kg . ha^{-1});
7. the vegetation type (being either grass/scrub, coniferous forest, deciduous forest or agriculture);
8. a comment (e.g. on the data source) in free text format.

The 8 parameters are set for a series of specific simulation years, year before present (BP) 1 being the most recent year of the simulations. Non-specified years will be linearly interpolated. The graphs visualize the recorded values over time.

An existing climate file can be imported using the button at the top of the form. Note that such an imported file must have a heading line containing the names of the variables given below in the data columns. The import form (not shown) allows to identify the variables and to insert lines with new data if so wished. After finishing the data import, the user returns to the climate scenario form in Fig. 6 and can add new data using this form as well.

The form can be closed by 2 buttons. Either the settings are saved to a file called <*Climate.txt*>, or the settings are not saved and an existing version of *Climate.txt* will be deleted.



Year BP = 1

No data values available

Precipitation: 0 Pot. Evapotranspiration: 0 mm/year

January temp: 0 July temp: 0 °C * 0.1

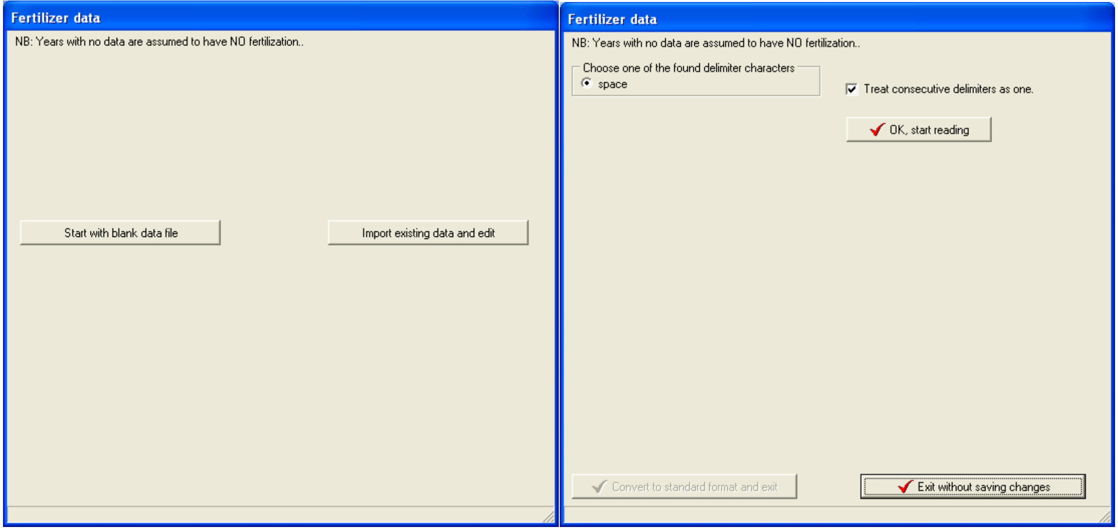
Plant residue: 0 Manure: 0 Mg C * 0.1/ha.year

Vegetation: grassscrub Comment: NoComment

Fig. 6 Appearance of a climate change form after importing an existing scenario

Defining a Fertilization scenario

The form in Fig. 7 and Fig. 8 is used to entry, import or modify a fertilization scenario. Fertilization scenarios are defined in any year Before Present by the parameters: *Ca, Mg, Na, K, Cl,* SO_4, HCO_3 and CO_3 in the form of inorganic fertilizer. All doses are input in mol.m^{-2}. Note that C from organic manure can be input via the climate scenario (previous section), but the abovementioned ions, if present in the manure, should be input via the fertilization forms (or file). The tables with the imported or typed data can be edited and lines can be inserted or deleted to include data for additional years or delete years. Note that years without data will be interpreted as years without fertilization, and also fertilization will be applied for a certain year BP even if the land use for this year is not *agriculture*. The form can be closed by 2 buttons. Either the settings are saved to a file called <*Fertilization.txt*>, or the settings are not saved (which has no consequences for an existing version of *Fertilization.txt*).



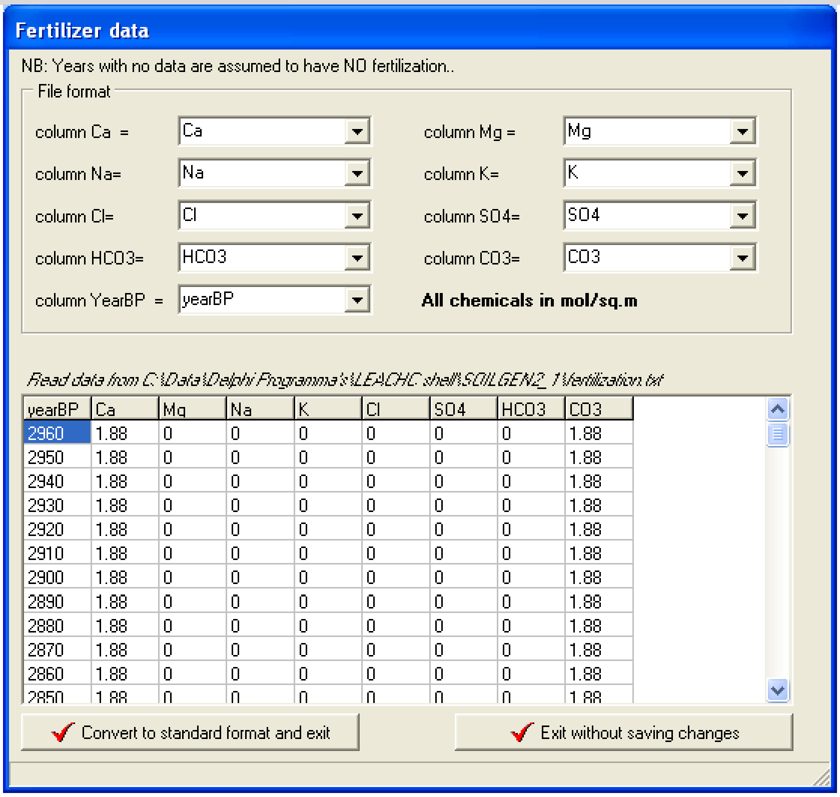
NB: Years with no data are assumed to have NO fertilization..

NB: Years with no data are assumed to have NO fertilization..

● space

☑ Treat consecutive delimiters as one.

Fig. 7 Fertilization scenario form after startup (left) and after choosing an import file (right)



NB: Years with no data are assumed to have NO fertilization..

column Ca = Ca
column Mg = Mg
column Na= Na
column K= K
column Cl= Cl
column SO4= SO4
column HCO3= HCO3
column CO3= CO3
column YearBP = yearBP

All chemicals in mol/sq.m

Read data from C:\Data\Delphi Programma's\LEACHC shell\SOILGEN2_1\fertilization.txt

yearBP	Ca	Mg	Na	K	Cl	SO4	HCO3	CO3
2960	1.88	0	0	0	0	0	0	1.88
2950	1.88	0	0	0	0	0	0	1.88
2940	1.88	0	0	0	0	0	0	1.88
2930	1.88	0	0	0	0	0	0	1.88
2920	1.88	0	0	0	0	0	0	1.88
2910	1.88	0	0	0	0	0	0	1.88
2900	1.88	0	0	0	0	0	0	1.88
2890	1.88	0	0	0	0	0	0	1.88
2880	1.88	0	0	0	0	0	0	1.88
2870	1.88	0	0	0	0	0	0	1.88
2860	1.88	0	0	0	0	0	0	1.88
2850	1.88	0	0	0	0	0	0	1.88

Fig. 8 Fertilization scenario form after importing or editing

Defining an Event scenario

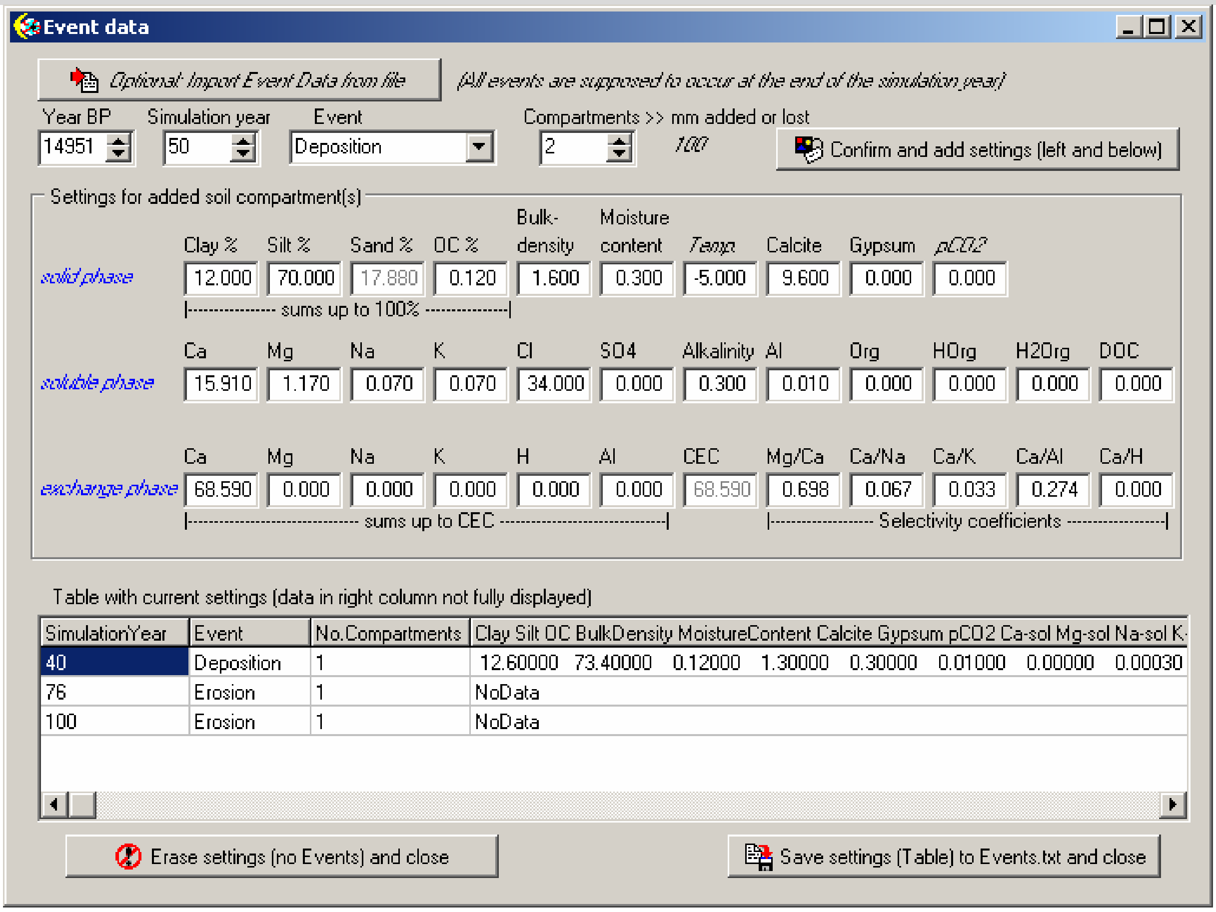
The form in Fig. 9 is used to entry, import or modify an event scenario. Currently, 6 types of events are distinguished:

1. Erosion events. Only the number of compartments that disappear at the top of the profile because of erosion have to be specified for a certain year;
2. Deposition events. The number of added compartments has to be specified as well as the properties of the added material;
3. Water tables. This feature has been added to allow simulation of a changing water table over time, for instance because a soil becomes drier when the coastline retreats. The number of soil components that corresponds to the average water table depth in a specified year has to be given.
4. Availability of measured Van Genuchten parameters for an indicated number of topsoil compartments in a certain simulation year (and valid until changed). These values override the default values estimated by the Hypres-pedotransfer function.
5. Specification of plowing. Indicate the depth of plowing and the mass fractions that are effectively mixed. Values remain valid in later simulation years until changed.
6. Specification if slash&burn occurs. Indicate the depth affected by the burning, the fractions of OC going into the atmosphere as CO_2, the fraction of OC transformed into charcoal (equivalent to the Inert Organic Matter pool) and the remainder fraction supposedly entering the humus pool.

An existing events file can be imported using the button on top of the form, which will open and import data to the form. Note that such an imported file must have a heading line containing the names of the variables given below in the data columns. After finishing the data import, the user form in Fig. 9 allows addition of new data as well. The import of new data is done by choosing a year, the type of event and, possibly, associated data.

The form can be closed by 2 buttons. Either the settings are saved to a file called <*Events.txt*>, or the settings are not saved and an existing version of *Events.txt* will be deleted.

Note: only 1 event can take place in 1 simulation year!



(All events are supposed to occur at the end of the simulation year)

Year BP	Simulation year	Event	Compartments >>	mm added or lost
14951	50	Deposition	2	100

Settings for added soil compartment(s)

	Clay %	Silt %	Sand %	OC %	Bulk-density	Moisture content	Temp	Calcite	Gypsum	pCO2
solid phase	12.000	70.000	17.880	0.120	1.600	0.300	-5.000	9.600	0.000	0.000

|---------------- sums up to 100% ---------------|

	Ca	Mg	Na	K	Cl	SO4	Alkalinity	Al	Org	HOrg	H2Org	DOC
soluble phase	15.910	1.170	0.070	0.070	34.000	0.000	0.300	0.010	0.000	0.000	0.000	0.000

	Ca	Mg	Na	K	H	Al	CEC	Mg/Ca	Ca/Na	Ca/K	Ca/Al	Ca/H
exchange phase	68.590	0.000	0.000	0.000	0.000	0.000	68.590	0.698	0.067	0.033	0.274	0.000

|------------------------------- sums up to CEC -------------------------------| |----------------- Selectivity coefficients -----------------|

Table with current settings (data in right column not fully displayed)

SimulationYear	Event	No.Compartments	Clay Silt OC BulkDensity MoistureContent Calcite Gypsum pCO2 Ca-sol Mg-sol Na-sol K-
40	Deposition	1	12.60000 73.40000 0.12000 1.30000 0.30000 0.01000 0.00000 0.00030
76	Erosion	1	NoData
100	Erosion	1	NoData

Fig. 9 Appearance of Events form after importing events from a file and during insertion of 1 additional deposition event

I.2.4 Output settings

The final settings to be made concern the model output, either on screen or as files. As observable from Fig. 4, an output file which summarizes scenario settings must be named. In case of multi-year scenario's the large number of output files can be a limitation and therefore the making of these – annual- output files can be prevented.

