MANUAL

Integrated Catchments model for Carbon (INCA-C)

Parameter description and Calibration strategy

May 2017

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OBS! This manual should be used simply as guidance. Many options and parameters have not been exhaustively explored or described and some parts of the information may not fully apply.

For questions and suggestions, please contact jose.ledesma@slu.se

1. Software and tools

- *inca_c_1.1_beta_7.exe* (Jan 2016): executable of the model
- *inca_c_cmd.exe* (Apr 2015): file necessary to run the MC tool for INCA-C
- *MCDemo.exe* (Jan 2016): executable of the MC tool (for both PERSiST and INCA-C)
- *MCDemo_Sensitivity.accdb* (May 2016): access file to work with results from MC tool for sensitivity/uncertainty analyses (same for both PERSiST and INCA-C)

2. Model and parameter descriptions

2.1 Brief model description

The Integrated Catchments model for Carbon (INCA-C) (Futter et al., 2007) is a dynamic, semi-distributed, process-based model that requires daily time series of precipitation, temperature, soil moisture deficit (SMD), and hydrologically effective rainfall (HER; precipitation net of evapotranspiration) (outputs from PERSiST) to simulate daily stream flow (hydrological sub-model, a simplified version of PERSiST) and daily DOC concentrations (biogeochemical sub-model). The following processes are represented in two soil layers (upper soil layer denoted as “organic” and lower soil layer denoted as “mineral”): (i) soil organic carbon (SOC) production through litter breakdown, (ii) temperature, moisture, and soil–solution chemistry dependent organic carbon sorption and desorption, and (iii) hydrologic controls on transport of DOC from soils to streamwaters. A “direct runoff” layer representing overland flow is also present. Key model parameters controlling DOC production and transport include soil thermal conductivity, temperature and soil moisture dependency of carbon processing rates including rates of DOC production, sorption and desorption in topsoil and subsoil, litter production, DOC production from litter, sensitivity of (de)sorption rates to soil–solution chemistry, and fraction of labile SOC of the SOC pool. Carbon pools include DOC, SOC, potentially dissolved carbon (PDC) and dissolved inorganic carbon (DIC).

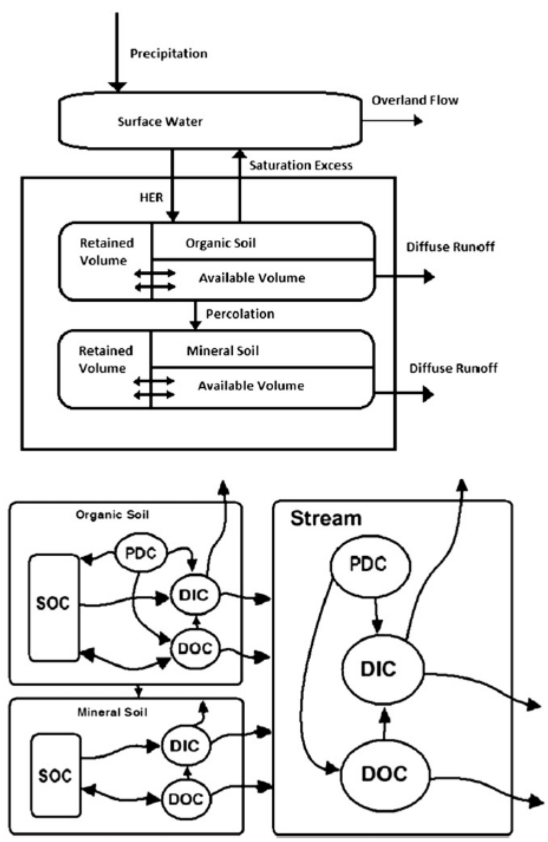


Fig. 2. Conceptualization of the two interconnected sub-models within INCA-C. Above, the hydrological sub-model with theoretical fluxes between water pools. Below, the biogeochemical carbon sub-model with theoretical transformations between different carbon pools.

2.2 Initial set up and necessary files

Model structure

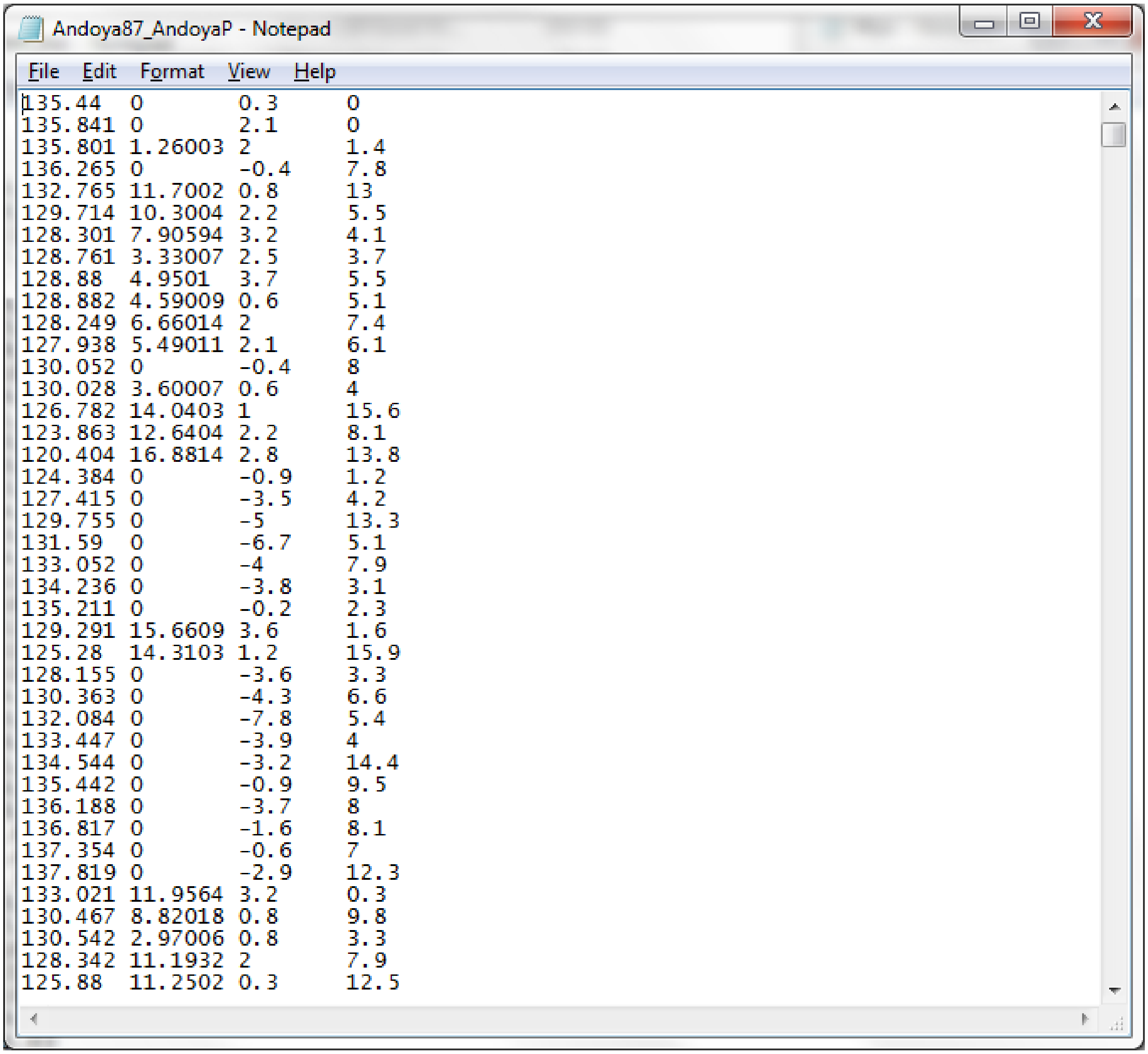
- *Reaches*: we can calibrate as many reaches as we want or have data for within our catchment, but commonly it is only use the main outlet. The number of reaches can be specified under Edit> Parameters> General parameters in the model interface or by using a previous .par file with the same number of reaches.

- *Land use types*: for every reach (sub-catchment), land use proportions are needed in order to divide the catchment among different classes (up to 6). Typical classifications include: wetland (bog, moorland), forest, grassland, arable, urban. The number of landscape units is 6 by default. If less just specified 0 in the proportions that can be assigned/changed under Edit> Parameters> Sub-catchment> Land use groups. The name of the different landscape units can be assigned/changed by opening the .par file with the notepad or under Edit> Options> Land Groups.

- *Soil configuration*: for every land use type, the soil is divided in 2 soil boxes by default, typically representing an upper organic soil layer and a lower mineral soil layer. Within the hydrological sub-model representation, INCA-C also simulates overland flow that can contain PDC and DOC, but no transformations are modelled in these third box.

Input and calibration data

- *.dat extension file*: can be created with the notepad. It contains daily time series of precipitation soils moisture deficit (in mm), hydrologically effective rainfall (in mm), temperature (in °C), and precipitation (in mm) for the available dates within the simulation period. Note that these are the only necessary input data to run the model and simulate flow and DOC. SMD and HER have to be obtained from PERSiST and the file is actually automatically generated as a model output. Within the file there are four column in the order SMD, HER, T, P and each row represents one day of the simulation period. No missing values are allowed (a complete time series is needed from day 1 to final date of simulation).


Andoya87_AndoyaP - Notepad

File Edit Format View Help

```
135.44  0       0.3     0
135.841 0       2.1     0
135.801 1.26003 2       1.4
136.265 0       -0.4    7.8
132.765 11.7002 0.8     13
129.714 10.3004 2.2     5.5
128.301 7.90594 3.2     4.1
128.761 3.33007 2.5     3.7
128.88  4.9501  3.7     5.5
128.882 4.59009 0.6     5.1
128.249 6.66014 2       7.4
127.938 5.49011 2.1     6.1
130.052 0       -0.4    8
130.028 3.60007 0.6     4
126.782 14.0403 1       15.6
123.863 12.6404 2.2     8.1
120.404 16.8814 2.8     13.8
124.384 0       -0.9    1.2
127.415 0       -3.5    4.2
129.755 0       -5      13.3
131.59  0       -6.7    5.1
133.052 0       -4      7.9
134.236 0       -3.8    3.1
135.211 0       -0.2    2.3
129.291 15.6609 3.6     1.6
125.28  14.3103 1.2     15.9
128.155 0       -3.6    3.3
130.363 0       -4.3    6.6
132.084 0       -7.8    5.4
133.447 0       -3.9    4
134.544 0       -3.2    14.4
135.442 0       -0.9    9.5
136.188 0       -3.7    8
136.817 0       -1.6    8.1
137.354 0       -0.6    7
137.819 0       -2.9    12.3
133.021 11.9564 3.2     0.3
130.467 8.82018 0.8     9.8
130.542 2.97006 0.8     3.3
128.342 11.1932 2       7.9
125.88  11.2502 0.3     12.5
```