The user can select a number of (maximally 6) time-depth diagrams to be displayed in the third tab sheet during runtime, to monitor important outcomes of the model. All the time-depth diagrams that can be selected for screen display are output files as well. These *.tdd files (see I.5) can be post-processed or displayed using separate software.

I.3 Input files

The table summarizes the major input files and states whether these are mandatory or not. All files are plain ASCII-textfiles and can be edited using a text editor.

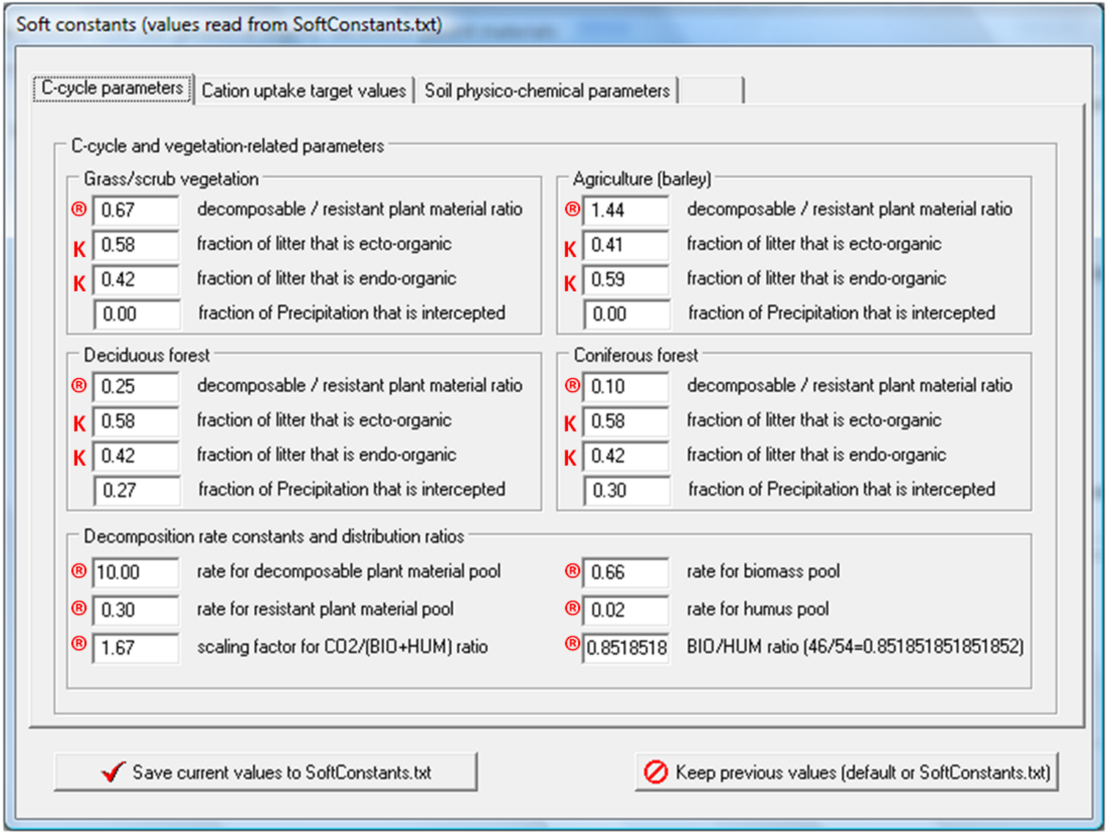
File with …	Mandatory?	Remarks on editing of these files
Soil properties	Yes	Lines containing explanatory text may not be removed; data lines may be inserted but must confirm to number of soil compartments, rainfall events, fertilization events or weeks. SoilGen assumes 365 rainfall and fertilizing events (possibly filled with values 0) and 53 weeks since standard periods of 1 year are simulated. Some values may not be altered, or are modified by SoilGen during runtime. Most data values may be edited via the user interface (see I.2.2). Example file in Appendix 1 (p.35).
Chemical equilibriums	Yes	Line order is not critical, but text may not be changed. Edit only the numbers in the first two columns. Example file in Appendix 2 (p.38).
C-cycling data	Yes	Line order and text may not be changed. Edit only the numbers.

		Example file in Appendix 3 (p.39).
Weathering data	Yes	Line order and text may not be changed. Edit only the numbers. Example file in Appendix 4 (p.40).
Bioturbation data	No	SoilGen needs a file called *BioturbINT.txt* if the effect of bioturbation is to be estimated. *BioturbINT.txt* contains bioturbation data for each simulation year. In case this file is missing, bioturbation is set to zero. With the user interface (section I.2.3), a simpler version of this file (e.g. *BioturbSET.txt*) can be created or imported containing only data at typical years. The user interface (linearly) interpolates these data to yearly values. There is no need to manually edit the values as this can be done via the user interface. Example file in Appendix 5.
Climate data	No	SoilGen needs a file *Climate.txt* if climate change is to be simulated. If this file is missing, a vegetation of deciduous forest is assumed with a fixed litter input. The climate is as specified in the soil properties input file. Example file in Appendix 6. With the user interface (section I.2.3), a climate change file can be imported or created containing data at typical years. The user interface (linearly) interpolates these data to yearly values.
pCO_2 data	No	If this file is missing, pCO_2-levels will be assumed constant at 0.000300 Bar. Per line the year_Before_Present and pCO_2 must be specified. The user interface (linearly) interpolates these data to yearly values. Example file in Appendix 7.
$\Delta^{14}C$ data	No	This file gives per year (CalBP) the values Delta 14C per mil for fresh litter added to the soil. Values for missing years are interpolated. No file = 0 per mil is assumed. 0 BP in this file means 1950 AD.
Fertilization data	No	SoilGen needs a file *Fertilization.txt* if the effect of fertilization is to be simulated. If this file is missing, no fertilization is assumed. With the user interface (section I.2.3), a fertilization file can be imported or created containing data at chosen years. Years undocumented in the file are assumed to have no fertilization. Example file in Appendix 8.
Event data	No	SoilGen needs a file *Events.txt* if the effect of pedogenetic relevant events is to be simulated. If this file is missing, it is assumed that no events occur. With the user interface (section I.2.3), an event file can be imported or created containing data at chosen years. Years undocumented in the file are assumed to have no events. Example file in Appendix 9.
Continuation	No	If one run has ended, SoilGen produces a subfolder with files that allow for a continuation run (e.g. for case studies that first simulate the past to reconstruct the present and then one or more future scenarios). The continuation possibility is detected automatically by SoilGen by the presence of 3 files that record the status at the end of the preceding run: • <continue.rec>, a binary file with the complete status of all relevant model variables; • <continuePhysicalWeathering.txt> with a specification of the particle size distribution; • <continueVanGenuchtenMeasured.txt> with a specification of VanGenuchten parameters that were measured and should remain valid in the continuation run.

I.4 Soft constants

Pressing the menu SoftConstants brings up a screen with a number of tab sheets. The data values in the tab sheets are read from a file SoftConstants.txt or, in case this file is not present, take the values

of the model defaults. If SoftConstants.txt is not present, SoilGen produces this file at program initialization. If values are changed by the user, and the “Save” button is pressed, SoftConstants.txt is updated and the previous version is renamed to”OldSoftConstants.txt” (earlier versions are not kept). The current version of SoilGen gives 3 tab sheets with softconstants.
In Fig. 10 the tab sheet with parameters relevant for the C-cycle routine is shown. (Default) parameter values equivalent to those from the RothC26.3 model are indicated by ®. Parameter values indicated by **K** are based on Kononova (1975). Remaining parameter values are used for the calculation of the evaporation of intercepted rain by leaves. In SoilGen2.18 some of these default values were modified after calibration (Yu et al., 2013).



C-cycle and vegetation-related parameters

Grass/scrub vegetation
® 0.67 decomposable / resistant plant material ratio
K 0.58 fraction of litter that is ecto-organic
K 0.42 fraction of litter that is endo-organic
0.00 fraction of Precipitation that is intercepted

Agriculture (barley)
® 1.44 decomposable / resistant plant material ratio
K 0.41 fraction of litter that is ecto-organic
K 0.59 fraction of litter that is endo-organic
0.00 fraction of Precipitation that is intercepted

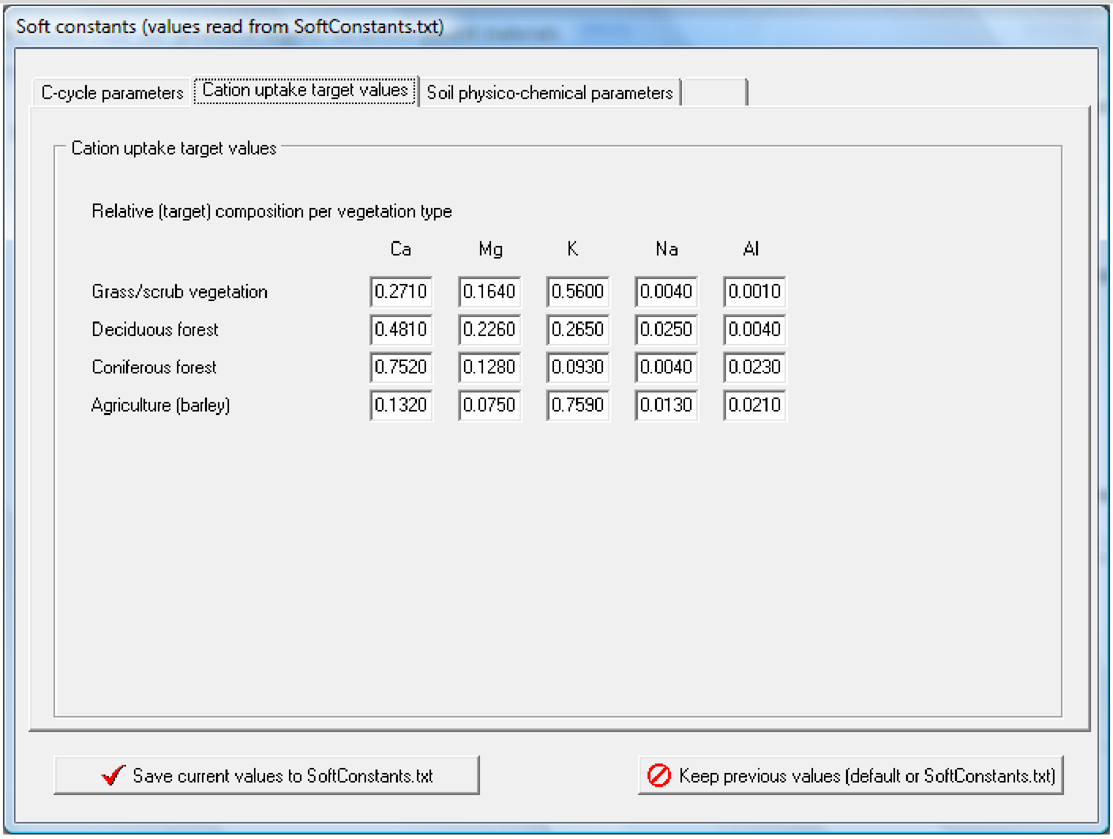
Deciduous forest
® 0.25 decomposable / resistant plant material ratio
K 0.58 fraction of litter that is ecto-organic
K 0.42 fraction of litter that is endo-organic
0.27 fraction of Precipitation that is intercepted

Coniferous forest
® 0.10 decomposable / resistant plant material ratio
K 0.58 fraction of litter that is ecto-organic
K 0.42 fraction of litter that is endo-organic
0.30 fraction of Precipitation that is intercepted

Decomposition rate constants and distribution ratios
® 10.00 rate for decomposable plant material pool
® 0.30 rate for resistant plant material pool
® 1.67 scaling factor for CO2/(BIO+HUM) ratio
® 0.66 rate for biomass pool
® 0.02 rate for humus pool
® 0.8518518 BIO/HUM ratio (46/54=0.851851851851852)

Fig. 10 Soft constants 1: Parameters relevant for C-cycle routine and interception evaporation

Fig. 11 shows a tab sheet with parameters that can be set for target cation composition per vegetation type. Default values are taken from Navrátil (2003) for forest vegetation, Thompson et al. (1997) for grass/scrubland and from Wyszkowski et al. (2006) for agriculture. Modified values should sum to 1 for each vegetation type.

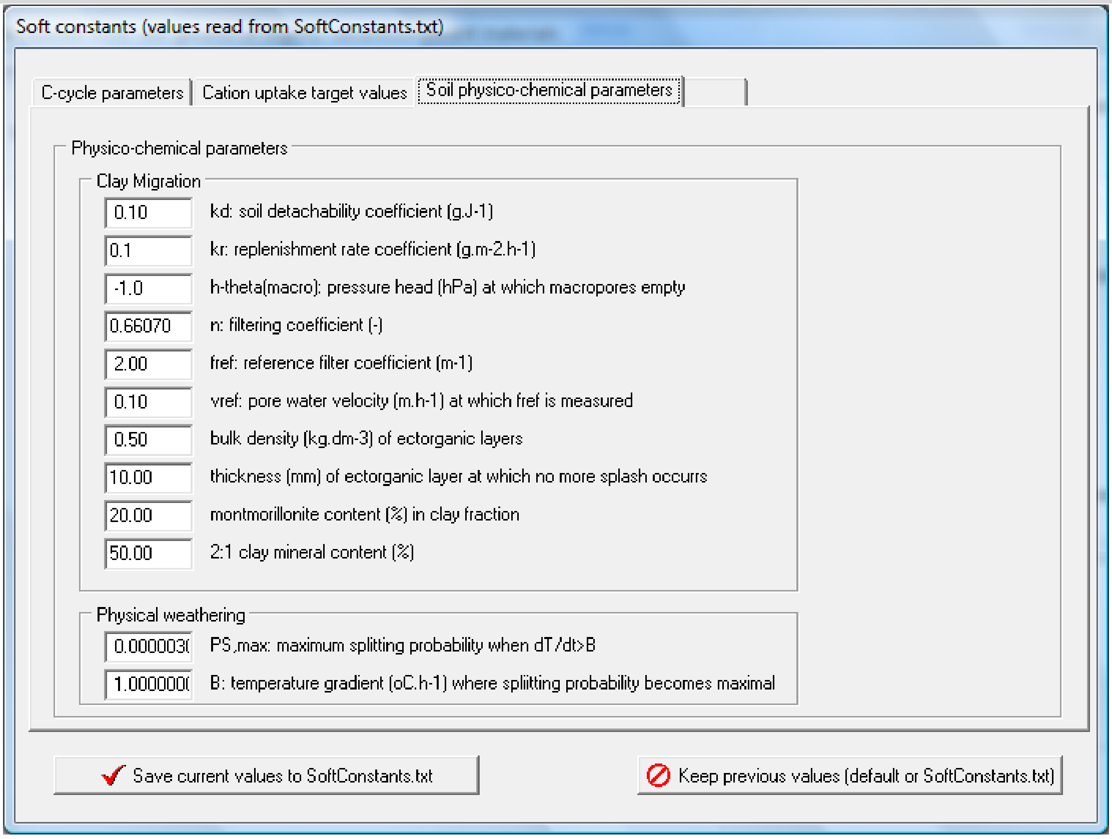


Relative (target) composition per vegetation type

	Ca	Mg	K	Na	Al
Grass/scrub vegetation	0.2710	0.1640	0.5600	0.0040	0.0010
Deciduous forest	0.4810	0.2260	0.2650	0.0250	0.0040
Coniferous forest	0.7520	0.1280	0.0930	0.0040	0.0230
Agriculture (barley)	0.1320	0.0750	0.7590	0.0130	0.0210

Fig. 11 Soft constants 2: Target cation composition per vegetation type

Fig. 12 shows a tab sheet with parameters for the processes clay migration and physical weathering. Values for *kd*, *kr*, f_{ref}, v_{ref} are taken from Jarvis et al., 1999. Values for $h(\theta_{macro})$, *n*, $P_{S,max}$ were obtained by calibration (Finke, 2012), a more extensive calibration is underway (2014). Other values are site characteristics.



Physico-chemical parameters

Clay Migration

0.10 kd: soil detachability coefficient (g.J-1)
0.1 kr: replenishment rate coefficient (g.m-2.h-1)
-1.0 h-theta(macro): pressure head (hPa) at which macropores empty
0.66070 n: filtering coefficient (-)
2.00 fref: reference filter coefficient (m-1)
0.10 vref: pore water velocity (m.h-1) at which fref is measured
0.50 bulk density (kg.dm-3) of ectorganic layers
10.00 thickness (mm) of ectorganic layer at which no more splash occurrs
20.00 montmorillonite content (%) in clay fraction
50.00 2:1 clay mineral content (%)

Physical weathering

0.000003 PS,max: maximum splitting probability when dT/dt>B
1.000000 B: temperature gradient (oC.h-1) where splitting probability becomes maximal

Fig. 12 Soft constants 3: Parameters for clay migration and physical weathering processes

I.5 Output files

The table summarizes the major output files and states whether these are always produced or not. All files are plain ASCII-files. The ☺ in the table indicate the years after the start of the simulations.

File	Status	Contents
Log file	Always	Summary of the simulated scenario in terms of used input and produced output
*.tdd	Always	Time-depth diagram data (data from 31-12 of every year per soil compartment) of specific model variables * (see Table 2) These files can be viewed and saved to bitmaps using external software (*TDGraph.exe*).
Messages.txt	Conditionally	Error messages during runtime
Dump.txt	Conditionally	Contains state of variables at time of a runtime error, at the start of the last runtime year, and at start of the simulation. This is an ASCII-text file, but is not interpretable from a text editor. Instead, re-starting SoilGen will cause detection of this file by the program and allow the user to analyze the state of the variables via a menu-option in the program.
LC☺.out	On request	Yearly output file of the solute transport and chemistry model (LEACHC)
RC☺.out	On request	Yearly output of the C-cycling sub-model
WE☺.out	On request	Yearly output of the weathering sub-model
Continuation files	Always	3 files that record the status at the end of the preceding run: • <continue.rec>, a binary file with the complete status of all relevant model variables; • <continuePhysicalWeathering.txt> with a specification of the particle size distribution; • <continueVanGenuchtenMeasured.txt> with a specification of

		VanGenuchten parameters that were measured and should remain valid in the continuation run.

Table 2 Output variables. All variables per soil compartment and at 31-12 of each year unless indicated otherwise. DPM=Decomposable Plant Material, RPM=Resistant Plant Material, IOM= Inert Organic Matter, OC=Organic Carbon.

Type	Variable	Dimension	Type	Variable	Dimension
Chemical	Alkalinity	mmol$^-$ dm^{-3}	Physical	Clay	mass% fine earth
	Ca^{2+} solution	mmol dm^{-3} **		Clay	volume%
	Mg^{2+} solution	mmol dm^{-3} **		Sand	mass% fine earth
	Na^+ solution	mmol dm^{-3} **		Silt	mass% fine earth
	K^+ solution	mmol dm^{-3} **		RHO	kg dm^{-3}
	Al^{3+} solution	mmol dm^{-3} **		Clay Dispersion Indic.	-
	Ca+Mg+Na+K	mmol dm^{-3}		PlantAvailableWater	volume fraction
	Cl^- solution	mmol dm^{-3} **		Porosity	volume fraction
	SO_4^{2-} solution	mmol dm^{-3} **		Theta	cm^3 cm^{-3}
	CO_3^{2-} solution	mmol dm^{-3} **		Potential	kPa
	HCO_3^-solution	mmol dm^{-3} **		ET	mm
	EC	mS m^{-1}		Flux	mm
	pH			Average Temperature	ºC
	Ca-exch.	mmol$^+$ kg^{-1} soil	Plant related	OC	mass% solid fraction
	Mg-exch.	mmol$^+$ kg^{-1} soil		DPM *	ton C ha^{-1}
	Na-exch.	mmol$^+$ kg^{-1} soil		RPM *	ton C ha^{-1}
	K-exch.	mmol$^+$ kg^{-1} soil		Biomass *	ton C ha^{-1}
	Al-exch.	mmol$^+$ kg^{-1} soil		Humus *	ton C ha^{-1}
	ESP	%		IOM *	ton C ha^{-1}
	Base Saturation	%		Roots	fraction
	CEC	mmol$^+$ kg^{-1} soil		Δ14C	per mil
	SAR	-		Age	14C years
	pCO2	bar		Fk-DPM	per mil Δ14C as fraction of all C in this pool
	$CaCO_3$	mass fraction		Fk-RPM	
	$CaSO_4$	mass fraction		Fk-BIO	
Element stocks in minerals	Ca-in-minerals	mol m^{-2}		Fk-HUM	
	Mg-in-minerals	mol m^{-2}		Fk-IOM	
	Na-in-minerals	mol m^{-2}	Weathering indices	CIA (Nesbitt+Young 1982)	%
	K-in-minerals	mol m^{-2}		IndexB (Kronberg+Nesbitt 1981)	-
	Fe-in-minerals	mol m^{-2}		CIW (Harnois 1988)	%
	Si-in-minerals	mol m^{-2}		PIA (Fedo et al. 1995)	%
	Al-in-minerals (not Gibbsite)	mol m^{-2}		WI (Price et al. 1991)	-
Minerals	Gibbsite	mol m^{-2}		CPA (Buggle et al 2011	%

***** also in ectorganic matter.

****** also as mmol m^{-2} in ectorganic matter.

Part II: Model concepts and processes

Model descriptions and applications have been published in

- Finke, P.A. and J.L. Hutson. 2008. Modelling soil genesis in calcareous löss. Geoderma 145 :462-479. (SoilGen1)
- Finke, P.A. 2012. Modeling the genesis of Luvisols as a function of topographic position in loess parent material. Quaternary International 265: 3-17. (SoilGen2)

II.1 Process coverage and structure

Table 3 summarizes how the Jenny (1941) factors of soil formation are linked to SoilGen and what existing model (LEACHC), model description (RothC 26.3) or new functionality was implemented to model the soil processes influenced by the Jenny factors. Reference is made to Hutson (2003a,b) and to Coleman and Jenkinson (2005) for detailed descriptions of the LEACHC and RothC 26.3 models.

Table 3 Process coverage of SoilGen model versions

Environmental factor		**Process coverage [1]**	
		SoilGen1 [5]	**Added in SoilGen2**
CLimate	Temperature	Heat flow [2]	
	Precipitation: water	Water flow [2]	
	Precipitation: solutes	Solute flow [2]	
	Evaporation	Evapotranspiration [2]	
Organisms	Vegetation	C-cycle [3], CO$_2$-production and diffusion, Selective cation uptake/release, Root distribution	
	Fauna	Bioturbation	
	Human influence	Fertilization [2]	Plowing
Relief	Slope	Runoff [2]	
	Erosion / Sedimentation		Removal or Addition of top layers
	Local variants of T, P, E		Heat/water/solute flow with P, E as f(exposition)
Parent material	Texture	Chemical Dissolution/Precipitation [2], Bioturbation, C-cycle	Physical weathering, Clay migration, CEC as f(clay, OC),
	Mineralogy		Cation release by weathering of primary minerals [4]
	Solute and exchange chemistry of Ca, Al, Mg, K, Na, …	Chemical equilibria [2] Cation exchange equilibria [2]	Arrhenius temperature correction Al-Gibbsite equilibrium, Exchangeable acidity, Base saturation
Time	Change of boundary conditions	Annual update of all boundary conditions	

[1] either simulated, as boundary condition or as initial state)

[2] based on LEACHC (Hutson, 2003)

[3] based on RothC26.3 (Coleman and Jenkinson, 2005)

[4] based on NUCSAM (Kros, 2002)

[5] Finke and Hutson (2008)

All though the temporal extent is large (X000 years), the time steps within the model may be small, depending on the dynamics of the processes. Most processes are modelled on the sub-day timescale. Fig. 14 gives a process order diagram within one year. The flow of water and solutes is computed with a maximum time step of 0.05 day, this is reduced in case of very large or small fluxes. CO$_2$-diffusion is computed with time steps of 0.1 day, which is reduced in case of numerical instability. The recalculation of chemical equilibriums is done once daily or every 80 water flow time steps, whichever value is smaller. The physical redistribution of soil matter due to dissolution/precipitation and bioturbation is calculated once per year since these changes are slow.

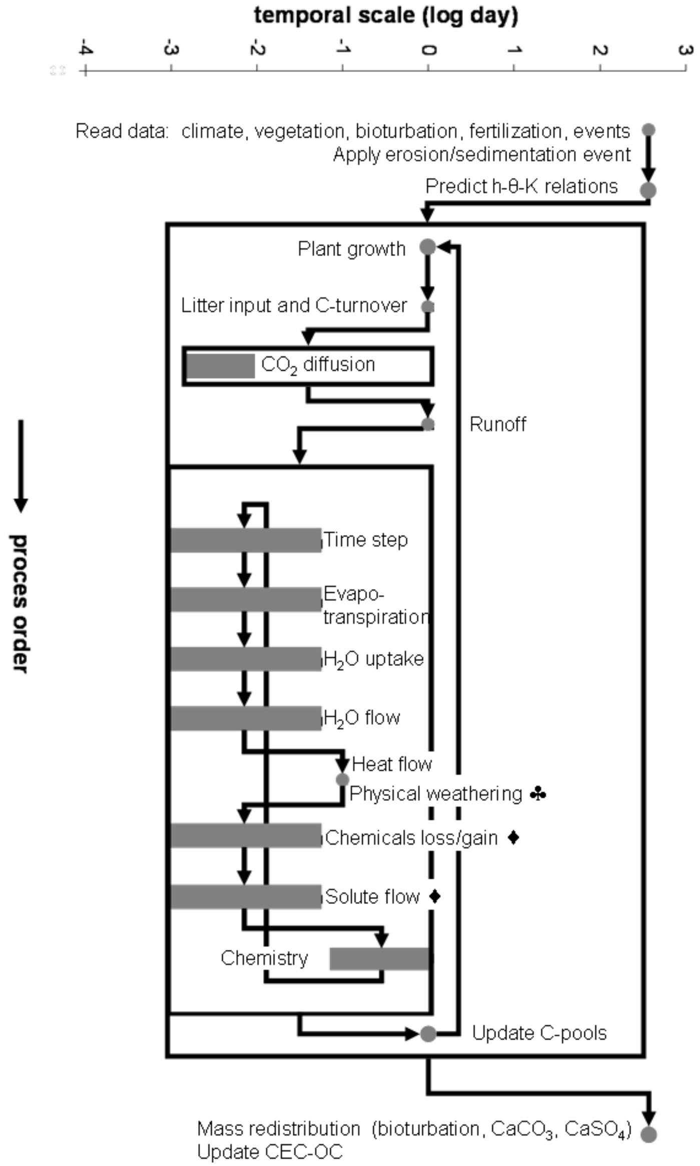


Fig. 14 Process flow (arrows) and temporal scales (solid boxes or dots) of the sub-processes in SoilGen2 in each one year. Open boxes indicate groups of processes that are repeated at daily of annual extent.

II.2 Model components

II.2.1 Flow of water, solutes, heat and CO2

The flows of water, solutes and heat are simulated using the LEACHC code. Below follows a brief characterization of the model. For details reference is made to Hutson (2003a).