- *.obs extension file*: can be created with the notepad. It contains daily time series of DOC data (in mg/L) and flow data (in m3/s) for each reach (sub-catchment) for the available dates within the calibration period. Note that the calibration period is not necessarily the same as the simulation period; it could be shorter if there are not enough observations to cover the period where input data are available. In that case earlier or later periods from the calibration period will be hindcast or forecast simulations. Missing values are allowed and do not need to be explicitly expressed as the date is used. Within the file, in the first row we write the reach number within a few "*" and as "Reach X". In the second row we write "AQUATIC DOC" within a few "-" Then, in two columns we paste the date in the left column as DD/MM/YYYY and the corresponding DOC values in mg/L in the right column. After the DOC data we do the same for flow data. We write the reach number (X) within a few "*" and as "Reach X", below we write "AQUATIC FLOW" within a few "-", and then in two columns we paste the date in the left column as DD/MM/YYYY and the corresponding flow values in m3/s in the right column. Analogously, if calibration is made for different reaches, the information is pasted in the same way below:

```
****************************** Reach 1 *************************
---------------------- AQUATIC DOC -------------------
25/8/2011       11.7
8/11/2011       13.2
13/6/2012       7.9
3/7/2012        11.2
24/7/2012       11.5
14/8/2012       10.5
28/8/2012       12.4
11/9/2012       14
25/9/2012       15.5
15/10/2012      14.2
23/10/2012      13.2
6/11/2012       10.1
13/11/2012      9.2
10/12/2012      7.3
29/1/2013       6.9
21/5/2013       7.4
18/6/2013       9.2
2/7/2013        12.1
16/7/2013       13.6
30/7/2013       13.9
6/8/2013        14.9
28/8/2013       18.7
3/9/2013        17
18/11/2013      8.3
2/12/2013       5.3
16/12/2013      4.6
6/1/2014        6.2
21/1/2014       7.6
10/2/2014       6.1
17/2/2014       6.4
3/3/2014        6.8
18/3/2014       2.8
31/3/2014       3.8
22/4/2014       5.4
5/5/2014        5.2
20/5/2014       6.4
****************************** Reach 1 *************************
---------------------------- AQUATIC FLOW ---------------------------
1/12/2012       0.012
2/12/2012       0.017
3/12/2012       0.013
4/12/2012       0.014
5/12/2012       0.012
6/12/2012       0.011
7/12/2012       0.013
8/12/2012       0.011
9/12/2012       0.011
10/12/2012      0.012
```

- *.par extension file*: this file contains all parameter values that can be adjusted using the model interface. Name of reaches, name of the landscape units, starting simulation date, time steps and such can all be easily specified within the model interface. Just as example:

bestParSet83 - Notepad

File Edit Format View Help

```
Andoya
"Bog","2","3","4","5","6"
"Bog","2","3","4","5","6"
0.01	0	0	0.001	0.001	0.001
0.012	0.00015	0.00015	0.01	0.01	0.01
0.008	8e-05	8e-05	0.01	0.01	0.01
7200	40000	80000	108567	200000	200000
796806	400000	200000	300000	10000	10000
30	20	10	20	5	5
0.15	3	3	2	5	5
547421	200000	100000	105401	10000	10000
12	10	5	118.635	10	10
0.15	3	3	5	1	1
1	1	1	1	1	1
3	20	20	20	20	20
1/1/2000
5331
0.0016324		0.0009824		0.00015	0.0008	0.0005	0.0005
0.00022351		1.7e-05	7.1e-05	0.01	0.01	0.01
0.010491		0.0009335		0.00095	0.002	0.0005	0.0005
0.000266831		0.0359	0.03125	4e-06	0.001	0.001
0	4e-06	9e-06	5e-05	0.0001	0.0001
0.00200966		1.0266	0.62169	0.00078	0.00078	0.00078
0.00101123		0.0002596		0.000235		0.0002	0.0001	0.0001
6.38501e-05		9.4e-05	0.000179		1e-06	0.0001	0.0001
0	0	0	0	0.0001	0.0001
0.0079624		0.00625	0.006396		0.0002	0.01	0.01
0.000610041		0.000193		4.4e-05	0	0.001	0.001
5	10	10	20	20	20
0.600389		1	0.5	0	1	1
1	30	1	1	1	1
365	300	365	365	365	365
0.179775		0.2	0.2	0.2	0.2	0.2
118.017	130	300	180.278	100	100
12	6	6	4.5	4.5	4.5
-0.01617		-0.01	-0.01	-0.03	-0.03	-0.03
2.3994	1.7	2.3	6.48896	3	3
24.8364	24	20	20	20	20
0	0	0	0	0	0
5.7597	2	2	3	3	3
0.012547		1	1	0.3	0.3	0.3
2.06924	0.9	0.8	0.7	0.7	0.7
15	20	12	6.6	6.6	6.6
0	0	0	0	0	0
0	0	0	0.0001	0	0
6	6	6	4.5	6	6
6	6	6	7.9	6	6
5	5	5	20	20	20
1	1	1	1	1	1
0	0	0	0	0	0
1000	1000	1000	1000	1000	1000
1	1	1	1	1	1
0	0	0	0	0	0
1000	1000	1000	1000	1000	1000
9.8167e-06		0	0	0	0	0
1	1	1	1	1	1
1.88636e-06		0	0	0	0	0
1	1	1	1	1	1
213.435	8.69	8.96376	0.536509		0.5	0.5
74.8914	6.3594	4.87714	15	15	15
1	51.465	72.3177	30	30	30
0.0010937		5	5	5	5	5
0.682059		0.1	0.1	0.1	0.1	0.1
220.3	0.9	0.9	0.9	0.9	0.9
0.140233		0.1	0.1	0.1	0.1	0.1
352.65	0.9	0.9	0.9	0.9	0.9
0.8596	0.900056		1	0.7	0.5	0.5
1.5247	1.84367	8	0.9	0.5	0.5
9.06519	6.91108	10	22	5	5
71560.9	609660	747060	33627.1	50000	50000
78986.6	296420	521170	60983.1	50000	50000
0.012
4
```

- *Other model input files*: abstraction, abstraction, effluent, system structure, organic fertilizer, terrestrial PDC inputs, aquatic PDC inputs, land use periods, deposition and/or spatial files are optional and not described here.

2.3 Model parameters

Below a description of all model parameters that can be adjusted under the “Edit>Parameters” menu. There are 4 type of parameters: sub-catchment, reach, instream and land phase (land use type). For every reach (sub-catchment) there will be some basic descriptive parameters. Landscape unit related-parameters are independent and for every reach (sub-catchment) every landscape unit will behave equally (e.g. forest type will have the same parameter values in every reach (sub-catchment), what will change will be the proportion of every landscape unit at every reach (sub-catchment)).

Sub-catchment…

Parameters that need to be specified for every sub-catchment (reach) considered. If we want to implement the same change in one parameter to all sub-catchments, the “Lock Sub-catchments” box at the down left corner of the menu can be checked.

Area> Physical attributes

Area (km2)

- *Description*: the area of the sub-catchment (km2).
- *Physical interpretation:* represents the surface area of the sub-catchment.
- *In the simulation (flow + DOC)*: important for calculating the magnitude of the flow, which will have an impact on the magnitude of the DOC as well.
- *Range*: from a few ha to tens of thousands of km2. The model has more problems in the smallest catchments, whereas mid to big size catchments can be better calibrated as long as T and P are representative.
- *Strategy/sensitivity*: fix the value at the beginning and do not change, meaningless to assess sensitivity.

Base Flow Index

- *Description*: base flow index (dimensionless).
- *Physical interpretation:* fraction of water that goes to the lower layer from the upper layer.
- *In the simulation (flow + DOC)*: lower values would produce faster responses in flow as more water will be available to drain in the upper layer, implying usually a higher DOC mobilization and therefore higher DOC simulated (and vice versa)
- *Range*: successful applications include values between 0.2 and 0.5, maybe lower but not higher.
- *Strategy/sensitivity*: adjust manually during initial manual calibration and include it in Monte Carlo (MC) analysis. It can be a sensitive parameter.

Direct runoff> Saturation excess control

Threshold soil zone flow

- *Description*: the threshold flow from the soil at which there is return flow to the direct runoff layer (m3/s).
- *Physical interpretation:* when the threshold value is exceeded, the water from the soil is returned to the surface.
- *In the simulation (flow + DOC)*: if a sufficiently high number is given (>0.2 m3/s), there will not be any effect on the simulations. If the value is very low, much more runoff will be generated from overland flow, which would usually imply faster flow responses and lower DOC mobilization (and vice versa).
- *Range*: from 0 to anything, usually given a value around 0.2 m3/s.
- *Strategy/sensitivity*: usually fix a high value at the beginning around 0.2 m3/s and do not change. Not sensitive parameter in that range and there are other more important parameters to control overland flow.

Direct runoff> Infiltration excess controls

Rainfall excess proportion

- *Description*: fraction of the hydrologically effective rainfall (HER; precipitation net of evapotranspiration) that goes to the direct runoff layer.
- *Physical interpretation:* fraction of the calculated amount of recharge water that do not infiltrate the soil but stays over the surface at every time step.
- *In the simulation (flow + DOC)*: in combination with the "Maximum infiltration rate" it can have a big influence on the amount of water flow generated as overland flow. Higher number would mean much more runoff will be generated from overland flow, which would usually imply faster flow responses and lower DOC mobilization (and vice versa).
- *Range*: usually give a value between 0 and 0.2.
- *Strategy/sensitivity*: adjust manually during initial manual calibration and include it in MC analysis. It can be a sensitive parameter.

Maximum infiltration rate

- *Description*: the maximum amount of water that can be infiltrated from the direct runoff layer to the upper layer in a day (mm/day).
- *Physical interpretation:* if the available water from precipitation or snowmelt exceeds the maximum infiltration rate, the difference will not infiltrate the soil but stays in the direct runoff layer.
- *In the simulation (flow + DOC)*: if a sufficiently high number is given (>20 mm/day to 50 mm/day or larger than any HER value in the series) there will not be influence as the amount of water it will never be exceeded

- *Range*: either give a sufficiently high number to not to have an influence (100 mm/day) or values around 10 mm/day to 50 mm/day.
- *Strategy/sensitivity*: maybe adjust manually during initial manual calibration and include it in MC analysis if the catchment is in a dry region but usually fix it at 100 mm/day and do not change.

Land use groups>

Land Use %

- *Description*: proportion of the specified landscape units (%).
- *Physical interpretation:* for every reach, it represents the percentage of surface area that every landscape unit (e.g.: wetland, forest, grassland, arable, urban) covers.
- *In the simulation*: it will determine the relative influence of each landscape unit in the overall simulation, which will depend on the specific parameter values at each unit.
- *Range*: 0% to 100% each with a total sum of 100%.
- *Strategy/sensitivity*: fix the value at the beginning and do not change, meaningless to assess sensitivity. Changes can be made to test effects of land use changes.