Water flow is modelled by the Richards' equation for transient vertical flow:

$$\frac{\partial h}{\partial t}C(\theta)=\frac{\partial}{\partial z}\left[K(\theta)\frac{\partial H}{\partial z}\right]-U(z,t) \qquad \text{-1-}$$

Where *C(θ)* is the differential water capacity $\partial\theta/\partial h$, *θ* is the volumetric water content (m^3/m^3), *h* is soil water pressure head (Pa.10), *K(θ)* is hydraulic conductivity (m.10^{-3}/d), *H* is hydraulic head (Pa.10) and *U(z,t)* is a sink term representing water lost at depth *z* and time *t* by transpiration. LEACHC solves the Richards' equation by application of finite differencing techniques. Steps taken are the rearranging and subsequent application of the Crank-Nicholson implicit method to estimate pressure heads at the end of the time step and application of a Gaussian elimination method (Thomas algorithm) to simultaneously solve the equations at all nodes in the soil profile. Note that all node distances are equal (often: 50 mm). The upper and lower nodes are outside the soil and are used to impose the upper boundary conditions for evaporation and infiltration and the lower boundary condition. The lower boundary condition is chosen by the model to cope with strong variations in the precipitation and evaporation regime over the last thousands of years: zero flux in case of an annual precipitation deficit and free drainage in case of an annual precipitation surplus. Deficit or surplus is determined at the start of the year by surplus=(P-P_{int})-PET, where P=precipitation (corrected for slope exposition if necessary), P_{int}=evaporation of intercepted rain (an input fraction of P, per vegetation type) and PET=Potential Evapotranspiration (corrected for slope exposition if necessary). The modified Campbell equations (Hutson & Cass) are used to obtain values for the differential water capacity and hydraulic conductivity from values of θ or h. However, input is in the form of Van Genuchten (1980) parameters (either measured or estimated by the Hypress pedotransfer function). The Van Genuchten parameters α, θ_{res}, θ_{sat} and m are used to calculate the a and b parameters of the Campbell equations (Campbell et al., 1977; Hutson, 2003a,b), according to a method by Sommer and Stöckle (2010); these are also needed to calculate gas diffusion. To account for the effect of temporarily frozen soils, the hydraulic conductivity is recalculated for soil temperatures below 0ºC using an impedance factor Ω (Lundin, 1989): $K=10^{-\Omega}$ *K. Ω was assigned the value 4.

Heat flow and temperature distribution are modelled by (Hutson, 2003a; Tillotson et al.,1980):

$$\frac{\partial T}{\partial t} = \frac{\partial}{\partial z}\left(\frac{K_t(\theta)}{\beta}\cdot\frac{\partial T}{\partial z}\right) \qquad \text{-2-}$$

Where T is temperature (ºC), $K_t(\theta)$ is thermal conductivity ($J.m^{-1}.s^{-1}.ºC^{-1}$) calculated at θ using the method presented by Wierenga et al. (1969) and β is the volumetric heat capacity determined from $\beta = \rho_s C_s + \theta C_w \rho_w$ with ρ_s and ρ_w the bulk densities of solids and water (1000 kg m^{-3}) respectively, C_s the gravimetric heat capacity of solids (840 J kg^{-1} $ºC^{-1}$) and C_w the gravimetric heat capacity of water (4200 J kg^{-1} $ºC^{-1}$). Equation 2 is solved for all profile nodes using an implicit central difference scheme with a Gaussian elimination method. The upper boundary condition is satisfied by a sinusoidal daily air temperature fluctuation derived from (input) daily averages and amplitudes of temperature. The lower boundary condition is a heat reservoir: the deepest compartment is assigned a thickness of 2 meter and there is a zero heat flux bottom boundary condition.

The flow of soluble matter is simulated using a finite difference approximation to the convection-dispersion equation (CDE) for each soluble compound:

$$\frac{\partial(\theta C)}{\partial t} = \frac{\partial}{\partial z}\left[\theta D(\theta,q) - qC\right] \pm \Phi \qquad \text{-3-}$$

Where C is the solute concentration (kg m^{-3}), $D(\theta,q)$ is the dispersion coefficient (mm^2 d^{-1}) being the combined effect of mechanical dispersion and aqueous diffusion, q is the water flux (mm d^{-1}) and Φ is a source or sink term (kg m^{-3} d^{-1}) representing the plant uptake or release by mineralization of organic matter. Note that solute concentrations depend on chemical equilibriums and partitioning between the exchange and solute phase (cf). A central-difference Crank-Nicholson approach is applied while solving eq. 3 to avoid numerical dispersion. Upper boundary conditions allow for surface infiltration, evaporation and zero flux, while the lower boundary condition depends on that for water flow: zero concentration for zero flux and constant concentration for free drainage.

The flow of CO_2 is assumed to be diffusive and is simulated by an explicit numerical solution to the gas regime equation:

$$\varepsilon \cdot \frac{\partial c}{\partial t} = D(T)_{gs} \cdot \frac{\partial^2}{\partial z^2} + P(z,t) \qquad \text{-4-}$$

Where ε is the air-filled porosity, c is the CO_2-concentration (partial pressure) in the soil air, P(z,t) is the CO_2 production in each soil compartment and $D(T)_{gs}$ is the gas diffusion coefficient in soil (m^2 s^{-1}), estimated by (Moldrup et al. 2000):

$$D(T)_{gs} = D(T)_0 \cdot (2\varepsilon_{100}^3 + 0.04\varepsilon_{100}) \cdot \left(\frac{\varepsilon}{\varepsilon_{100}}\right)^{2+3/b} \qquad \text{-5-}$$

with ε_{100} is the air-filled porosity at -100 cm pressure head, b is the Campbell soil water retention parameter (see above) and $D(T)_0$ is the gas diffusion coefficient in free air obtained by (assuming a constant pressure of 101.3 kPa):

$$D(T)_0 = 1.39\times10^{-5}\cdot\left(\frac{T+273.16}{273.16}\right)^{1.75} \qquad \text{-6-}$$

With T in ºC.

II.2.2 Plant related processes

SoilGen distinguishes 4 vegetation types (grass/scrub, conifers, deciduous wood and agriculture), each of which is characterized by: (i) a rooting density function, (ii) preferential cation uptake controlled by fixed cation ratios in the plant, (iii) C-decomposition rates, (iv) the fraction of dead C that enters the soil system as leaf and root litter, (v) the distribution of litter input over the year and (vi) a partitioning coefficient to fraction the fresh litter in resistant and decomposable components. Furthermore, the yearly amount of produced C-litter is input to the model (and normally depends on the vegetation). The belowground C-cycle (visualized in Fig. 15) is modelled according to the concepts of the RothC 26.3 model (Jenkinson and Coleman, 1994). Dead plant material, split in an ectorganic (leaf litter) and endorganic (root litter) part (Kononova, 1975), is divided into a resistant and a decomposable fraction according to a vegetation-dependent ratio. Both fractions decompose into biomass, humus and CO_2 at rates that are determined by the fraction that is decomposing, soil temperature, soil moisture deficit, soil cover fraction and the time increment. Biomass and humus continue to decompose into biomass, humus and CO_2 in next time steps. For a detailed description and values of rate factors reference is made to Coleman and Jenkinson (2005). The C-submodel is applied at daily intervals, where the produced CO_2 enters the gas regime equation (eq. 4). The CO_2 profile at the end of each day gives the pCO_2 values for the chemical equilibriums for this day.

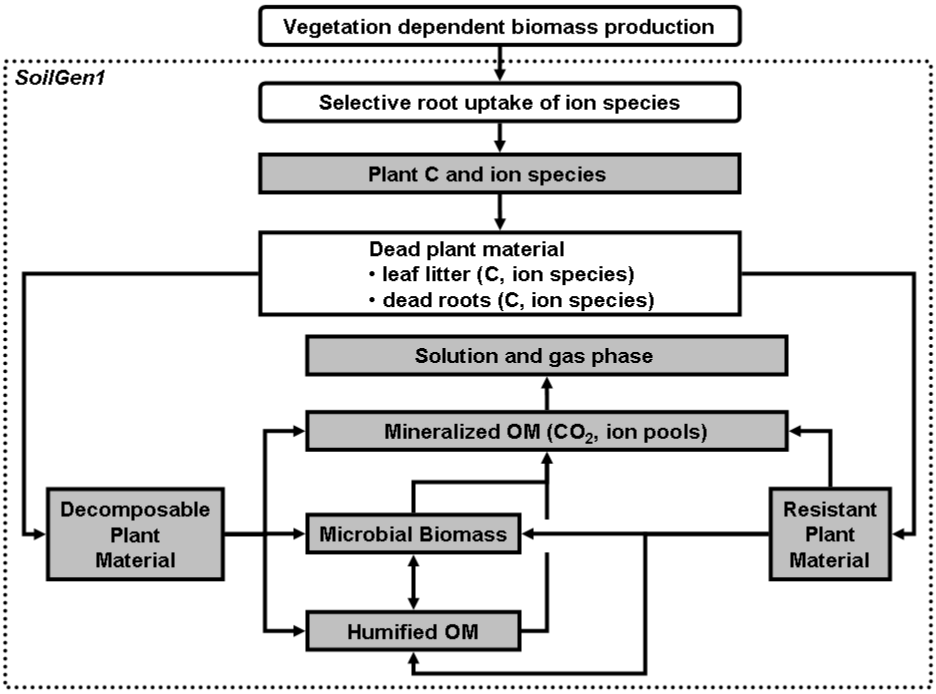


Fig. 15 C-cycling in SoilGen (based on Coleman&Jenkinson, 2005). Greyshaded boxes indicate pools, rounded boxes indicate processes and the rectangular white box is for conceptualization only

Uptake of the cations Ca, Mg, K, Na and Al by vegetation occurs via the transpiration stream and is forced to reflect the relative proportions of those elements measured in the plant (stable vegetation assumption). Each vegetation is characterized by a content of the basic cations Ca, Mg, K, Na and Al. Typical contents for agriculture (Barley) were obtained from Wyszkowski et al. (2006), for grass/scrub from Thompson et al. (1997), and for coniferous and deciduous wood from Navrátil (2003). These contents are rescaled to cation mass fractions summing up to 1 (Table 4). The calculation of cation and anion uptake per soil compartment then proceeds as follows:

1. A general cation uptake factor is calculated as the minimal occurring ratio between one of the 5 cations actually present in the solution in the soil compartment and the associated cation mass fraction.
2. An uptake fraction for each cation in the soil compartment is calculated by the multiplication of

the general cation uptake factor and the cation-specific mass fraction. This fraction is applied to this cation in solution in the soil compartment to calculate actual plant uptake. If one of the cations has 0 concentration, non-preferential uptake is assumed.

3. The uptake charge from the soil compartment in the transpiration stream is calculated, and it is checked if the sum of the anion charges of Cl, SO_4, CO_3, HCO_3 in solution in the soil compartment can balance this charge. There is no preferential uptake of any anion. If there is no charge balance, a correction ratio to the cation uptake is calculated satisfying 0-charge of total uptake.

The absolute uptake in one time step is thus limited by the element concentrations in the rooted soil compartments, by the transpiration flux and by a charge balance condition.

Table 4 Relative concentrations of Ca, Mg, K, Na and Al in 4 vegetation types

Vegetation	Source	Relative concentration (-)				
		Ca	Mg	Na	K	Al
Coniferous forest	Navrátil, 2003	0.752	0.128	0.004	0.093	0.023
Deciduous forest	Navrátil, 2003	0.481	0.226	0.025	0.265	0.004
Grass/scrub	Thompson et al., 1997	0.271	0.164	0.004	0.560	0.001
Agriculture	Wyszkowski et al., 2006	0.132	0.075	0.013	0.759	0.021

Cations are stored in the same plant biomass pools distinguished in the C-cycle, and those cations entering the mineralized (CO_2) pool actually enter the soil solution either at the soil surface (leaf litter) or in the rooted compartments (root turnover).

SoilGen keeps track of the ^{14}C age of the soil organic matter by assigning fresh organic matter (litter inputs) the $\Delta^{14}C$ value (user) input per year BP, tracing ^{14}C activity while C is transferred between the pools while also applying annual radioactive decay. The $\Delta^{14}C$ of the soil organic matter is output, as are ^{14}C activity ratios to total C in each one of the pools. Also the convention 14C age is calculated in each simulation year by

Age_{yearAD}=(-5568/ln(2))*(ln((((delta14c-1)*1000)/1000)+1)+((yearAD-1950)/(5730/ln(2))))

II.2.3 Chemical processes

The chemical phases simulated in SoilGen are depicted in Fig. 16. Processes that influence the composition of the solution phase are described briefly hereunder.

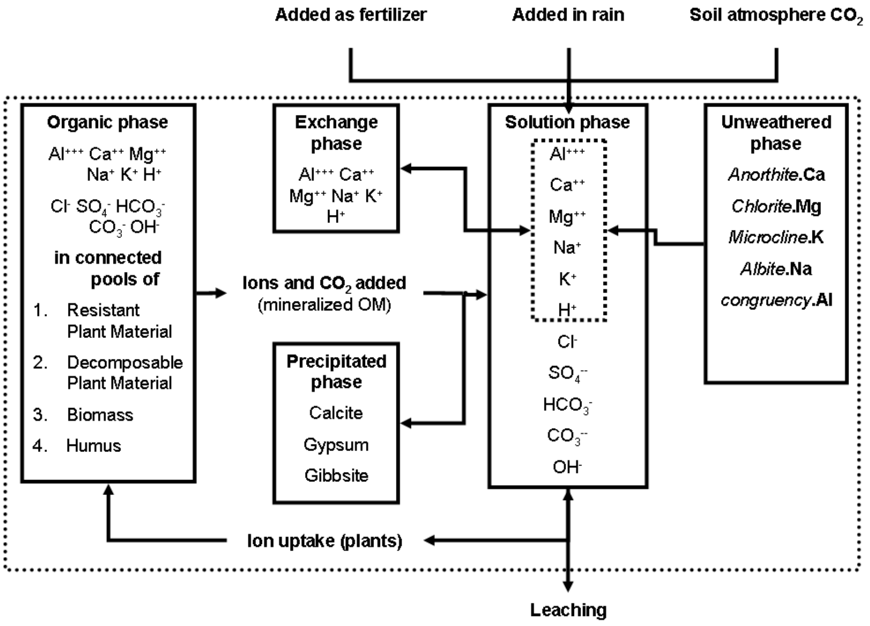


Fig. 16 Ions and chemical phases in SoilGen

II.2.3.1 Weathering of primary minerals

The description below refers to SoilGen versions up till (inclusive) 2.24.

The weathering flux FX ($mol_c.ha^{-1}.y^{-1}$) of the cations Ca, Mg, K and Na from primary silicate minerals to the soil solution is described by (Van Grinsven, 1988):

$$FX = \rho * T * kX * cH^{\alpha(X)},$$

where ρ is dry soil bulk density ($kg.m^{-3}$), T is thickness soil compartment (m), kX is a weathering rate constant ($m^3.mol_c^{-1}.y^{-1}$) for cation X, cH is the H concentration ($mol_c.m^{-3}$) and $\alpha(X)$ (-) is a parameter. Cation dependent values for kX and $\alpha(X)$ were taken from De Vries (1994) and Kros (2002, p.43). The weathering flux of Al from primary minerals is modelled as the result of congruent weathering of Anorthite, Chlorite, Microcline and Albite releasing respectively the Ca, Mg, K and Na:

$$FAl = 3 * FCa + 0.6 * FMg + 3FK + 3FNa$$

After entering the soil solution, Al-concentrations are equilibrated with gibbsite at the occurring soil pH.

II.2.3.2 Exchange phase

Soil CEC is partly determined by the mineral surfaces, partly by organic matter. As organic matter content may change and clay may migrate, the CEC may change. A 2-domain CEC model was formulated, in which the initial total CEC of the soil is partitioned into a part attributable to the initial organic carbon (OC) and another part attributable to the mineral fraction. This partitioning was done using the regression equation by Foth and Ellis (1997: p.57) based on 12,000 data sets to identify contributions of OC (%) and clay (%):

$$CEC = f * (32 + 36.7 * OC + 1.96 * Clay),$$

where CEC in $mmol^+$/kg soil and *f* is a factor matching the empirical CEC after Foth and Ellis (1997) to the initial CEC in the simulated pedon. The CEC_{OC} is henceforth a variable determined by $f*36.7*OC$ and the CEC_{clay} follows the evolution of the clay content in any layer as determined by clay migration (cf. next section) and physical weathering. This approach simplifies reality as it does not take into account the possible effect of pH-change on CEC.

II.2.3.3 Equilibration

The solution phase is brought in equilibrium with the precipitated and exchange phases by satisfying the following thermodynamic equilibriums: (i) Henry's Law constant for CO_2, (ii) the dissociation constant of H_2CO_3, (iii) the dissociation constant of water, (iv) the solubility constants of gypsum, calcite and gibbsite, (v) ion pair stability constants for the species named in Fig. 16, (vi) Gapon selectivity constants for the exchange/solution phase equilibriums for Ca-Mg-Na-K.
Calculation of the equilibrium distribution is done via an iterative procedure, which is an expansion of Hutson (2003a) to (additionally) include

- Gibbsite-Al-pH equilibrium ;
- Al and H as exchangeable cations;
- Modification of all chemical constants for temperature (Arrhenius correction).

The equilibration is done via the next procedure:

(i) for the initial values of the pH and elements in solution, the ionic strength is calculated, which is used to calculate activity coefficients for all ion species and equilibrium constants using the Davies' relationship (Stumm and Morgan, 1970);
(ii) the levels of HCO_3^-, CO_3^{2-}, $CaSO_4$, $Al(OH_3)$ and $CaCO_3$ are calculated using pH and pCO_2 (which is daily adjusted);
(iii) the cation levels are partitioned between the solution and the exchange phases according to the Gapon equations;
(iv) Steps (i) to (iii) are repeated until the result is stable;
(v) With a stable result, the charge balance is checked, and if an unbalance exists, pH is adjusted and the procedure restarts at step (i).

The search for an optimal value of pH (in terms of charge balance) is done with a bisection method. For a detailed description of the calculations involved, reference is made to Hutson (2003a).

II.2.4 Processes causing redistribution of soil phases

II.2.4.1 Bioturbation

The processes considered in SoilGen that are able to change the distribution of solid phase and liquid phase components are bioturbation, tillage and mass changes due to accumulation or mineralization of OC, dissolution or precipitation of calcite and gypsum, physical weathering and clay transport. Erosion and sedimentation are considered in the sense that these processes can remove or add entire compartments at the top of the soil profile. Central assumption in SoilGen is that the volume of each soil compartment is constant over time, all though in reality a volume of soil may lose porosity (collapse) due to the removal of calcite, or may gain porosity due to biological activity. Thus, in the terminology of Brimhall and Dietrich (1987) a strain equal to 0 was assumed. The errors thus introduced do not affect calculated mass percentages, but may have some influence on soil physical characteristics.

Redistribution of mass by bioturbation is done in 2 steps:

(i) The percentage of the mass subject to vertical redistribution by soil meso- and macrofauna in each compartment is determined. Currently, this percentage is input and was made to vary over the Holocene time extent with the vegetation, climate and soil depth. Whole-soil values of bioturbation for different vegetations from Gobat et al. (1998, p.122) were taken as reference. Bioturbation mass percentages of all mineral pools (clay, silt, sand, including calcite and gypsum), soil water and elements in solution and OC-pools are put in the vertical mixing pool. In this pool, values are averaged and masses are re-assigned to the bioturbated soil compartments according to the bioturbation mass percentages.

(ii) For each bioturbated compartment, the bioturbated mass is mixed with the non-bioturbated mass to obtain one set of soil properties per soil compartment.

Tillage is considered an extreme form of bioturbation, where the mass % involved in turbation is set to 50% (Ullrich and Volk, 2009) over the plowing depth (input) per default, but may be changed via the events.txt file.

An additional effect of bioturbation is the increasing gas diffusion. Singer et al. (2001) measured a CO_2-diffusion of $5x10^{-4}$ cm^2/s in the absence and $4.45x10^{-3}$ cm^2/s in the presence of earthworms. This factor 8.9 increase of $D(T)_{gs}$ (eq. 5) is applied to those compartments with bioturbation.

II.2.4.2 Changes in soluble compounds (calcite and gypsum)

Mass lost or gained due to the dissolution or precipitation of calcite and gypsum is added to the total mass in any compartment, thus affecting bulk density and porosity.

II.2.4.3 Physical weathering

Physical weathering is the process that breaks up soil particles by strain caused by temperature gradients associated with variations in thermal expansion inside the particle, by ice growth or growth of other crystals of larger size than the porosity permits. The net effect of physical weathering is a reduction in grain size. Gradually, this produces material in the clay fraction that may be moved by clay migration. Recently, Minasny and McBratney (2001) developed a mechanistic model to estimate soil production by physical weathering of bedrock as an exponential decline function of soil thickness, but this model does not predict textural change. Salvador-Blanes et al. (2007) modelled fragmentation of soil particles as a probabilistic process, whereby the resistance to fragmentation is a function of soil depth, thus mimicking the effect of decreasing temperature fluctuations with increasing soil depth. Because of the current scope on unconsolidated materials, physical weathering is modelled as a probabilistic process as by Salvador-Blanes et al. (2007) and like suggested by Takeshi et al. (1999), but with a clear connection to soil temperature gradients. The model divides the fine earth fraction in particle size classes with boundaries at 2048-1024-512-256-128-64-32-16-8-4-2 µm. These class boundaries are chosen because these are powers of 2. It is assumed that all particles are cubes with a ribbon size halfway between the class limits: 1536, 768, 384, 192, 96, 48, 24, 12, 12, 6, 3, and 1 µm. Each particle needs to be split in half 7 times to obtain 8 equally sized particles in the next smaller particle size class. This splitting of a particle is assumed to be a probabilistic Bernoulli process, where the splitting probability depends on the temperature gradient over a certain time interval *dt*:

$$P_s = \begin{cases} P_{s,\max} & if \ \dfrac{dT}{dt} > B \\ \dfrac{P_{s,\max} * \dfrac{dT}{dt}}{B} & if \ \dfrac{dT}{dt} \le B \end{cases}$$

Where $P_{s,max}$ is the maximal split probability and B is a threshold temperature gradient over dt where P_s becomes maximal.

The expected number N of potential splitting events needed to achieve m=7 successful splits assumedly follow the negative binomial distribution and are estimated by:

$$E(N) = {}^{m}\!/\!_{P_s}$$

Thus, the number of grains in any particle size class *i* that is split in *dt* is given by the number

$$S_{i,dt} = \min(k_{i,t-dt}\,,\ {k_{i,t-dt}}/{E})\,,$$

where $k_{i,t-dt}$ is the number of grains in particle size class at the start of *dt*, and

$$k_{i,t} = k_{i,t-dt} - a * S_{i,dt} + b * 8 * S_{i-1,dt}\,,$$

where *a* =0 for the clay fraction (*i* =11) and a =1 else; *b* =0 for the coarsest sand fraction (*i* =1) and *b* =1 else.

In most applications, the value of *B* was fixed to 1 ºC.h^{-1} and $P_{s,max}$ was subject to calibration (Finke, 2012).

II.2.4.4 Clay migration

Clay migration is initiated at the surface by splash detachment, which brings part of the clay in the top soil compartment in the dispersed state. In all compartments, the amount of dispersed clay depends on how much the salt concentration falls below a threshold value. This is re-evaluated at the start of each time step. Transport of the dispersed clay fraction and associated exchangeable cations during this time step is modelled like solute transport with the Convection-Dispersion Equation but with particle filtering as an additional sink term.

Splash detachment is simulated following the approach by Jarvis et al. (1999) with modifications as their model was intended for agricultural soils and thus did not include the reducing effect of a humus profile on splash detachment (c.f. step b) nor the effect of bioturbation (cf. step c). The mass balance of dispersible particles at the surface layer is given by:

$$\frac{dA_s}{dt} = -D + P\,,$$

where A_s is the mass of dispersible particles at the soil surface (g.m^{-2}), *D* is splash detachment rate (g.m^{-2}.h^{-1}) and *P* is the replenishment rate (g.m^{-2}.h^{-1}).

The following steps are taken to calculate mass balance components:

a. Initialization of pools of clay, dispersible clay in the upper 1 mm and in the whole top soil compartment (usually 50 mm). The maximal % of dispersible clay (DC_{max}) is estimated with CEC (mmol $^+$/kg soil), OC (%) and clay content (%) using the regression equations 3.1 and 3.2 of Brubaker et al. (1992):

$$DC_{max} = \begin{array}{ll} 0.635 * clay & \text{if } (\text{CEC} - 3 * \text{OC})/\text{clay} <= 0.4 \\ 0.340 * clay & \text{if } (\text{CEC} - 3 * \text{OC})/\text{clay} > 0.4 \end{array}$$

The initial value of the dispersible clay pool, DC_s, is set equal to DC_{max}. The initial value of A_s is then calculated by

$$A_s = DC_s * \rho * 0.01\,,$$

with ρ for dry soil bulk density (kg.m^{-3}) and 0.01 for unit conversion.

b. For each rainfall event, *D* is estimated by

$$D = k_d * E * R * (1 - sc) * DC_s\,,$$

where k_d is the soil detachability coefficient (g.J^{-1}) set to the value 15 as calibrated by Jarvis et al. (1999) and *sc* (-) accounts for the proportion of the soil covered by ground vegetation or the humus profile. *D* is also corrected each time step for the fraction of the soil surface that is actually hit by raindrops (depending on the size of the time step and the rainfall intensity). Furthermore, *R* (mm.h^{-1}) is rainfall intensity, DC_s is the amount of readily available dispersible particles (g.g^{-1} soil) at the surface 1 mm with initial value equal to DC_{max} in step a, and *E* (J.m^{-2}.mm^{-1}) is kinetic energy of the rainfall calculated using the relation from the revised universal soil loss equation (Brown and Foster, 1987):

$$E = 29 * \{1 - 0.72 * \exp(-0.05 * R)\}$$

c. The replenishment rate *P* is calculated according to Jarvis et al. (1999):

$$P = k_r * \left(1 - \frac{DC_s}{DC_{max}}\right),$$

where k_r is the replenishment rate coefficient (g.m^{-2}.h^{-1}) set to the value 0.1 as calibrated by Jarvis et al. (1999). The value of *P* is restricted so that it cannot exceed the amount present in the surface 1 mm layer after bioturbation.

The fraction of clay in a transportable dispersed state *fDC* in every soil compartment is calculated by:

$$fDC = \{1-(SC/CSC)\} * \theta_{macro} * fVC \text{ ,}$$

where *SC* is the total electrolyte concentration ($\text{mmol}_c.\text{dm}^{-3}$ water), which is calculated by the model per time step and *CSC* ($\text{mmol}_c.\text{dm}^{-3}$ water) is the critical salt concentration at which soil clay mixtures stay flocculated. Also *CSC* is calculated by the model, using simulated soil parameters and a regression relation based on experimental data from Goldberg and Forster (1990). θ_{macro} is the volumetric water fraction (m^3 water.m^{-3} soil) in macropores and *fVC* is the fraction of the soil volume taken by clay. $\theta_{macro} * fVC$ accounts for the clay fraction that is in contact with rapidly flowing water in macropores. θ_{macro} is estimated from the water retention characteristic at a pressure head *h* (hPa) near saturation, and *h* was subject to calibration. It will henceforth be indicated as $h(\theta_{macro})$.
The removal of particles from suspended transport in soil water by filtering (*F*, $\text{g.m}^{-3}.\text{h}^{-1}$) is calculated with (Jarvis et al., 1999):

$$F = f_{ref} * v_{ref}{}^{n} * v^{1-n} * c * \theta \text{ ,}$$

where f_{ref} (m^{-1}) is a reference filter coefficient, v_{ref} (m.h^{-1}) is the pore water velocity at which f_{ref} is measured. Values of 2 m^{-1} at 0.1 m.h^{-1} were taken from Jarvis et al. (1999). Furthermore, *v* is the current pore water velocity, *c* is the particle concentration (g.m^{-3} water) and *n* is an empirical exponent. In SoilGen, *c* is a vector containing the dispersible and transportable clay calculated using eq. 14, but also the associated exchangeable cations Ca, Mg, Na, K, H and Al. For values of *n* of 0 and 1, respectively, this equation reduces to the equation for clean bed filtering or the equation for the sink term in reactive transport models. Values of *n* between 0 and 1 will give a loss by filtering that increases with higher pore water velocities in natural structured porous media. Such results were predicted theoretically (Song and Elimech, 1993) and were also experimentally derived (Kretschmar et al., 1997). Jarvis et al. (1999) found that particle leaching was highly sensitive to parameter *n* and obtained a value of 0.7 by calibration. As this sensitivity was confirmed in experimental runs with SoilGen2, the value of *n* was subjected to calibration (Finke, 2012).