Constants> Physical attributes

CO2 (DIC) saturation concentration

- *Description*: saturation concentration for CO2.
- *Physical interpretation:* saturation concentration for CO2.
- *In the simulation*: to control degassing but this parameter never really worked and it is not really used by the model.
- *Range*: 0.00015.
- *Strategy/sensitivity*: leave the default value and do not change.

Atmospheric partial pressure of CO2

- *Description*: the partial pressure of CO2 in the atmosphere (atm).
- *Physical interpretation:* it represents the partial pressure of CO2 in the atmosphere.
- *In the simulation*: to control degassing but this parameter never really worked and it is not really used by the model.
- *Range*: 0.00035 atm.
- *Strategy/sensitivity*: leave the default value and do not change.

Henry's law constant for CO2

- *Description*: Henry's law constant for CO2.
- *Physical interpretation:* Henry's law constant for CO2.
- *In the simulation*: to control degassing but this parameter never really worked and it is not really used by the model.

- *Range*: 2.265.
- *Strategy/sensitivity*: leave the default value and do not change.

Deposition> Atmospheric deposition loads

Dry

- *Description*: dry deposition of sulfate or any other strong acidifying anion in the catchment (kg/ha/year).
- *Physical interpretation:* it represents a constant dry amount of strong acidifying anions that the catchment receives in a year per unit of area.
- *In the simulation (DOC)*: it is used to reproduce the solubility control of strong acidifying anions on the DOC mobilization so higher numbers would reduce DOC in stream (and vice versa), and this will have to be determined also with the parameter controlling the rate of (de)sorption to soil–solution chemistry under Land Phase> Processes> Sulphate.
- *Range*: if known, the specific value for the catchment in kg/ha/year, otherwise 0.
- *Strategy/sensitivity*: if used, it should be a known value, so fix at the beginning and do not change, meaningless to assess sensitivity.

Wet

- *Description*: wet deposition of sulfate or any other strong acidifying anion in the catchment (kg/ha/year).
- *Physical interpretation:* it represents a constant wet amount of strong acidifying anions that the catchment receives in a year per unit of area.
- *In the simulation (DOC)*: it is used to reproduce the solubility control of strong acidifying anions on the DOC mobilization so higher numbers would reduce DOC in stream (and vice versa), and this will have to be determined also with the parameter controlling the rate of (de)sorption to soil–solution chemistry under Land Phase> Processes> Sulphate.
- *Range*: if known, the specific value for the catchment in kg/ha/year, otherwise 0.
- *Strategy/sensitivity*: if used, it should be a known value, so fix at the beginning and do not change, meaningless to assess sensitivity.

Reach…

Parameters that need to be specified for every sub-catchment (reach) considered. If we want to implement the same change in one parameter to all reaches, the “Lock Reaches” box at the down left corner of the menu can be checked.

Dimensions> Dimensions

Length

- *Description*: length of the main stem of the specific reach (m).

- *Physical interpretation:* represents the total length of the reach.
- *In the simulation (flow + DOC)*: necessary to estimate residence times of the water in the stream. It has some influence on the flashiness of the flow, lower values would produce faster responses and vice versa, in both the flow and the DOC simulation.
- *Range*: depends on the size of the sub-catchment, from as low as 100 m to as much as 1000000 m. In very short systems it could be that we need to give a higher value than the real one in order for the model not to crash as some in-stream processes need some longer residence time in order to be calculated (model may run out of water).
- *Strategy/sensitivity*: give a rough estimate at the beginning and do not change or slightly modify it manually later on. Meaningless to assess sensitivity.

Average width

- *Description*: width of the main stem of the reach (m).
- *Physical interpretation:* represents the average stream width in the sub-catchment.
- *In the simulation (flow + DOC)*: necessary to estimate residence times of water in the stream. Appears to have no effect.
- *Range*: depends on the size of the sub-catchment, from as low as 1 m to as much as 100 m.
- *Strategy/sensitivity*: give a rough estimate at the beginning and do not change or slightly modify it manually later on. Meaningless to assess sensitivity.

Latitude

- *Description*: latitude (degrees).
- *Physical interpretation:* it represents the geographical latitude where the catchment is located.
- *In the simulation*: used to calculate solar radiation, appears to have no influence in the simulation.
- *Range*: the specific value for the catchment.
- *Strategy/sensitivity*: fix the value at the beginning and do not change. Meaningless to assess sensitivity.

Longitude

- *Description*: longitude (degrees).
- *Physical interpretation:* it represents the geographical longitude where the catchment is located.
- *In the simulation*: used to calculate solar radiation, appears to have no influence in the simulation.
- *Range*: the specific value for the catchment.
- *Strategy/sensitivity*: fix the value at the beginning and do not change. Meaningless to assess sensitivity.

Area

- *Description*: area of the main stem of the reach (km2).

- *Physical interpretation:* it represents the surface area covered by the stream, just the result of multiplying the estimated length with the estimated average width.
- *In the simulation*: not influential.
- *Range*: the specific value obtained after multiplying the estimated length with the estimated average width.
- *Strategy/sensitivity*: fix the value at the beginning and do not change. Meaningless to assess sensitivity.

Dimensions> Velocity / flow information

Flow a

- *Description*: flow velocity multiplier (dimensionless).
- *Physical interpretation:* parameter to determine flow velocity as $v = a*Q^b$
- *In the simulation (flow + DOC)*: important to control water residence times in the stream. It has an important influence on the flashiness of the flow, higher values would produce faster responses and vice versa, consequently for the DOC simulation as well.
- *Range*: successful applications include values between 0.005 and 0.2 but the range of exploration could be between 0.001 and 0.5.
- *Strategy/sensitivity*: adjust manually during initial manual calibration and include it in the MC analysis. It is usually a sensitive parameter but not always (e.g. small catchments).

Flow b

- *Description*: flow velocity exponent (dimensionless).
- *Physical interpretation:* parameter to determine flow velocity as $v = a*Q^b$
- *In the simulation*: important to control water residence times in the stream. It has an important influence on the flashiness of the flow, higher values would produce faster responses and vice versa, consequently for the DOC simulation as well.
- *Range*: successful applications include values between 0.7 and 0.95 but the range of exploration could be between 0.5 and 1.
- *Strategy/sensitivity*: adjust manually during initial manual calibration and include it in MC analysis. It is usually a sensitive parameter but not always (e.g. small catchments).

PDC>

Open water PDC settling velocity

- *Description*: velocity in which PDC is transferred to the stream bed sediment (m/day).
- *Physical interpretation:* it represents the rate at which the PDC exported to the stream sediments into the stream bed.
- *In the simulation*: this parameter is usually not used and a high value (around 40 m/day) as it does not influence flow or DOC simulation (it does influence PDC simulation).
- *Range*: a realistic value is not necessary because it is not used.

- *Strategy/sensitivity*: fix at 40 m/day at the beginning and do not change.

Open water PDC -> DOC

- *Description*: the rate at which PDC is transformed into DOC in the aquatic phase (/day).
- *Physical interpretation:* it represents the amount of PDC that can be transformed into DOC in a day in the stream.
- *In the simulation*: this parameter is not really used so its influence has not been assessed.
- *Range*: a realistic value can actually be 0 /day in small systems.
- *Strategy/sensitivity*: fix as 0 /day at the beginning and do not change.

Litter fall rate

- *Description*: amount of litter falling directly into the stream per unit of area per day (kg/ha/day).
- *Physical interpretation:* it represents the amount of leaves and other litter that fall directly into the stream.
- *In the simulation (DOC)*: it has very little influence.
- *Range*: if a value is known give it but there is no much influence of this parameter in the simulation and a value of 0 kg/ha/day is usually given.
- *Strategy/sensitivity*: set as 0 kg/ha/day at the beginning and do not change.

<u>DOC></u>

DOC -> DIC self-shading factor

- *Description*: as DOC increase, factor decreasing the rate in which DOC is mineralized to DIC as a consequence of photodegradation (mg/L).
- *Physical interpretation:* it allows to slow things down (i.e. decrease the rate of mineralization of DOC into DIC from photodegradation) as DOC increases and creates browner waters that hinder light to penetrate deep in the aquatic system.
- *In the simulation (DOC)*: the higher the value the lower the shading effect and the higher the photodegradation which would imply a lower DOC simulated during high radiation periods (and vice versa). A value of 0 mg/L implies complete shade effect (no photodegradation). Only useful when the parameter “DOC -> DIC radiation multiplier” is given a number, i.e. when photodegradation is considered.
- *Range*: if photodegradation is not considered give a value of 0 mg/L (the usual case). Otherwise (lake-type systems) give a value between 0.001 and 0.01 mg/L.
- *Strategy/sensitivity*: if considered, adjust manually during initial manual calibration and include it in MC analysis. It can be sensitive.

DOC -> DIC radiation multiplier

- *Description*: multiplier controlling the rate of photodegradation (DOC to DIC) in the aquatic system (kg m2/kW).

- *Physical interpretation:* it represents a factor controlling the amount of DOC that can be mineralized to DIC as a consequence of photodegradation in the aquatic system.
- *In the simulation (DOC)*: the higher the value the higher the photodegradation which would imply a lower DOC simulated during high radiation periods (and vice versa). A value of 0 kg m2/kW implies no photodegradation. Only useful when photodegradation is considered.
- *Range*: if photodegradation is not considered give a value of 0 mg/L (the usual case). Otherwise (lake-type systems) give a value between 0.00001 and 0.001 kg m2/kW.
- *Strategy/sensitivity*: if considered, adjust manually during initial manual calibration and include it in MC analysis. It can be sensitive.

Open water DOC -> DIC microbial

- *Description*: velocity in which DOC is transformed into DIC in the stream as a consequence of microbial degradation (/day).
- *Physical interpretation (DOC):* it represents the amount of DOC that can be transformed into DIC in a day by the microbial community in the stream (/day).
- *In the simulation (DOC)*: higher values would lead to larger transformation of DOC into DIC therefore a smaller DOC simulated (and vice versa).
- *Range*: useful values can be in the wide range between 0.00001 /day and 0.1 /day. If microbial degradation in the stream is not considered (probably only considered in lake-type systems) give a value of 0 /day.
- *Strategy/sensitivity*: if considered, adjust manually during initial manual calibration and include it in MC analysis. It can be sensitive.

Open water DOC -> PDC

- *Description*: velocity in which DOC is transformed into PDC in the stream (/day).
- *Physical interpretation:* it represents the amount of DOC that can be transformed into PDC in a day in the stream.
- *In the simulation*: it has not been assessed.
- *Range*: difficult to justify transformation of DOC into PDC or at least difficult to have data so a value of 0 /day is usually given.
- *Strategy/sensitivity*: fix as 0 /day at the beginning and do not change.

DIC>

Open water DIC mass transfer rate

- *Description*: parameter controlling the mass transfer of DIC to the atmosphere in the aquatic phase (m/day).
- *Physical interpretation:* it represents the amount of DIC evading the stream to the atmosphere.