II.2.4.5 Effects on soil physical parameters

Mass changes, as induced by bioturbation but also by changes in OC due to decomposition of organic matter, changes in calcite or gypsum content due to dissolution or precipitation and changes in texture due to physical weathering and clay migration in all compartments are used to (annually) recalculate mass percentages of the solid phase components OC, Clay, Silt and Sand. Subsequently, bulk density and porosity are recalculated and the Hypres pedotransfer function (Wösten et al., 1999) is applied to recalculate the Van Genuchten parameters based on texture, OC and bulk density.

II.3 Slope effects on precipitation and potential evapotranspiration

It has long been recognized that the size and bearing of a slope in combination with the speed and bearing of the wind carrying the precipitation affect the net precipitation received by a unit area (Lyles et al., 1969). The net potential evapotranspiration is affected by slope properties as well. To calculate the net effect of wind speed, slope angle and their bearings, first the wind speed in the direction of the slope is calculated:

$$V_2 = V_1 * \cos(\delta - \gamma) \text{ ,}$$

where V_2 is the wind speed in slope direction, V_1 is the wind speed in wind direction, δ is the upslope bearing and γ is the wind bearing.
The diversion angle β from vertical rainfall is induced by wind and is calculated according to Mauersberger (2001, p.30):

$$\beta = abs(\arctan(V_2 / v_r)) \text{ ,}$$

where v_r is the mean fall velocity of raindrops (e.g. estimated from rainfall intensity, Schmidt, 1992, p.412). In SoilGen2 v_r has the fixed value 5 m/s.
The rainfall R_2 on a sloped area of 1 m^2 with slope angle α, wind effect β and their bearings δ and γ respectively, is then given by (e.g., Erpul et al., 2008):

$$R_2 = R_1 * (1 - X * \tan(\beta) * \tan(\alpha) * \cos(\delta + X\gamma)) \text{ ,}$$

where R_1 is the precipitation at the horizontal plane and X is an exposition indicator, with values 1 for windward and -1 for leeward exposition.
The net potential evapotranspiration PE_2 is calculated by a correction of the measured PE_1 for latitude, slope angle and slope azimuth. It was assumed that potential evapotranspiration responds linearly to differences in incoming radiation for different slopes. Then, the correction factor is the ratio between

the potential solar radiation on a horizontal surface at given latitude, summarized for one year, and the potential solar radiation on a slope α with bearing δ converted to map area for the same period and latitude. This ratio was calculated with an implementation of the algorithm developed by Swift (1976). This correction factor is however only applied to short vegetations (grassscrub and agriculture) because the effect of exposition on a forest floor is assumed to be minimal.

II.4 Calibration, verification status and applications

II.4.1 Calibration and verification status

The following activities have contributed to the verification status of SoilGen:

- The water flow, C-cycling and chemical weathering routines have been tested as part of the models from which they were taken, cf. Addiscott and Wagenet (1985), Dann et al. (2006), Jabro et al. (2006), Jalali and Rowell (2003), Kros et al. (1999) and Smith et al. (1997).
- The process of decalcification has received special attention in Finke and Hutson (2008) and Finke (2012) via calibration of the Calcite dissolution constant by comparison with a meta-model by Egli and Fitze (2001). Results indicate that the model is fairly well calibrated and the quality of the hydrological inputs determines the adequacy of the model predictions.
- The processes of clay migration and physical weathering were provisionally calibrated (Finke 2012) resulting in the conclusion that the development of E and Bt-horizons can be modelled with SoilGen although predicted clay contents in Bt-horizons are clearly lower than measurements. A more thorough calibration has been done since then (Finke et al., 2015).
- The C-submodel has been verified for temperate deciduous forests in Belgium and China (Yu et al., 2013) by a combination of sensitivity analysis and calibration with measurements.
- In Finke (2012), the adequacy of modeling the depth distribution of clay, silt, sand, OC, pH, calcite, CEC, BS and exchangeable Na, K, Ca and Mg, was tested at 3 different topographic positions. The over-all dissimilarity (all above variables combined) between simulated and measured values (in a range from 0=perfect to 1=totally dissimilar) varied between 0.23 and 0.28 (Finke, 2012). Best values were obtained for OC, CEC and texture.

Reference is made to Finke and Hutson (2008), Finke (2012), Yu et al. (2013) and Finke et al. (2015) for precise quantification of the adequacy of modelled processes in SoilGen.

II.4.2 Applications

SoilGen has been applied in a number of case studies:

- Finke and Hutson (2008) applied it to evaluate the effect of late-glacial to Holocene climate transitions on Hungarian and Belgian loess soils with special emphasis on the effect of bioturbation (climosequence research);
- Finke (2012) applied it to a toposequence in loess in Belgium;
- Sauer et al. (2012) applied it on two chronosequences in marine terraces in Norway;
- Finke et al. (2013) applied it to test soil variability patterns in highly variable loess soils with special emphasis on terrain controls on soil formation;
- Zwertvaegher et al. (2010, 2012) applied it in a cover sand area to reconstruct land characteristics and land qualities at prehistoric times for archaeological land evaluation.

Ongoing studies imply

- calibration and application on Holocene palaeosoils in the Chinese loess with special emphasis on the soil C;
- application on agricultural scenarios in France.

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Appendix 1: Example soil data input file (LeachC)

Comments added in grey part; file in white part of table. Blue marked text should not be changed. Yellow marked text can be changed via the user interface (see p.9). Red marked text can be changed in this file and will be applied for all simulated years.

```
ALLsoil0 < DOS Filename, 8 characters with no extension. Used in batch runs (started as LEACHC<filename).
--------------------------------------------------------------------------
                      LEACHC SALINITY DATA FILE.
A value must be present for each item, although it may not be used in the
simulation.  The file is read free format with blank delimiters. Preserve
division and heading records.  The number of depth segments may be changed.
**************************************************************************************************************
 1      <Date format (1: month/day/year;  2: day/month/year).  Dates must be 6 digits, 2 each for day, mo, yr.   Do not change
 010199 <Starting date.  No date in the input data should precede this date.                                     Do not change
 123199 <Ending date or day number.  The starting date is day 1. (A value <010101 is treated as a day number).   Do not change
 0.05   <Largest time interval within a day (0.1 day or less).                                                   Via GUI
 1      <Number of repetitions of rainfall, crop and chemical application data.                                  Do not change
 15  <Profile depth (mm), preferably a multiple of the segment thickness.                                        Via GUI
 50     <Segment thickness (mm).  (The number of segments should be between about 8 and 30.                      Via GUI
 2      <Lower boundary condition: 1:fixed depth water table; 2:free drainage, 3:zero flux 4:lysimeter.          ProgrDecision
 1100  <If the lower boundary is 1 or 4: initial water table depth (mm).                                         Not relevant
---------------------------------------------------------------------------
The steady-state flow option uses constant water fluxes during the application
periods specified in the rainfall data table, and a uniform water content
specified here.  Steady-state flow implies a lab column, and crop and evaporation data are ignored.
---------------------------------------------------------------------------
  1     < Water flow: 1: Richards; 2: Addiscott tipping bucket; 3: steady-state.                                 Do not change
  0.4   < Steady-state flow water content (volume fraction); 999: saturated column.                              Not relevant
**************************************************************************************************************
**************************************************************************************************************
 1      <Number of output files: 1: OUT only; 2: OUT + SUM; 3: OUT + SUM + BTC                                   Not relevant
--------------------------------------
--- For the *.OUT file :
 1      <Units for depth data: 1: ug/kg, 2: mg/m2 per segment depth. (Not used in LEACHC, leave as 1)            Not relevant
 1      <Node print frequency (print data for every node (1), alternate nodes (2).                               Not relevant
 2      <Print options: 1 or 2.  Use to specify one of the following options.                                    Not relevant
 5      <Option 1: Print at fixed time intervals (days between prints).                                          Not relevant
 1      <Option 2: No. of prints (the times for which are specified below)                                       Not relevant
 3      <Tables printed: 1: mass balance; 2: + depth data; 3: + crop data                                        Not relevant
 0      <Reset *.OUT file cumulative values each print? 0: No, 1: Yes                                            Not relevant
---------------------------------------
--- For the * .SUM file :
 .05      <Summary print interval (d)  (999 for calendar month printouts)
 0   <Surface to [depth 1?] mm      ( Three depth segments for the                                               Not relevant
 0   <Depth 1 to [depth 2?] mm       summary file. Zero defaults to nodes                                        Not relevant
 0   <Depth 2 to [depth 3?] mm       closest to thirds of the profile)                                           Not relevant
 2   <4th segment: Root zone (1); profile (2); Depth 3 to lower boundary (3)                                     Not relevant
---------------------------------------
--- For the *.BTC (breakthrough) file :
 1.0    <Incremental depth of drainage water per output (mm)                                                     Not relevant
--------------------------------------------------------------------------
-- List here the times at which the *.OUT file is desired for print option 2.
-- The number of records must match the 'No. of prints' under option 2 above.
        Date or    Time of day          (At least one must be specified
        Day no.  (to nearest tenth)      even if print option is not 2)
        --------  ----------------
        123199         .5                                                                                        Not relevant
*************************************************************************
*************************************************************************
                  SOIL PHYSICAL PROPERTIES
-------------------------------------------------------------------------
-- Retentivity model 0 uses listed Campbell's retention parameters, otherwise
-- the desired particle size-based regression model is used.
-------------------------------------------------------------------------
 Soil |                     |Retention|   Starting   |   Roots   | Starting
layer | Clay  Silt  Organic |  model  |theta or pot'l|  (for no  | temp (C)
 no.  |             carbon  |         |(one is used) |  growth)  | (not read in
      |   %     %     %     |         |          kPa | (relative)| LEACHW)
 ---    ----  ----   ----     ------   -----   -----    ------    -----------
  1      12.6 73.4   0.12        5      .3  -1500.      .05         -5.                                          Best via GUI
etcetera                                                                                                         Best via GUI
 30      12.6 73.4   0.12        5      .3  -1500.      .05         -5.                                          Best via GUI
---------------------------------------------------------------------------
   1    < Use listed water contents (1) or potentials (2) as starting values.                                    Autoset to 2
Particle density:  Clay    Silt and sand    Organic matter  (kg/dm3) (to calculate porosity)
                   2.65         2.65              1.10                                                           Best via GUI
***************************************************************************
For a uniform profile: Any non-zero value here will override those in
the table below.
----------------------------------------------------------------------
  0.0  0.0  <Soil bulk density and particle density (kg/dm3) .                                                   Not relevant
 -0.0       <'Air-entry value' (AEV) (kPa).                                                                      Not relevant
  0.0       <Exponent (BCAM) in Campbell's water retention equation.                                             Not relevant
  0   -0.0  <Conductivity (mm/day) and corresponding matric potential (kPa) (for potential-based version of      Not relevant
eq. 2.5).
  0.0       <Pore interaction parameter (P) in Campbell's conductivity equation.                                 Not relevant
  0.0       <Dispersivity (mm).                                                                                  Not relevant
  0.0       <For Addiscott flow: Matric potential (kPa) at field capacity                                        Not relevant
  0.0       <                  : Division between mobile and immobile water (kPa)                                Not relevant
*********************************************************************************************************
 Soil  |  Soil retentivity |   Bulk  |  Match K(h) curve at: | Dispersivity |  For Addiscott flow option:
 segment      parameters   | density |   K    Matric  using  |              |  Field     Mobile/immobile
 no.   |    AEV     BCAM   |         |         potl      P   |              | capacity      threshold
       |    kPa            |  kg/dm3 |  mm/d    kPa          |     mm       |   kPa            kPa
 -----    ------   -----     -------   ----  -----   -----       -----        -------       ---------
   1       -1.      3.       1.30      10    -00.    1.0        100.         -5.0           -200.            } Program
```

```
etcetera                                                                                                          } Decision
  30       -1.      3.      1.30       10     -00.     1.0        100.          -5.0           -200.              } + via GUI
*********************************************************************************************************
*********************************************************************************************************
Runoff according to the SCS curve number approach.  Curve number listed here will be
adjusted by slope. During periods of crop growth, CN2 replaced by value for crop.
(Procedure according to J.R. Williams (1991). Runoff and Water Erosion.
Chap 18, Modeling Plant and Soil Systems, Agronomy 31.)
----------------
 75   <Curve number (CN2).  In LEACHM, water content use to adjust CN2 based on top 20 cm.                       Fixed value
 0    <Slope, %. Used to adjust CN2 according to equation of Williams (1991).                                     Via GUI !
** (Set slope to 0 to bypass the runoff routine.  Runoff owing to profile saturation will still be
accumulated)
*************************************************************************
*************************************************************************
                          CROP DATA
-------------------------------------------------------------------------
  Data for at least one crop must be specified, even if no crop desired.
  For fallow soil, set flag below to 0, or germination past the simulation end date.
-------------------------------------------------------------------------
  1      <Plants present: 1 yes, 0 no.                                                                            ManagedProgram
  1      <No. of crops (>0)                                                                                       ManagedProgram
  -15 <Wilting point (soil) kPa.                                                                                  AdvancedUsers
  -30 <Min.root water potl(kpa).                                                                                  AdvancedUsers
  1.1    <Maximum ratio of actual to potential T.                                                                 AdvancedUsers
  1.05   <Root resistance.                                                                                        AdvancedUsers
---------------------------------------------------------------------  --kg/ha--- ----------
Growth  Perennial  N_uptake              Date or day of          Rel.  Crop    Pan   |  Crop     Min Harvested
1: No   1: Yes    1:to maturity                 Maturity          root  cover  factor | uptake    N  fraction
2: Yes  2: No     2:to harvest  Germ. Emerg.  Root  Cover  Harv. depth fraction      |  N    P   fixed
------  -------   ------------  ------------------------------------ -----  ------  ----   -----kg/ha---- -------
   1       1        1          010199 030199 040199 050199 110199 1.     1       1.      102  20   0    .88       AdvancedUsers
***********************************************************************
***********************************************************************
           INITIAL PROFILE DATA - SOLUBLE CATIONS AND ANIONS (AND DOC)
    -- (can be exchangeable + soluble if exchangeable set to 0) --
     Depth      Ca     Mg      Na      K      Cl     SO4     Alkal.     Al  Org3-  HOrg2- H2Org-    DOC-ignored
    segment                  mmol/l                          mmol-/l                mmol/l          % -fr(BIOM)
     -----    ------ ------ ------ ------ ------ ------    ------ ------ ------ ------ ------ ------
       1      15.910 1.170  0.070  0.070 34.000   0.000    0.300    0.010 0.000   0.000  0.000 0.0100         Best via GUI
Etcetera                                                                                                          Best via GUI
      30      15.910 1.170  0.070  0.070 34.000   0.000    0.300    0.010 0.000   0.000  0.000 0.0100         Best via GUI
----------------------------------------------------------------------
Concentration (mmmol/l) below profile, used with lower boundaries 1 or 5
                0.0     0.0     0.0     0.0     0.0     0.0     0.0     0.0     0.0     0.0     0.0     0.0    Not relevant
 5     < Depth (mm) of water in mixing cell (boundaries 1 and 5 only)                                             Not relevant
***********************************************************************
***********************************************************************
     Depth       Ca         Mg         Na         K         CEC        H         Al
    segment                        mmol+/kg
     ----    -------    -------    -------    -------    -------    -------    -------
      1       68.5900    13.0100    0.7000    1.5000    83.80011    0.0001     0.00001                          Best via GUI
etcetera                                                                                                          Best via GUI
      30      68.5900    13.0100    0.7000    1.5000    83.80011    0.0001     0.00001                          Best via GUI
**************************************************************************
**************************************************************************
             SELECTIVITY COEFFICIENTS         pCO2   Calcite  Gypsum   SELECTIVITY COEFFICIENTS
    Segment  Mg/Ca     Ca/Na      Ca/K         (atm)   (mass fraction)   Ca/Al      Ca/H
     ---- --------- --------- ---------        -----   ------- ------- --------- ---------
      1    0.69820    0.06700   0.03310        0.01000  0.1200   0.0000 0.27416    0.00051                      Best via GUI
etcetera                                                                                                          Best via GUI
      30   0.69820    0.06700   0.03310        0.01000  0.1200   0.0000 0.27416    0.00051                      Best via GUI
**************************************************************************
**************************************************************************
*  CHEMICAL EQUILIBRATION PROCEDURE:
*     Which of the following conditions apply to the initial data:
*  0: Selectivity coefficients are correct.  Recalculate equilibrium composition from sum of solution and
exchangeable.
*  1: Solution and exchangeable cations are in equilibrium, calculate selectivity coefficients.
*  2: Selectivity coefficients and soluble cations are correct, calculate exchangeable cations.
  0         < Enter 0, 1 or 2                                                                                     ProgrDecision
  80        < Time steps between calls to chemical equilibration subroutine. Called daily if capacity model       AdvancedUsers
used.
**************************************************************************
DIFFUSION
---------
 120        <Molecular diffusion coefficient in water (mm2/day)                                                   Best via GUI
**************************************************************************
**************************************************************************
                    CHEMICAL AMENDMENT APPLICATIONS
                       ----------------------
 365    <  Number of broadcast applications. (At least 1.  Can be past last date.)
----------------------------------------------------------------------
    Date       Incorporation    Ca    Mg    Na     K    Cl    SO4  HCO3   CO3  Al
or day number (segments, >0)             ------mol/sq.m-------
   ------      ------------   ----- ----- ----- ----- ----- ----- ----- -----DO NOT DELETE 365 DATA LINES BELOW
    10199           1          0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00                           } Managed
Etcetera: NB: fertilizer inputs will be automatically inserted here (1 october any year)                          } by
   123199           1          0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00                           } program
**************************************************************************
**************************************************************************
                    CULTIVATIONS
                    ------------
 1  < Number of cultivations.  At least one must be specified.  Can be past last day.
 ------------------------------------------------------
 Date or   Depth of cultivation
 day no.            mm
 -------          -----
 0102             200                                                                                             AdvancedUsers
**************************************************************************
**************************************************************************
      RAIN AND RAIN WATER COMPOSITION  (Include irrigation here, or specify
```

```
      -------------------------------    in a separate file.)
365  < Number of water applications. Some or all can be past last day.(See manual on setting automated
irrigation thresholds)
  0  < For a separate irrigation file, set to 1 and edit and rename CHEMTEST.SCH.
--------------------------------------------------------------------------
      Start      Amount  Surface flux      Water composition (can be 0)
Date/day  Time             density     Ca     Mg     Na     K     Cl    SO4  Alkalinity Al
-------  --day-  --mm--  ---mm/d----      ----------  mmol/l-----------
 10199       0.5      0.0     100.0      0.005 0.010 0.140 0.010 0.150 0.035 -0.040 0.000      Best via GUI
etcetera                                                                                        Best via GUI
123199       0.5      3.0     100.0      0.005 0.010 0.140 0.010 0.150 0.035 -0.040 0.000      Best via GUI
**************************************************************************
**************************************************************************
          POTENTIAL ET (WEEKLY TOTALS, mm), DEPTH TO WATER TABLE (mm)
          MEAN WEEKLY TEMPERATURES AND MEAN WEEKLY AMPLITUDE (degrees C)
--------------------------------------------------------------------------
      Week no.    ET   Water table  Mean temp  Amplitude
      ----------------------------------------------
        1        0.6      0            3.5         1.7                                         Best via GUI
etcetera                                                                                        Best via GUI
       53        0        0            0.4         0.5                                         Best via GUI
```

Appendix 2: Example chemistry input data

Comments added in grey part; file in white part of table.

```
0   0   EQUILIBRIUM CONSTANT + dH (kJ.mol-1) FILE FOR SOILGEN (values 25oC; dH for temp. corrections)
0   0   DO NOT CHANGE TEXT, ONLY NUMBERS. LINE ORDER IS NOT CRITICAL.
3.4041E-02   -19.983   KH  Henrys law constant for CO2 (log = -1.468 )
1.0000E-14   55.907   KW  Stability constant of water (log = -14.000 )
4.4463E-07   9.109   KA1 First dissociation constant of H2CO3 (log = -6.352 )
4.6881E-11   14.899  KA2 Second dissociation constant of H2CO3 (log = -10.329 )
5.9704E-04   -14.832   KD1 Stability constant of CaCO3 (log = -3.224 )
7.8343E-02   -11.255   KD2 Stability constant of CaHCO3+ (log = -1.106 )
4.9774E-02   -8.205   KD3 Stability constant of CaOH+ (log = -1.303 )
5.0119E-03   -6.904   KD4 Stability constant of CaSO4 (log = -2.300 )
1.0471E-03   -11.351   KD5 Stability constant of MgCO3 (log = -2.980 )
8.5114E-02   -3.305   KD6 Stability constant of MgHCO3+ (log = -1.070 )
2.7542E-03   -10.837   KD7 Stability constant of MgOH+ (log = -2.560 )
4.2658E-03   -19.037   KD8 Stability constant of MgSO4 (log = -2.370 )
1.9953E-01   -4.686   KD9 Stability constant of NaSO4- (log = -0.700 )
5.3703E-02   -37.279   KD10 Stability constant of NaCO3- (log = -1.270 )
1.4125E-01   -9.414   KD11 Stability constant of KSO4- (log = -0.850 )
2.6303E-05   -0.456   SP1 Solubility product of gypsum (log = -4.580 )
3.3113E-09   -9.611   SP2 Solubility product of calcite (log = -8.480 )
2.2387E+09   -95.395   KSP Solubility product of Gibbsite (log = 9.350 )
1.0233E-05   49.790   KAl1 Stability constant AlOH_2p (log = -4.990 )       } Not used in SoilGen
1.0000E-10   92.048   KAl2 Stability constant AlOH2_p (log = -10.000 )      } Not used in SoilGen
1.0000E-23   184.347   KAl4 Stability constant AlOH4_m (log = -23.000 )     } Not used in SoilGen
1.0471E+07   4.602   Kf1 Stability constant AlF_2p (log K = 7.020 )         } Not used in SoilGen
5.7544E+12   8.368   Kf2 Stability constant AlF2_p (log K = 12.760 )        } Not used in SoilGen
1.0715E+17   10.460   Kf3 Stability constant AlF3 (log K = 17.030 )         } Not used in SoilGen
5.3703E+19   9.205   Kf4 Stability constant AlF4_m (log K = 19.730 )        } Not used in SoilGen
8.3176E+20   7.531   Kf5 Stability constant AlF5_2m (log K = 20.920 )       } Not used in SoilGen
2.4547E+08   0.000   Ko1 Stability constant AlOrg (log K = 8.390 )          } Not used in SoilGen
1.2303E+13   0.000   Ko2 Stability constant AlHOrg_p (log K= 13.090 )       } Not used in SoilGen
1.7378E-02   0.000   Kg1 Stability constant H2Org_m (log K= -1.760 )        } Not used in SoilGen
1.2589E-06   0.000   Kg2 Stability constant HOrg_2m (log K= -5.900 )        } Not used in SoilGen
1.4791E-07   0.000   Kg3 Stability constant Org_3m (log K= -6.830 )         } Not used in SoilGen
1.4791E+03   14.477   KHF Dissociation constant HF (log K = 3.170 )         } Not used in SoilGen
2.5119E-11   19.623   KCaF Solubility product of CaF2 (log K = -10.600 )    } Not used in SoilGen
0   0   END OF FILE
```

Appendix 3: Example C-cycling input data file

Comments added in grey part; file in white part of table.

```
Data file with C-turnover data for SoilGen
C-turnover modelled using the approach of Roth-C26.3 model. Refs:
Jenkinson, D.S., Coleman, K., 1994. Calculating the annual input of organic
                                 matter to soil from measurements of total organic carbon
                                 and radiocarbon. European Journal of Soil Science 45, 167-174
Coleman, K., Jenkinson, D.S., 2005. RothC-26.3: a model for the turnover of carbon in soil.
                                 Model Description and Users Guide. November 1999 Issue
                                 (Modified April 2005).
                                 http://www.rothamsted.bbsrc.ac.uk/aen/carbon/download.htm
DO NOT CHANGE TEXT NOR LINE ORDER, ONLY CHANGE NUMBERS
[initial profile data: distribution C over various pools (%) (all soil compartments)]
[DPMpool  RPMpool  BIOpool  HUMpool  IOMpool]
0 0 0 0 100
```

NB: all in IOMpool= constant!

```
[monthly inputs: distribution of inputs (%) of PlantResidues and Manure for all vegetations per month]
[month PlantResiduesIN ManureIN for grassscrub]
1  0  0
2  0  0
3  0  0
4  0  0
5  6  0
6  23  0
7  29  0
8  24  0
9  18  0
10  0  0
11  0  0
12  0  0
400  [mm maximum rootable depth]
```

NB: overrides other root depths!

```
[month PlantResiduesIN ManureIN for deciduouswood]
1  0  0
2  0  0
3  0  0
4  0  0
5  0  0
6  0  0
7  0  0
8  0  0
9  20  0
10  70  0
11  10  0
12  0  0
1000  [mm maximum rootable depth]
```

NB: overrides other root depths!

```
[month PlantResiduesIN ManureIN for coniferouswood]
1  10  0
2  10  0
3  10  0
4  0  0
5  0  0
6  0  0
7  0  0
8  0  0
9  10  0
10  20  0
11  20  0
12  20  0
1000  [mm maximum rootable depth]
```

NB: overrides other root depths!

```
[month PlantResiduesIN ManureIN for agriculture]
1 0 0
2 0 0
3 0 0
4 0 80
5 0 20
6 0 0
7 0 0
8 50 0
9 50 0
10 0 0
11 0 0
12 0 0
400  [mm maximum rootable depth]
```

NB: overrides other root depths!

Appendix 4: Example weathering data file

Comments added in grey part; file in white part of table.

Wheathering data file for SoilGen. Weathering is described according to:	
Van Grinsven, J.J.M. van, 1988. Impact of atmospheric deposition on soils.	
Quantification of chemical and hydrological processes.	
PhD-thesis, Wageningen University, Netherlands (Ch. 10).	
Kros, J. 2002. Evaluation of biogeochemical models at local and regional scale.	
PhD-thesis. Wageningen University, Netherlands (ch.2.1)	
IF YOU EDIT THIS FILE: DO NOT CHANGE TEXT NOR LINE ORDER, ONLY CHANGE NUMBERS.	
[Weathering rates]	
0.226 kCa we,pm = Weathering rate Ca from primary minerals (m3.molc-1.y-1)	Kros, 2002 Chapter 2.1
0.85 alfa(Ca) = parameter describing effect pH on weathering rate (-)	Kros, 2002 Chapter 2.1
0.192 kMg we,pm = Weathering rate Mg from primary minerals (m3.molc-1.y-1)	Kros, 2002 Chapter 2.1
1.54 alfa(Mg) = parameter describing effect pH on weathering rate (-)	Kros, 2002 Chapter 2.1
0.233 kK we,pm = Weathering rate K from primary minerals (m3.molc-1.y-1)	Kros, 2002 Chapter 2.1
1.02 alfa(K) = parameter describing effect pH on weathering rate (-)	Kros, 2002 Chapter 2.1
0.0843 kNa we,pm = Weathering rate Na from primary minerals (m3.molc-1.y-1)	Kros, 2002 Chapter 2.1
0.87 alfa(Na) = parameter describing effect pH on weathering rate (-)	Kros, 2002 Chapter 2.1
3 =coefficient for congruent weathering Anorthite (Ca) with respect to Al (-)	Kros, 2002 Chapter 2.1
0.6 =coefficient for congruent weathering Chlorite (Mg) with respect to Al (-)	Kros, 2002 Chapter 2.1
3 =coefficient for congruent weathering Microcline (K) with respect to Al (-)	Kros, 2002 Chapter 2.1
3 =coefficient for congruent weathering Albite (Na) with respect to Al (-)	Kros, 2002 Chapter 2.1
[Al-chemistry]	
0.000167 =Elovich rate constant (kg-1.y-1)	Kros2002Ch2.1 Not used!
9.8 =Elovich exponent constant (m3.molc-1)	Kros2002Ch2.1 Not used!
[Initial profile data: Ca, Mg, K, Na (primary minerals) and Al (Gibbsite)(all soil compartments)]	
0.00006179 ="free" Al (molc.kg-1, e.g. estimated from dithionite or oxalate extraction; initial Gibsite pool)	} Profile dependent;
0.00031564 =Ca (molc.kg-1 soil, e.g. from total analysis corrected for "free"Al and Fe)	} assumed constant
0.00048382 =Mg (molc.kg-1 soil, e.g. from total analysis corrected for "free"Al and Fe)	} over all
0.00050958 =K (molc.kg-1 soil, e.g. from total analysis corrected for "free"Al and Fe)	} profile
0.00047435 =Na (molc.kg-1 soil, e.g. from total analysis corrected for "free"Al and Fe)	} compartments!