- *In the simulation*: it only has an effect on the DIC simulation, which is usually not assessed, the higher the value the more DIC will be lost to the atmosphere in the aquatic and the lower the DIC simulated there.
- *Range*: give a value of around 10 m/day.
- *Strategy/sensitivity*: fix at the beginning and do not change (unless the purpose of the study is to actually simulate DIC in the stream).

DIC -> PDC (photosynthesis)

- *Description*: parameter controlling the rate of photosystems (/day).
- *Physical interpretation:* it represents speed of the photosynthesis process in a day, in which DIC is transformed into PDC.
- *In the simulation*: only affecting DIC and PDC which are usually not assessed, the higher the number the higher the PDC and the lower the DIC simulated in the stream (and vice versa).
- *Range*: usually photosynthesis is not considered to be important process in the stream and a value of 0 /day is given.
- *Strategy/sensitivity*: usually give a value of 0 /day at the beginning and do not change.

<u>Effluent / Abstraction></u>

To show the parameters in this tab, the “Reach has discharge / abstraction” box at the down left corner in this menu has to be checked.

Abstraction Flow

- *Description*: rate of water removal from reach (m3/s).
- *Physical interpretation:* represents the constant removal of water from the stream for (e.g.) agriculture or industrial use. If not constant, this can be also specified as a time series as input .abs file in the model.
- *In the simulation (flow + DOC)*: would produce a daily decrease in simulate stream flow equal to the specified value and a consequent effect on DOC.
- *Range*: usually not used because data not available so 0 m3/s, but depending on the system could have a wide range of values and could be helpful.
- *Strategy/sensitivity*: it should be a known value, so fix at the beginning and do not change, meaningless to assess sensitivity.

Effluent Flow

- *Description*: rate of water addition to reach (m3/s).
- *Physical interpretation:* represents the constant addition of water to the stream from (e.g.) industrial activities including water treatment plants. If not constant (e.g. intermittent natural water sources) this can be also specified as a time series as input .ets file in the model.
- *In the simulation (flow + DOC)*: would produce a daily increase in simulate stream flow equal to the specified value and a consequent effect on DOC.

- *Range*: usually not used because data not available so 0 m3/s, but depending on the system could have a wide range of values and could be helpful.
- *Strategy/sensitivity*: it should be a known value, so fix at the beginning and do not change, meaningless to assess sensitivity.

Effluent DOC concentration

- *Description*: concentration of DOC in the effluent (mg/L).
- *Physical interpretation:* it represents the constant DOC concentration in the specified effluent.
- *In the simulation (DOC)*: it would produce a proportional increment in the simulated DOC relative to the amount of water added in the effluent.
- *Range*: usually not used because data not available so 0 mg/L, but depending on the system could have a wide range of values and could be helpful.
- *Strategy/sensitivity*: it should be a known value, so fix at the beginning and do not change, meaningless to assess sensitivity.

<u>Instream…</u>

Some very basic parameters describing the aquatic phase

<u>Parameters></u>

Minimum water temperature

- *Description*: minimum water temperature (°C).
- *Physical interpretation:* represents the minimum possible temperature of the stream.
- *In the simulation (DOC)*: it does not really have an influence, especially if in-stream processes are not considered.
- *Range*: usually a realistic value around 0-2 °C works.
- *Strategy/sensitivity*: fix the value at the beginning and do not change, meaningless to assess sensitivity.

Water temperature lag factor

- *Description*: parameter used to smooth out the water temperature in comparison to the air temperature (dimensionless).
- *Physical interpretation:* water temperature changes are usually more gradual and slow than air temperature changes so this parameter is used to account for that.
- *In the simulation*: not really connected to anything so no influence.
- *Range*: any number between 5 and 10 works.
- *Strategy/sensitivity*: fix the value at the beginning and do not change.

Initial Values> River dynamics

Flow

- *Description*: the initial flow during the date that was set as initial date of simulation (m3/s).
- *Physical interpretation:* represents the initial flow in stream.
- *In the simulation (flow + DOC)*: important to start the simulation at the right flow magnitude. It will only influence the initial period.
- *Range*: depends on the size of the sub-catchment, from as low as 0.0001 m3/s to as much as 500 m3/s. If the value is not known, give an estimation according the climate data and similar periods where flow is known.
- *Strategy/sensitivity*: fix the value at the beginning and do not change, meaningless to assess sensitivity.

Water temperature

- *Description*: the initial water temperature during the date that was set as initial date of simulation (°C).
- *Physical interpretation:* initial water temperature in the stream.
- *In the simulation*: not really connected to anything so no influence.
- *Range*: give a rough estimate.
- *Strategy/sensitivity*: fix the value at the beginning and do not change, meaningless to assess sensitivity.

Initial Values> Open water carbon

PDC concentration

- *Description*: the initial PDC concentration in the stream during the date that was set as initial date of simulation (mg/L).
- *Physical interpretation:* initial PDC concentration in the stream.
- *In the simulation*: does not have any real influence.
- *Range*: give a value around 1 mg/L.
- *Strategy/sensitivity*: fix the value at the beginning and do not change, meaningless to assess sensitivity.

DOC concentration

- *Description*: the initial DOC concentration in the stream during the date that was set as initial date of simulation (mg/L).
- *Physical interpretation:* initial DOC concentration in the stream.
- *In the simulation (DOC)*: important to start the simulation at the right DOC magnitude. It will only influence the initial period.

- *Range*: if known, give the value, otherwise give an estimate taking into account the periods of known DOC concentrations.
- *Strategy/sensitivity*: fix the value at the beginning and do not change, meaningless to assess sensitivity.

DIC concentration

- *Description*: the initial DIC concentration in the stream during the date that was set as initial date of simulation (mg/L).
- *Physical interpretation:* initial DIC concentration in the stream.
- *In the simulation*: only has some influence on the initial period in the DIC simulation.
- *Range*: give the value if known, otherwise a rough estimate, maybe 1 to 2 mg/L.
- *Strategy/sensitivity*: fix the value at the beginning and do not change, meaningless to assess sensitivity.

Land Phase…

These parameters are applied at the land use scale, which means that one set of these parameters must be provided for each land use type defined in the parameter file. If we want to implement the same change in one parameter to all land use types, the “Lock parameter sets” box at the top right corner of the menu can be checked.

The basics of the model is based on the transformation processes between different carbon pools in the form of $dX/dt = f(M) \cdot f(T) \cdot [k1 \cdot Y - k2 \cdot X]$, where, every day (every time step), there are transformation between carbon pool *X* and carbon pool *Y* (e.g. sorption/desorption, production/consumption) controlled by k1 and k2 rates, and those are a function of the moisture M status and the temperature T. The amount transferred is in kg. Thus, the most sensitive parameters in the model are moisture and temperature related parameters, together with transformation rate parameters (especially in the upper soil box and the ones relating to DOC).

Processes> SOC

Organic layer SOC to DOC

- *Description*: the rate at which SOC is transformed into DOC in the upper layer (/day).
- *Physical interpretation:* it represents the amount of SOC that can be transformed into DOC in the upper layer in a day.
- *In the simulation (DOC)*: higher values would simulate more DOC and would decrease SOC pools in the upper layer (and vice versa).
- *Range*: it depends on the values given to other transformation rates as they are all related but in general in the order of 0.0001 to 0.01 /day.
- *Strategy/sensitivity*: adjust manually during initial manual calibration and include it in the MC analysis. Sensitive.

Organic layer SOC to DIC

- *Description*: the rate at which SOC is transformed into DIC in the upper layer (/day).
- *Physical interpretation:* it represents the amount of SOC that can be transformed into DIC in the upper layer in a day.
- *In the simulation (DOC)*: higher values would tend to simulate less DOC and more DIC and would decrease SOC pools in the upper layer (and vice versa).
- *Range*: it could be considered 0 /day, otherwise values around 1E-08 to 1E-04 but it also depends on the values given to other transformation rates.
- *Strategy/sensitivity*: adjust manually during initial manual calibration and include it in the MC analysis. It can be sensitive.

Mineral layer SOC to DOC

- *Description*: the rate at which SOC is transformed into DOC in the lower layer (/day).
- *Physical interpretation:* it represents the amount of SOC that can be transformed into DOC in the lower layer in a day.
- *In the simulation (DOC)*: higher values would simulate more DOC and would decrease SOC pools in the lower layer (and vice versa).
- *Range*: it depends on the values given to other transformation rates as they are all related but in general in the order of 1E-06 to 0.0002 /day.
- *Strategy/sensitivity*: adjust manually during initial manual calibration and include it in the MC analysis. It can be sensitive.

Mineral layer SOC to DIC

- *Description*: the rate at which SOC is transformed into DIC in the lower layer (/day).
- *Physical interpretation:* it represents the amount of SOC that can be transformed into DIC in the lower layer in a day.
- *In the simulation*: higher values would tend to simulate less DOC and more DIC and would decrease SOC pools in the lower layer (and vice versa).
- *Range*: it could be considered 0 /day, otherwise values around 1E-08 to 1E-04 but it also depends on the values given to other transformation rates.
- *Strategy/sensitivity*: adjust manually during initial manual calibration and include it in the MC analysis. It can be sensitive.

<u>Processes> PDC</u>

Organic layer PDC to SOC

- *Description*: the rate at which PDC is transformed into SOC in the upper layer (/day).
- *Physical interpretation:* it represents the amount of PDC that can be transformed into SOC in the upper layer in a day.

- *In the simulation (DOC)*: higher values would decrease the simulated DOC, as less PDC would be available to be transformed to DOC (and vice versa). Important parameter to control PDC in direct runoff.
- *Range*: it depends on the values given to other transformation rates as they are all related but in general in the order of 0.0001 to 0.02 /day.
- *Strategy/sensitivity*: adjust manually during initial manual calibration and include it in the MC analysis. It can be sensitive.

Organic layer PDC to DIC

- *Description*: the rate at which PDC is transformed into DIC in the upper layer (/day).
- *Physical interpretation:* it represents the amount of PDC that can be transformed into DIC in the upper layer in a day.
- *In the simulation (DOC)*: higher values would decrease the simulated DOC, as less PDC would be available to be transformed to DOC (and vice versa). Important parameter to control PDC in direct runoff.
- *Range*: it depends on the values given to other transformation rates as they are all related but in general in the order of 0.0001 to 0.01 /day.
- *Strategy/sensitivity*: adjust manually during initial manual calibration and include it in the MC analysis. It can be sensitive.

Organic layer PDC to DOC

- *Description*: the rate at which PDC is transformed into DOC in the upper layer (/day).
- *Physical interpretation:* it represents the amount of PDC that can be transformed into DOC in the upper layer in a day.
- *In the simulation (DOC)*: higher values would increase the simulated DOC (and vice versa). Important parameter to control PDC in direct runoff.
- *Range*: it depends on the values given to other transformation rates as they are all related but in general in the order of 0.00001 to 0.01 /day.
- *Strategy/sensitivity*: adjust manually during initial manual calibration and include it in the MC analysis. It can be sensitive.

Daily PDC input to organic layer

- *Description*: the amount of material as PDC received by the upper layer per day and per km2 (kg/day).
- *Physical interpretation:* it represents the additions of PDC to the upper soil layer in a day.
- *In the simulation (DOC)*: higher values would tend to simulate more DOC (and vice versa).
- *Range*: a value around 1 kg/day should work and be reasonable, but this process is better controlled with the parameter “Litterfall”.
- *Strategy/sensitivity*: adjust manually during initial manual calibration and include it or not in the MC analysis. Not very sensitive, better focus on the parameter “Litterfall”.

Direct runoff PDC to DOC

- *Description*: the rate at which PDC is transformed into DOC in the direct runoff layer (/day).
- *Physical interpretation:* this parameter was added to represent for the common relationship between high flow and high DOC in forest catchments where the model had problems.
- *In the simulation (DOC)*: higher values would increase the DOC simulated during high flow conditions (and vice versa). Important parameter to control PDC in direct runoff.
- *Range*: it can be 0 /day in wetland-type catchment as the discharge-DOC relationship is actually negative and in other cases it can have a value around 0.0000001 to 0.01 /day.
- *Strategy/sensitivity*: adjust manually during initial manual calibration and include it in the MC analysis. Sensitive.

<u>Processes> DOC</u>

Organic layer DOC to SOC

- *Description*: the rate at which DOC is transformed into SOC in the upper layer (/day).
- *Physical interpretation:* it represents the amount of DOC that can be transformed into SOC in the upper layer in a day.
- *In the simulation (DOC)*: higher values would simulate less DOC and would increase SOC pools in the upper layer (and vice versa).
- *Range*: it depends on the values given to other transformation rates as they are all related but in general in the order of 0.00001 to 0.001 /day.
- *Strategy/sensitivity*: adjust manually during initial manual calibration and include it in the MC analysis. Sensitive.

Organic layer DOC to DIC

- *Description*: the rate at which DOC is transformed into DIC in the upper layer (/day).
- *Physical interpretation:* it represents the amount of DOC that can be transformed into DIC in the upper layer in a day.
- *In the simulation (DOC)*: higher values would simulate less DOC and more DIC (and vice versa).
- *Range*: it depends on the values given to other transformation rates as they are all related but in general in the order of 0.00001 to 0.001 /day.
- *Strategy/sensitivity*: adjust manually during initial manual calibration and include it in the MC analysis. It can be sensitive.

Mineral layer DOC to SOC

- *Description*: the rate at which DOC is transformed into SOC in the lower layer (/day).
- *Physical interpretation:* it represents the amount of DOC that can be transformed into SOC in the lower layer in a day.
- *In the simulation (DOC)*: higher values would simulate less DOC and would increase SOC pools in the lower layer (and vice versa). Important to control base flow simulation.

- *Range*: it depends on the values given to other transformation rates as they are all related but in general in the order of 0.0001 to 0.1 /day.
- *Strategy/sensitivity*: adjust manually during initial manual calibration and include it in the MC analysis. It can be sensitive.

Mineral layer DOC to DIC

- *Description*: the rate at which DOC is transformed into DIC in the lower layer (/day).
- *Physical interpretation:* it represents the amount of DOC that can be transformed into DIC in the lower layer in a day.
- *In the simulation (DOC)*: higher values would simulate less DOC and more DIC (and vice versa).
- *Range*: it depends on the values given to other transformation rates as they are all related but in general in the order of 0.000001 to 0.001 /day.
- *Strategy/sensitivity*: adjust manually during initial manual calibration and include it in the MC analysis. It can be sensitive.

<u>Processes> DIC</u>

Organic layer CO2 mass transfer velocity

- *Description*: parameter (not used anymore) controlling mass transfer velocity of CO2 in the upper layer (/day).
- *Physical interpretation:* it controls the amount of CO2 that can be transferred from the soil (upper layer) to the atmosphere in a day.
- *In the simulation*: does not have any real influence.
- *Range*: any number as this parameter is not in use anymore.
- *Strategy/sensitivity*: fix a value at the beginning and do not change.

Mineral layer CO2 mass transfer velocity

- *Description*: parameter (not used anymore) controlling mass transfer velocity of CO2 in the lower layer (/day).
- *Physical interpretation:* it controls the amount of CO2 that can be transferred from the soil (lower layer) to the atmosphere in a day.
- *In the simulation*: does not have any real influence.
- *Range*: any number as this parameter is not in use anymore.
- *Strategy/sensitivity*: fix a value at the beginning and do not change.

<u>Processes> Enzymatic latch</u>

To simulate the increase in biological processes during dry conditions that can lead to a higher DOC flux. When the SMD goes above certain threshold ("Organic layer critical SMD threshold" and "Mineral layer critical SMD threshold"), as in a very dry environment, this triggers a process by which the transformation rate from SOC to DOC increase by a specified rate ("Organic layer enzymatic latch rate" and “Mineral layer enzymatic latch rate”), and then decreases linearly to the base level during a specified time (“Organic layer return time” and “Mineral layer return time”). For dry catchments or to address scenarios with drier conditions.

Organic layer return time

- *Description*: see above.
- *Physical interpretation:* see above.
- *In the simulation*: higher values would increase the period of higher DOC after the SMD threshold is reached (and vice versa).
- *Range*: a few weeks.
- *Strategy/sensitivity*: only use if we know the process occurs and/or in dry catchments.

Organic layer enzymatic latch rate

- *Description*: see above.
- *Physical interpretation:* see above.
- *In the simulation*: higher values would increase the simulated DOC during dry periods, a value of 0 /day would not do anything.
- *Range*: if used, values in the order of 0.0001 and 0.01 /day.
- *Strategy/sensitivity*: only use if we know the process occurs and/or in dry catchments.

Organic layer critical SMD threshold

- *Description*: see above.
- *Physical interpretation:* see above.
- *In the simulation*: if the value is above the highest SMD in the record, nothing will happen, from there, the lower values the more periods with potential to simulate DOC.
- *Range*: depends on the SMD time series, around 50-100 mm maybe.
- *Strategy/sensitivity*: only use if we know the process occurs and/or in dry catchments.

Mineral layer return time

- *Description*: see above.
- *Physical interpretation:* see above.
- *In the simulation*: higher values would increase the period of higher DOC after the SMD threshold is reached.
- *Range*: a few weeks.
- *Strategy/sensitivity*: only use if we know the process occurs and/or in dry catchments.

Mineral layer enzymatic latch rate

- *Description*: see above.
- *Physical interpretation:* see above.

- *In the simulation*: higher values would increase the simulated DOC during dry periods, a value of 0 /day would not do anything.
- *Range*: if used, values in the order of 0.0001 and 0.01 /day.
- *Strategy/sensitivity*: only use if we know the process occurs and/or in dry catchments.

Mineral layer critical SMD threshold

- *Description*: see above.
- *Physical interpretation:* see above.
- *In the simulation*: if the value is above the highest SMD in the record, nothing will happen, from there, the lower values the more periods with potential to simulate DOC.
- *Range*: depends on the SMD time series, around 50-100 mm maybe.
- *Strategy/sensitivity*: only use if we know the process occurs and/or in dry catchments.

Processes> Sulphate

This is only relevant when there is a .dts file used, i.e. an input file with deposition time series of an strong acidifying anion; or when a constant deposition is specified under Sub-catchment>Deposition> Atmospheric deposition loads. These parameters try to represent the decrease in carbon solubility when there is an strong acidifying anion present in the soils solution, i.e. limiting the SOC desorption into DOC, such as dDOC/dt = -(k2 + b1 · [anion]exp b2) · DOC + k1 · SOC.

Organic layer b1

- *Description*: see above.
- *Physical interpretation:* see above.
- *In the simulation*: higher number would decrease the simulated DOC, a value of 0 would mean no influence.
- *Range*: if used, values in the range of 1E-06 to 1E-03.
- *Strategy/sensitivity*: if used, adjust manually during initial manual calibration and include it in MC analysis. It can be a sensitive parameter.

Organic layer b2

- *Description*: see above.
- *Physical interpretation:* see above.
- *In the simulation*: higher number would decrease the simulated DOC.
- *Range*: usually 1 or a bit higher.
- *Strategy/sensitivity*: if used, adjust manually during initial manual calibration and include it in MC analysis. It can be a sensitive parameter.

Mineral layer b1

- *Description*: see above.

- *Physical interpretation:* see above.
- *In the simulation*: higher number would decrease the simulated DOC, a value of 0 would mean no influence.
- *Range*: if used, values in the range of 1E-06 to 1E-03.
- *Strategy/sensitivity*: if used, adjust manually during initial manual calibration and include it in MC analysis. It can be a sensitive parameter.

Mineral layer b2

- *Description*: see above.
- *Physical interpretation:* see above.
- *In the simulation*: higher number would decrease the simulated DOC.
- *Range*: usually 1 or a bit higher.
- *Strategy/sensitivity*: if used, adjust manually during initial manual calibration and include it in MC analysis. It can be a sensitive parameter.

<u>Initial values> Direct runoff</u>

Flow

- *Description*: initial flow in the direct runoff layer (m3/s).
- *Physical interpretation:* it represents the initial overland flow (m3/s).
- *In the simulation (flow + DOC)*: higher values would simulate higher flow at the beginning of the time series simulation.
- *Range*: give a value of 0 m3/s as initial flow conditions are set with the Instream>Initial Values> River dynamics> “Flow” parameter.
- *Strategy/sensitivity*: fix as 0 m3/s at the beginning and do not change.

PDC

- *Description*: initial amount of PDC in the direct runoff layer (kg/ha).
- *Physical interpretation:* it represents the initial amount of PDC in the direct runoff layer per unit of area.
- *In the simulation (DOC)*: higher values would increment the simulated DOC at the beginning of the simulation period (and vice versa). Important to keep this value more or less stable during the simulation in direct runoff PDC tab.
- *Range*: around 10000 kg/ha (±50%) is a reasonable estimate.
- *Strategy/sensitivity*: give an estimate at the beginning and do not change or slightly manually adjust later.

DOC

- *Description*: initial DOC concentration in the direct runoff layer (mg/L).
- *Physical interpretation:* it represents the initial DOC concentration in the direct runoff layer.

- *In the simulation*: does not really have an influence.
- *Range*: as direct runoff water represents overland flow it will have a rainfall type of signal so values around 1-2 mg/L are reasonable.
- *Strategy/sensitivity*: give an estimate at the beginning and do not change or slightly manually adjust later. Not sensitive.

Initial values> Organic layer

Flow

- *Description*: initial flow in the upper soil layer (m3/s).
- *Physical interpretation:* it represents the initial flow from the upper layer.
- *In the simulation (flow + DOC)*: higher values would simulate higher flow at the beginning of the time series simulation.
- *Range*: give a value of 0 m3/s as initial flow conditions are set with the Instream>Initial Values> River dynamics> "Flow" parameter.
- *Strategy/sensitivity*: fix as 0 m3/s at the beginning and do not change.