Appendix 5: Example bioturbation input file

```
1 0 250 350 8 7 0
5 0 250 350 8 7 0
10 0 250 350 8 7 0
100 0 250 350 8 7 0
1000 0 250 350 8 7 0
7500 0 250 350 8 7 0
```

Data per column:

1. Year= simulation year (oldest year = 1);
2. Upper depth of bioturbation (usually 0: the soil surface) in mm below current soil surface;
3. Depth of maximal bioturbation (mm below current soil surface);
4. Lower depth of bioturbation (mm below current soil surface);
5. Magnitude of bioturbation at upper depth (promille of total soil mass at this depth);
6. Magnitude of (maximal) bioturbation at depth of maximal bioturbation (promille of mass);
7. Magnitude of bioturbation at lower depth of bioturbation (usually 0).

Appendix 6: Example climate input file

```
YearBP  P  EP  JanT  JulT  PlantsInC(t/ha,y)  ManureInC(t/ha,y)  Vegetation  Period
15000  250  494  -6.7  13.6  1.7  0.0  grassscrub  LateGlacial
14750  300  510  -5.9  14.4  7.0  0.0  coniferouswood  Bölling
14500  700  516  -5.7  14.7  10.0  0.0  deciduouswood  Bölling
14250  700  511  -5.9  14.4  10.0  0.0  deciduouswood  Bölling
14000  800  526  -5.2  15.1  6.0  0.0  coniferouswood  MDryas
13750  800  541  -4.5  15.8  10.0  0.0  coniferouswood  Alleröd
13500  800  538  -4.6  15.7  10.0  0.0  coniferouswood  Alleröd
13250  800  559  -3.6  16.7  10.0  0.0  coniferouswood  Alleröd
13000  700  581  -2.6  17.7  10.0  0.0  coniferouswood  Alleröd
12750  700  555  -3.8  16.5  3.4  0.0  grassscrub  YDryas
12500  700  547  -4.2  16.1  3.4  0.0  grassscrub  YDryas
12250  700  546  -4.2  16.1  3.4  0.0  grassscrub  YDryas
11960  616  549  -4.0  16.2  5.0  0.0  coniferouswood  YDryas
11860  625  558  -3.4  16.3  5.0  0.0  coniferouswood  YDryas
11760  640  550  -3.5  15.8  5.0  0.0  grassscrub  YDryas
11660  661  557  -3.1  16.1  5.0  0.0  grassscrub  YDryas
11560  663  567  -2.7  16.6  5.0  0.0  grassscrub  YDryas
11460  662  551  -3.5  15.8  5.0  0.0  grassscrub  YDryas
11360  666  549  -3.7  15.8  5.0  0.0  grassscrub  YDryas
11260  665  552  -3.7  16.1  5.0  0.0  grassscrub  YDryas
11160  673  578  -2.0  17.0  3.4  0.0  grassscrub  YDryas
11060  681  577  -2.3  17.1  3.4  0.0  grassscrub  YDryas
10960  702  574  -2.1  16.7  3.4  0.0  grassscrub  YDryas
10860  729  587  -1.2  17.0  3.4  0.0  grassscrub  YDryas
10760  720  589  -0.9  16.8  3.4  0.0  grassscrub  YDryas
10660  748  587  -1.2  17.0  3.4  0.0  grassscrub  YDryas
10560  787  596  -0.6  17.2  3.4  0.0  grassscrub  YDryas
10460  781  600  -0.4  17.3  3.4  0.0  grassscrub  YDryas
10360  773  608  0.2  17.6  3.4  0.0  grassscrub  YDryas
10260  764  609  0.3  17.6  8.5  0.0  deciduouswood  Preboreal
10160  789  607  0.3  17.5  8.5  0.0  deciduouswood  Preboreal
10060  820  615  0.8  17.6  8.5  0.0  deciduouswood  Preboreal
9960  832  619  1.2  17.7  9.0  0.0  coniferouswood  Preboreal
9860  859  621  1.2  17.8  9.0  0.0  coniferouswood  Preboreal
9760  850  619  1.2  17.6  10.0  0.0  coniferouswood  Preboreal
9660  855  624  1.5  17.8  10.0  0.0  coniferouswood  Preboreal
9560  847  618  1.1  17.7  10.0  0.0  coniferouswood  Preboreal
9460  869  623  1.6  17.6  10.0  0.0  deciduouswood  Boreal
9360  830  618  1.1  17.6  10.0  0.0  deciduouswood  Boreal
9260  828  614  0.7  17.6  10.0  0.0  deciduouswood  Boreal
9160  830  615  0.8  17.6  10.0  0.0  deciduouswood  Boreal
9060  830  615  0.9  17.6  11.9  0.0  deciduouswood  Atlanticum
Et cetera
160  845  646  3.2  18.1  11.0  0.0  deciduouswood  Subatlanticum
60  849  642  3.0  18.0  11.0  0.0  deciduouswood  Subatlanticum
```

Meaning of column headers:

- YearBP = years before present
- P = annual precipitation (mm), not corrected for interception
- evaporation EP = potential annual evapotranspiration (mm) JanT =
- average january temperature (^{o}C) JulT = average july temperature (^{o}C)
- PlantsInC(t/ha,y) = annual amount of C added to the soil in the form of leaf litter and root litter
- ManureInC(t/ha,y) = annual amount of C added to the soil in the form of organic manure (if agriculture)
- Vegetation = one of the following types: grassscrub, coniferouswood, deciduouswood, agriculture
- Period = a free format text description of the period

Appendix 7: Example pCO2 input file

```
yearBP pCO2
14950  0.000275
14900  0.000275
14850  0.000275
150    0.000300
40     0.000310
1      0.000390
```

Meaning of column headers:

- YearBP = years before present
- pCO2= partial CO2-pressure in the atmosphere, in bar

Appendix 8: Example Δ14C input file

```
CalBP  Delta 14C per mil
15000  277.5
14990  277.0
14980  276.6
14970  276.2
14960  275.7
….
20  -16.4
15  -17.2
10  -20.0
5  -22.5
0  -24.5
-6  21.1
-7  37.9
-8  100.7
-9  213.3
-10  225.6
-11  215.9
-12  260.6
….
-38  175.8
-39  166.8
-40  154.9
-41  141.2
-42  135.5
-43  130.1
-44  119.4
-45  114.2
```

Appendix 9: Example fertilization input file

```
yearBP  Ca  Mg  Na  K  Cl  SO4  HCO3  CO3  (mol/sq.m)
2960  1.88  0  0  0  0  0  0  1.88
2950  1.88  0  0  0  0  0  0  1.88
2940  1.88  0  0  0  0  0  0  1.88
2930  1.88  0  0  0  0  0  0  1.88
2920  1.88  0  0  0  0  0  0  1.88
2910  1.88  0  0  0  0  0  0  1.88
2900  1.88  0  0  0  0  0  0  1.88
2890  1.88  0  0  0  0  0  0  1.88
2880  1.88  0  0  0  0  0  0  1.88
2870  1.88  0  0  0  0  0  0  1.88
2860  1.88  0  0  0  0  0  0  1.88
2850  1.88  0  0  0  0  0  0  1.88
2840  1.88  0  0  0  0  0  0  1.88
Et cetera
100  1.88  0  0  0  0  0  0  1.88
90  1.88  0  0  0  0  0  0  1.88
80  1.88  0  0  0  0  0  0  1.88
70  1.88  0  0  0  0  0  0  1.88
60  0.28  0  0  0  0  0  0  0.28
59  0.28  0  0  0  0  0  0  0.28
58  0.28  0  0  0  0  0  0  0.28
Et cetera
3  0.28  0  0  0  0  0  0  0.28
2  0.28  0  0  0  0  0  0  0.28
1  0.28  0  0  0  0  0  0  0.28
```

Meaning of column headers:

- YearBP = years before present
- Ca, MG, etc: amounts in fertilization at soil surface, in mol.m^{-2}

Appendix 10: Example events input file

Individual lines are marked

```
SimulationYear Event No.Compartments Clay Silt OC BulkDensity MoistureContent Calcite Gypsum pCO2    } title row
Ca-sol Mg-sol Na-sol K-sol Cl-sol SO4-sol Alkalinity Al-sol Org3-sol HOrg-sol H2Org-sol DOC Ca-exch
Mg-exch Na-exch K-exch H-exch Al-exch CEC Mg/Ca-select Ca/Na-select Ca/K-select Ca/Al-select Ca/H-
select
10 Deposition 2  12.0 78.8    0.12000    1.60000    0.30000    0.10000    0.00000    0.00030       } row with
15.91000    1.17000    0.07000    0.07000   34.00000    0.00000    0.30000    0.01000    0.00000    sedimentation data
0.00000    0.00000    0.00000   68.59000    0.00010    0.00010    0.00010    0.00010    0.00010
68.59050    0.69820    0.06700    0.03310    0.27416    0.00051
50 Deposition 1  12.0 78.8    0.12000    1.60000    0.30000    0.10000    0.00000    0.00030       } row with
15.91000    1.17000    0.07000    0.07000   34.00000    0.00000    0.30000    0.01000    0.00000    sedimentation data
0.00000    0.00000    0.00000   68.59000    0.00010    0.00010    0.00010    0.00010    0.00010
68.59050    0.69820    0.06700    0.03310    0.27416    0.00051
100 Deposition 1  12.0 78.8    0.12000    1.60000    0.30000    0.10000    0.00000    0.00030      } row with
15.91000    1.17000    0.07000    0.07000   34.00000    0.00000    0.30000    0.01000    0.00000    sedimentation data
0.00000    0.00000    0.00000   68.59000    0.00010    0.00010    0.00010    0.00010    0.00010
68.59050    0.69820    0.06700    0.03310    0.27416    0.00051
2250 Deposition 1  12.0 78.8    0.12000    1.60000    0.30000    0.10000    0.00000    0.00030     } row with
15.91000    1.17000    0.07000    0.07000   34.00000    0.00000    0.30000    0.01000    0.00000    sedimentation data
0.00000    0.00000    0.00000   68.59000    0.00010    0.00010    0.00010    0.00010    0.00010
68.59050    0.69820    0.06700    0.03310    0.27416    0.00051
4000 Deposition 2  12.0 78.8    0.12000    1.60000    0.30000    0.10000    0.00000    0.00030     } row with
15.91000    1.17000    0.07000    0.07000   34.00000    0.00000    0.30000    0.01000    0.00000    sedimentation data
0.00000    0.00000    0.00000   68.59000    0.00010    0.00010    0.00010    0.00010    0.00010
68.59050    0.69820    0.06700    0.03310    0.27416    0.00051
6580 SlashBurn 1 0.70 0.03 0.27                                                                      } SlashBurn, 1 comp.
7000 Erosion 2 NoData                                                                                } erosion 2 comp.
7001 WaterTable 10 NoData                                                                            } watertable 10th comp
7002 WaterTable 11 NoData                                                                            } watertable 11th comp
7004 VGNChange 4 VGN1.txt                                                                            Input VanGenuchten-
                                                                                                     parameters for the top
                                                                                                     4 compartments is to
                                                                                                     be read from
                                                                                                     "VGN1.txt"; for other
                                                                                                     compartments it is
                                                                                                     estimated by the
                                                                                                     program.
```

Example of Van Genuchten File (4 compartments):

```
Theta-Sat  Theta-Res alpha n  gamma ksat(mm/day)
0.42 0.01  0.0084  1.441  -1.497  129.8
0.42 0.01  0.0084  1.441  -1.497  129.8
0.42 0.01  0.0084  1.441  -1.497  129.8
0.42 0.01  0.0084  1.441  -1.497  129.8
```

Appendix 11: USDA curve number (CN2)

Runoff is calculated using the USDA Soil Conservation Service (SCS) procedure known as the "curve number technique" (Soil Conservation Service 1972). The procedure uses total precipitation in a calendar day to estimate runoff. Runoff curves are specified by numbers which vary from 0 (no runoff) to 100 (all runoff). The SCS handbook provides a list of runoff curve numbers for various hydrological soil groups and soil-cover complexes. To determine the runoff curve number for cropland soils, it is necessary to decide which of four hydrologic soil groups best describes the soil. Description of the groups is given in Table 10.11. The curve number (CN2) is determined from the soil texture and slope of the site using information in Tables 10.1 and 10.2. The curve number is further modified for the degree of conservation practices followed as indicated in Table10. 2.

NOTE: In SoilGen2.18 CN2 is fixed to 75. A protocol to decide on the value of CN2 based on texture, clay mineralogy and infiltrability still needs to be developed.

Table 10.1. The soil hydrology groups needed for selection of a runoff curve number for croplands.

Hydrologic group	**Description**
A. Lower Runoff Potential	Includes deep sands with very little silt and clay, also deep, rapidly permeable loess.
B. Moderately Low Runoff Potential	Mostly sandy soils less deep than A, and loess less deep or less aggregated than A, but the group as a whole has above-average infiltration after thorough wetting.
C. Moderately High Runoff Potential	Comprises shallow soils and soils containing considerable clay and colloids, though less than that of group D. The group has below-average infiltration after thorough wetting.
D. Highest Runoff Potential	Includes mostly clays of high swelling percentage, but the group also includes some shallow soils with nearly impermeable sub-horizons near the surface.

Table 10.2. Runoff curve numbers (CN2) for various hydrological conditions, slopes, and conservation practices.

	Hydrologic conditions			
Slope (%)	A	B	C	D
0-2	61	73	81	84
2-5	64	76	84	87
5-10	68	80	88	91
>10	71	83	91	94