SOC

- *Description*: initial amount of SOC in the upper layer (kg/ha).
- *Physical interpretation:* it represents the initial soil carbon pool in the upper layer per unit of area.
- *In the simulation (DOC)*: higher values would lead to a higher simulation of DOC throughout the simulation period.
- *Range*: in the order of 10000 to 20000 kg/ha for very low carbon content soils to as much as 80000 kg/ha for peatlands.
- *Strategy/sensitivity*: give an estimate at the beginning and maybe slightly manually adjust later. Sensitive

DOC

- *Description*: initial DOC concentration in the upper layer (mg/L).
- *Physical interpretation:* it represents the initial DOC concentration in the upper layer.
- *In the simulation (DOC)*: small influence at the beginning of the simulation period.
- *Range*: give realistic values depending on the soil and land use type, from 1-2 mg/L for very mineral soils to as much as 100 mg/L for very organic soils.
- *Strategy/sensitivity*: give an estimate at the beginning and do not change or slightly manually adjust later. Not really sensitive.

DIC

- *Description*: initial DIC concentration in the upper layer (mg/L).
- *Physical interpretation:* it represents the initial DIC concentration in the upper layer.

- *In the simulation*: small influence at the beginning of the DIC simulation.
- *Range*: give a rough estimate depending on the soil/land use type.
- *Strategy/sensitivity*: give an estimate at the beginning and do not change or slightly manually adjust later. Not sensitive for DOC.

Initial values> Mineral layer

Flow

- *Description*: initial flow in the lower soil layer (m3/s).
- *Physical interpretation:* it represents the initial flow from the lower layer.
- *In the simulation (flow + DOC)*: higher values would simulate higher flow at the beginning of the time series simulation.
- *Range*: give a value of 0 m3/s as initial flow conditions are set with the Instream>Initial Values> River dynamics> “Flow” parameter.
- *Strategy/sensitivity*: fix as 0 m3/s at the beginning and do not change.

SOC

- *Description*: initial amount of SOC in the lower layer (kg/ha).
- *Physical interpretation:* it represents the initial soil carbon pool in the lower layer per unit of area.
- *In the simulation (DOC)*: higher values would lead to a higher simulation of DOC throughout the simulation period.
- *Range*: in the order of 10000 to 20000 kg/ha for very low carbon content soils to as much as 80000 kg/ha for peatlands.
- *Strategy/sensitivity*: give an estimate at the beginning and maybe slightly manually adjust later.

DOC

- *Description*: initial DOC concentration in the lower layer (mg/L).
- *Physical interpretation:* it represents the initial DOC concentration in the lower layer.
- *In the simulation (DOC)*: small influence at the beginning of the simulation period.
- *Range*: give realistic values depending on the soil and land use type, from 1-2 mg/L for very mineral soils to as much as 100 mg/L for very organic soils.
- *Strategy/sensitivity*: give an estimate at the beginning and do not change or slightly manually adjust later. Not really sensitive.

DIC

- *Description*: initial DIC concentration in the lower layer (mg/L).
- *Physical interpretation:* it represents the initial DIC concentration in the lower layer.
- *In the simulation*: small influence at the beginning of the DIC simulation.
- *Range*: give a rough estimate depending on the soil/land use type.

- *Strategy/sensitivity*: give an estimate at the beginning and do not change or slightly manually adjust later. Not sensitive for DOC.

Initial values> Temperature

Initial soil temperature

- *Description*: initial soil temperature (°C).
- *Physical interpretation:* it represents the initial temperature in the soil at the start of the simulation period.
- *In the simulation*: does not really do anything.
- *Range*: give an estimate based on real data or the air temperature at the beginning of the simulation period.
- *Strategy/sensitivity*: fix at the beginning and do not change.

Constants> Volume> Volume constants

Organic layer retention volume

- *Description*: amount of water per km2 in the upper layer below which water no longer freely drains (m3).
- *Physical interpretation:* it represents the volume of water in the upper layer at the permanent wilting point, i.e. the pool of DOC in the upper layer that is not drained but can be exchanged with other soil boxes.
- *In the simulation (DOC)*: higher values would lead to a lower DOC concentration simulation as less DOC is available to be drained. Important to get the timing of the DOC peaks (the dynamics in general) correct.
- *Range*: values around 50000 to 200000 m3 work well.
- *Strategy/sensitivity*: adjust manually during initial manual calibration and definitely include it in MC analysis. It is usually a sensitive parameter.

Mineral layer retention volume

- *Description*: amount of water per km2 in the lower layer below which water no longer freely drains (m3).
- *Physical interpretation:* it represents the volume of water in the lower layer at the permanent wilting point, i.e. the pool of DOC in the lower layer that is not drained but can be exchanged with other soil boxes.
- *In the simulation (DOC)*: higher values would lead to a lower DOC concentration simulation as less DOC is available to be drained.
- *Range*: values around 30000 to 100000 m3 work well.
- *Strategy/sensitivity*: adjust manually during initial manual calibration and definitely include it in MC analysis. It is usually a sensitive parameter.

Constants> Time> Time constants

Direct runoff residence time

- *Description*: characteristic time constant for water drainage (days).
- *Physical interpretation:* it represents the residence time of water in the direct runoff layer as a proxy to the hydrological connectivity.
- *In the simulation (flow + DOC)*: lower values would produce faster responses (increase flashiness) and vice versa.
- *Range*: typical values might vary between 0.5 day and 1.5 days.
- *Strategy/sensitivity*: adjust manually during initial manual calibration and include it in MC analysis. It is usually a sensitive parameter.

Organic layer residence time

- *Description*: characteristic time constant for water drainage (days).
- *Physical interpretation:* it represents the residence time of water in the upper layer as a proxy to the hydrological connectivity. Only applies to the fraction of water which is above the "Retention volume", i.e. the water than can actually move. In other words, it represents how much time it takes for the water that comes to the specific soil box to leave.
- *In the simulation (flow + DOC)*: lower values would produce faster responses (increase flashiness) and vice versa.
- *Range*: In small flashy catchments, the upper soil box can also have values near 1 day, while big streams around 5 days.
- *Strategy/sensitivity*: adjust manually during initial manual calibration and include it in MC analysis. It is usually a sensitive parameter.

Mineral layer residence time

- *Description*: characteristic time constant for water drainage (days).
- *Physical interpretation:* it represents the residence time of water in the lower layer as a proxy to the hydrological connectivity. Only applies to the fraction of water which is above the "Retention volume", i.e. the water than can actually move. In other words, it represents how much time it takes for the water that comes to the specific soil box to leave.
- *In the simulation (flow + DOC)*: lower values would produce faster responses (increase flashiness) and vice versa.
- *Range*: In small flashy catchments, the lower soil box can also have values near 10 days, while big streams around 20-30 days or more.
- *Strategy/sensitivity*: adjust manually during initial manual calibration and include it in MC analysis. It can be sensitive.

Constants> DICmax

Organic layer DICmax

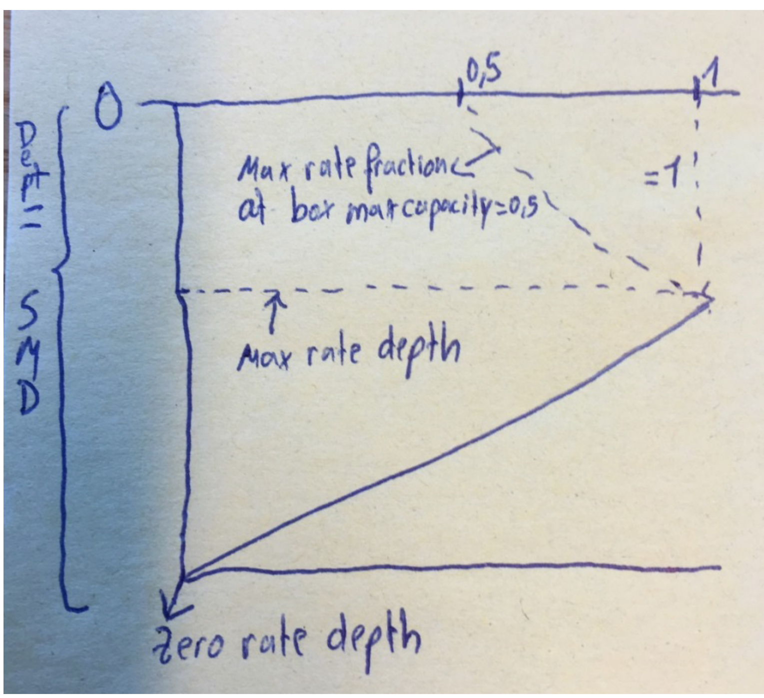
- *Description*: parameter not in use.
- *Physical interpretation:* nothing.
- *In the simulation*: does nothing.
- *Range*: any value.
- *Strategy/sensitivity*: fix at the beginning and do not change.

Mineral layer DICmax

- *Description*: parameter not in use.
- *Physical interpretation:* nothing.
- *In the simulation*: does nothing.
- *Range*: any value.
- *Strategy/sensitivity*: fix at the beginning and do not change.

Thresholds> Soil Moisture Deficit> Limiting factors

These parameters are used to regulate transformation rates at different moisture conditions. Above a specified SMD ("Zero rate depth"), processes are turned off, and below they linearly increase until the base level at another specified SMD value ("Max rate depth"). Below the "Max rate depth", another parameter ("Max rate fraction at box max capacity") controls the decrease in transformation rates until SMD=0.



Maximum soil moisture deficit

- *Description*: not in use anymore.
- *Physical interpretation:* not in use anymore.
- *In the simulation*: not in use anymore.
- *Range*: not in use anymore.
- *Strategy/sensitivity*: not in use anymore.

Zero rate depth

- *Description*: see above.
- *Physical interpretation:* see above.
- *In the simulation (DOC)*: lower values would reduce the simulated DOC.
- *Range*: depending on the SMD time series.
- *Strategy/sensitivity*: adjust manually during initial manual calibration and include it in MC analysis. It is usually sensitive.

Max rate depth

- *Description*: see above.
- *Physical interpretation:* see above.
- *In the simulation (DOC)*: lower values would reduce the simulated DOC.
- *Range*: it should be lower than “Zero rate depth” to make sense. If value is higher than the maximum SMD in the time series, these processes are not considered.
- *Strategy/sensitivity*: adjust manually during initial manual calibration and include it in MC analysis. It is usually sensitive.

Max rate fraction at box max capacity

- *Description*: see above.
- *Physical interpretation:* see above.
- *In the simulation (DOC)*: lower values would decrease the simulated DOC.
- *Range*: it should be between 0 (meaning at SMD=0 processes are turned off) and 1 (meaning processes are equal to the base line from the “Max rate depth” to SMD=0.
- *Strategy/sensitivity*: adjust manually during initial manual calibration and include it in MC analysis. It can be sensitive.

<u>Thresholds> Sustainable Flows> Limiting factors</u>

Minimum organic layer flow

- *Description*: minimum threshold flow in the upper layer (m3/s).
- *Physical interpretation:* it is used to always simulate a minimum flow in the upper layer, not really used anymore as it breaks the water balance.

- *In the simulation*: not assessed.
- *Range*: give a value of 0 m3/s.
- *Strategy/sensitivity*: set as 0 m3/s at the beginning and do not change.

Minimum mineral layer flow

- *Description*: minimum threshold flow in the upper layer (m3/s).
- *Physical interpretation:* it is used to always simulate a minimum flow in the lower layer, not really used anymore as it breaks the water balance.
- *In the simulation*: not assessed.
- *Range*: give a value of 0 m3/s.
- *Strategy/sensitivity*: set as 0 m3/s at the beginning and do not change.

Sub-models> Soil Temperature> Summer / winter temperatures

Difference between summer/winter maximums

- *Description*: difference soil temperature between the maximum in summer and in winter (°C).
- *Physical interpretation:* it represents the difference between the maximum soil temperature in the summer and in the winter.
- *In the simulation*: it does not really do anything.
- *Range*: values around 5 to 15 °C are reasonable.
- *Strategy/sensitivity*: fix at the beginning and do not change, not sensitive.

Thermal conductivity of soil

- *Description*: thermal conductivity of the soil (W/m K).
- *Physical interpretation:* it represents the thermal conductivity of the soil.
- *In the simulation (DOC)*: lower values would tend to decrease the simulated DOC.
- *Range*: depending on the type of soil, from around 0.1 W/m K to around 2 or 3 W/m K.
- *Strategy/sensitivity*: adjust manually during initial manual calibration and include it in MC analysis. It is usually sensitive.

Specific heat capacity due to freeze/thaw

- *Description*: specific heat capacity due to freeze/thaw.
- *Physical interpretation:* it represents head capacity at around freezing conditions.
- *In the simulation (DOC)*: higher values would lead to a higher DOC simulation during periods with temperatures around 0 °C.
- *Range*: around 5 to 15.
- *Strategy/sensitivity*: give a rough estimate at the beginning and do not change or slightly modify it manually later on. Not really sensitive.

Sub-models> Soil Temperature> Snow pack effects

Snow depth factor

- *Description*: parameter relating depth of snow with depth of water.
- *Physical interpretation:* it represents the relationship between depth of snow and amount of water in the snow pack.
- *In the simulation (DOC)*: a higher negative value would decrease the DOC during snow conditions.
- *Range*: give a value around -0.01
- *Strategy/sensitivity*: manually adjust around -0.01. Not very sensitive but do not change too much from -0.01.

Sub-models> Temperature Response> COUP Model response function

Response to a 10 °C soil temperature change for each process

- *Description*: it multiplies the process rates by the specified value for every 10 degrees increment with respect to the base level soil temperature at which the processes are multiplied by 1.
- *Physical interpretation:* it represents the increase in biological production with soil temperature.
- *In the simulation (DOC)*: lower values would give a higher absolute DOC simulation with a lower span or range in variation and vice versa.
- *Range*: values around 5 to 6 are unrealistic but give good simulations, although not always. According the theory, an increase in temperature of 10 °C should double process rates so a value of 2 is reasonable.
- *Strategy/sensitivity*: play with values around 2 in the manual calibration. If included in the MC analysis do not include “Base temperature for each process at which the response is 1”. This is a sensitive parameter.

Base temperature for each process at which the response is 1

- *Description*: the base line soil temperature at which the process rates are 1 (°C).
- *Physical interpretation:* it represents the reference soil temperature to control temperature dependence on process rates.
- *In the simulation (DOC)*: lower value would tend to increase the simulated DOC and vice versa.
- *Range*: values around 5 to 15 °C.
- *Strategy/sensitivity*: adjust manually during initial manual calibration and if included in the MC analysis do not include “Response to a 10 °C soil temperature change for each process”. This is a sensitive parameter.

Sub-models> Snow Pack> Snow accumulation sub-model

Initial depth (as water equivalent)

- *Description*: initial depth of snow pack (mm).

- *Physical interpretation:* represents the size of the snow pack over the ground.
- *In the simulation*: does not really do anything, only coupled to the modelling of soil temperature.
- *Range*: depends on the system.
- *Strategy/sensitivity*: give a rough estimate at the beginning and do not change. Meaningless to assess sensitivity.

Degree day factor for snowmelt

- *Description*: temperature-dependent rate at which snow melts (mm/°C).
- *Physical interpretation:* it represents the amount of snow (in mm depth of water) that melts for every degree Celsius that the temperature is above threshold temperature for snow pack to melt ("Snow melt temperature").
- *In the simulation (flow + DOC)*: a higher value will imply faster responses, i.e. more flashy responses and higher peaks as the snow will melt quicker and contribute to flow much faster (but also leave faster) and vice versa.
- *Range*: successful applications include values as low as 0.5 mm/°C and up to 3.5 mm/°C. It could vary between 0.5 mm/°C and 4 mm/°C, but 3 mm/°C is maybe already in the upper range of realistic values and 1 mm/°C in the lower realistic range. We might give lower values to forest than to open areas such as wetlands ("At times, the melt rate in the forest was half that of the open site" according to Woo and Heron, 1987).
- *Strategy/sensitivity*: adjust manually during initial manual calibration and maybe include it in MC analysis. Not very sensitive.

Water equivalent factor

- *Description*: parameter relating depth of snow with depth of water.
- *Physical interpretation:* it represents the relationship between depth of snow and amount of water in the snow pack.
- *In the simulation (flow + DOC)*: higher values would produce higher flow peaks after snowmelt and probably higher DOC.
- *Range*: around 0.1 to 1.
- *Strategy/sensitivity*: manually adjust during initial manual calibration and do not change or slightly adjust later on. Not very sensitive.

<u>Fertiliser> Addition</u>

Fertiliser addition start day

- *Description*: day in the calendar for literfall addition.
- *Physical interpretation:* it represents the initial day for literfall in the year.
- *In the simulation*: not assessed.
- *Range*: usually assumed a one year round literfall (average) starting at day 1, so 1.

- *Strategy/sensitivity*: fix to 1 at the beginning and do not change.

Fertiliser addition period

- *Description*: number of days with literfall in a year (days).
- *Physical interpretation:* it represents the number of days from the initial day that there will be literfall.
- *In the simulation*: not assessed.
- *Range*: usually assumed a one year round litterfall (average) so 365.
- *Strategy/sensitivity*: fix to 365 at the beginning and do not change.

<u>Fertiliser> Inputs</u>

Litterfall

- *Description*: the amount of literfall per unit of area per day in the catchment (kg/ha/day).
- *Physical interpretation:* it represents the amount of literfall falling every day in the catchment and can go to PDC and DOC later on.
- *In the simulation (DOC)*: higher values would increase the simulated DOC and the PDC in the direct runoff layer (and vice versa).
- *Range*: a value around 0.2 kg/ha/day is reasonable but successful simulations have had as much as 1 kg/ha/day (e.g. agricultural additions).
- *Strategy/sensitivity*: adjust manually during initial manual calibration and include it in the MC analysis. It can be a sensitive parameter.

<u>Partitioning> Organic layer</u>

Fast pool fraction

- *Description*: fraction of the total SOC in the upper layer that belongs to the fast pool.
- *Physical interpretation:* the upper layer is divided into a fast SOC pool where carbon produced and easily leachable and a slow carbon pool where carbon is not available at the time step.
- *In the simulation (DOC)*: higher values would lead to higher simulated DOC and vice versa.
- *Range*: from 0.5 to 0.9 or more, depending on the soil type.
- *Strategy/sensitivity*: adjust manually during initial manual calibration and include it in the MC analysis. It can be a sensitive parameter.

Rate constant

- *Description*: parameter controlling speed of equilibration between fast and slow pools in the upper layer.
- *Physical interpretation:* it represents the speed at which carbon can go from the slow pool to the fast pool in the upper layer after fast pool is leaching the carbon.
- *In the simulation*: does not seem to have a big influence

- *Range*: values around 100.
- *Strategy/sensitivity*: adjust manually during initial manual calibration and include it in the MC analysis. Not really sensitive.

Partitioning> Mineral layer

Fast pool fraction

- *Description*: fraction of the total SOC in the lower layer that belongs to the fast pool.
- *Physical interpretation:* the lower layer is divided into a fast SOC pool where carbon produced and easily leachable and a slow carbon pool where carbon is not available at the time step.
- *In the simulation (DOC)*: higher values would lead to higher simulated DOC and vice versa.
- *Range*: from 0.1 to 0.9, depending on the soil type.
- *Strategy/sensitivity*: adjust manually during initial manual calibration and include it in the MC analysis. It can be a sensitive parameter.

Rate constant

- *Description*: parameter controlling speed of equilibration between fast and slow pools in the lower layer.
- *Physical interpretation:* it represents the speed at which carbon can go from the slow pool to the fast pool in the lower layer after fast pool is leaching the carbon.
- *In the simulation*: does not seem to have a big influence.
- *Range*: values around 100.
- *Strategy/sensitivity*: adjust manually during initial manual calibration and include it in the MC analysis. Not really sensitive.

3. Model calibration and uncertainty and sensitivity analyses

Based on de Wit et al. (2016).

3.1 Manual calibration

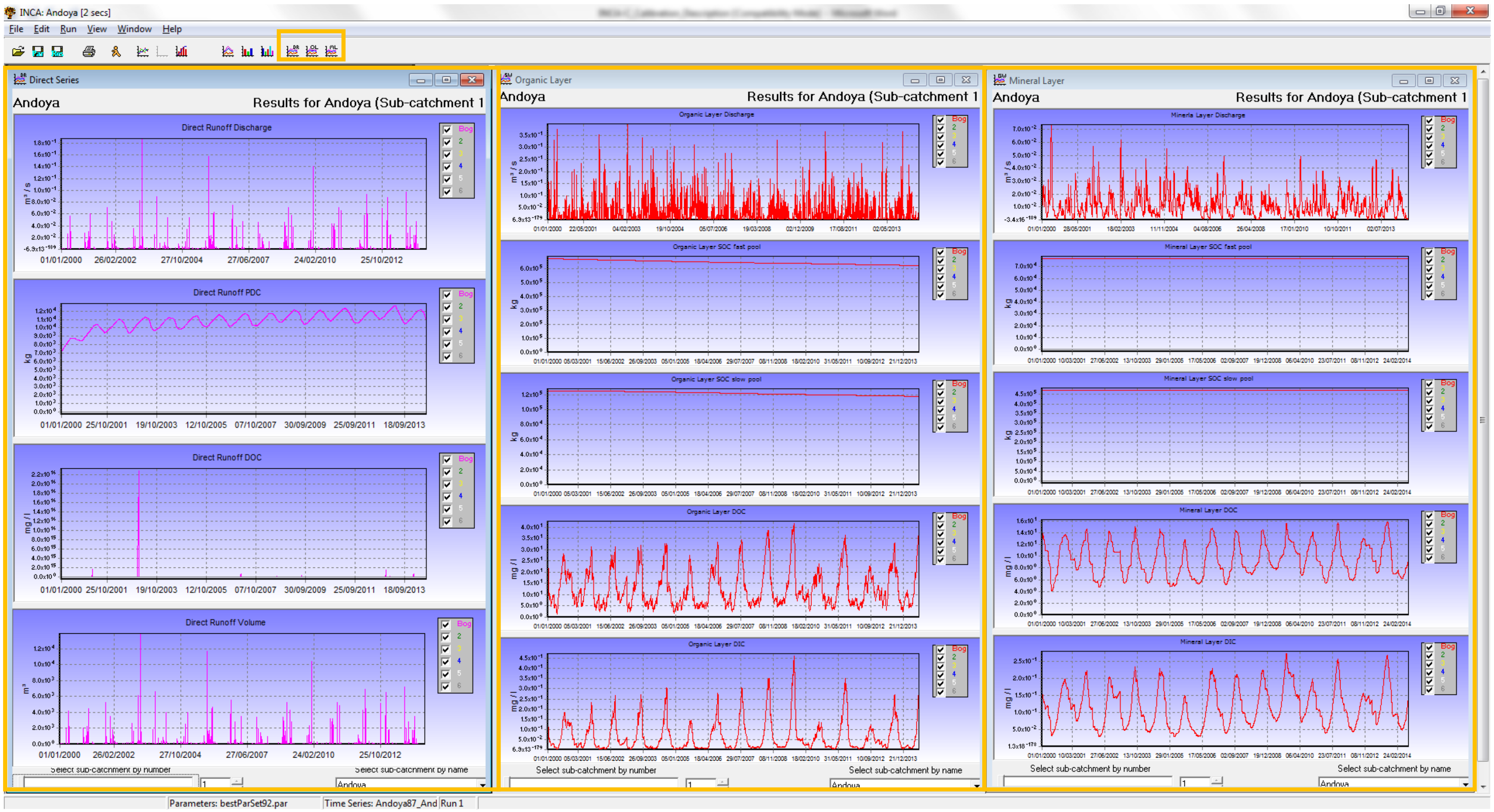
.par file, .dat file, and .obs file are loaded into the model through File>Open….

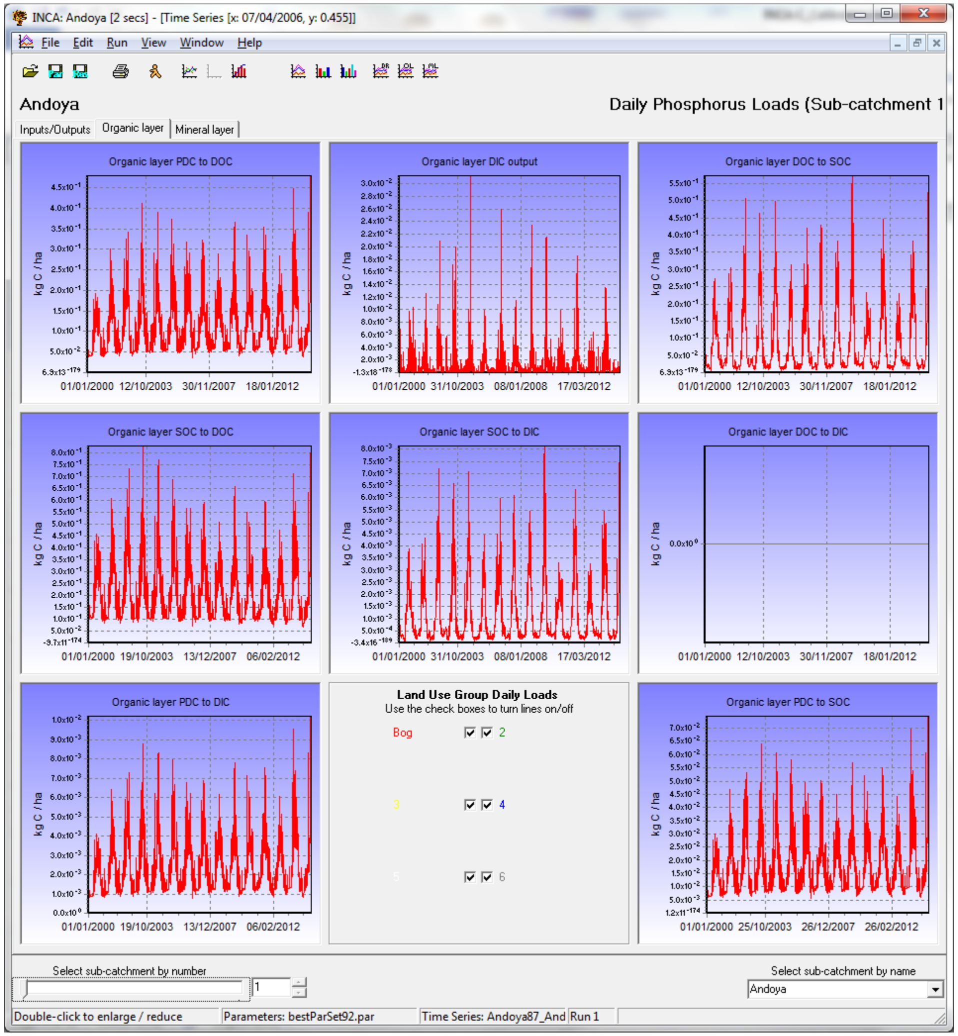
As starting point in the calibration, we can use .par file from a previous successful INCA-C application. This will ensure that parameter values are within the usual range of good performance. From here, manual iterations of usually sensitive parameters and with a physical interpretation are done based on visual inspection of model simulations versus observed data, for both the hydrological sub-model (flow) and the biogeochemical sub-model (DOC).

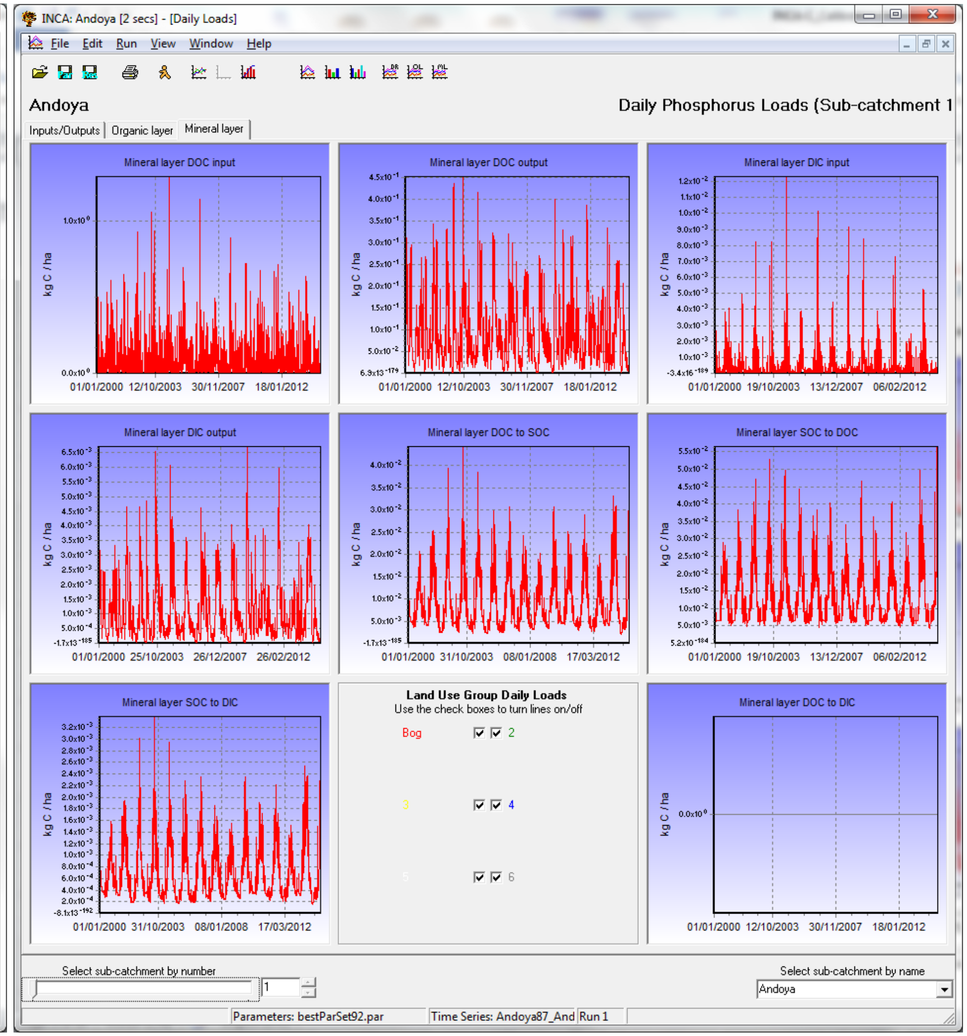
An important aim at this stage is to ensure a simulation of flow that is similar to the best performing parameter set simulation of flow given by PERSiST. Therefore, ideally, all the parameters that have an influence on the flow simulation can be fixed at this stage after we succeed fitting the flow in a similar way that was fit in PERSiST. The Monte Carlo tool (see below) can be used to help reaching this aim by only varying parameters with influence in flow.

The manual iteration is repeated until a reasonable capture of the observed DOC dynamics is reached (e.g.: at least N-S = 0.1-0.2).

At this point (and especially check after Monte Carlo), it is important to ensure that direct runoff PDC is relatively constant during the simulation period (see second graph in left panel in first figure below) and that we are not losing or gaining too much carbon in the soil (second and third graphs in middle and right panels in the first figure below). To access these panels corresponding to direct runoff, organic layer (upper soil layer) and mineral layer (lower soil layer) we use the most right icons in the INCA-C interface marked as “DR”, “OL”, and “ML” (see first figure below). It is also important to check that other dynamics (DR, OL, ML discharge, OL and ML DOC) and absolute values (e.g.: more DOC in the upper than lower soil) are sensible (see other graphs in first figure below). It is also important to make sure the transformations between different carbon pools (PDC, SOC, DOC, DIC) are consistent (see two last figures below).


INCA: Andoya [2 secs]
File Edit Run View Window Help
Direct Series
Andoya
Results for Andoya (Sub-catchment 1
Direct Runoff Discharge
Direct Runoff PDC
Direct Runoff DOC
Direct Runoff Volume
Organic Layer
Organic Layer Discharge
Organic Layer SOC fast pool
Organic Layer SOC slow pool
Organic Layer DOC
Organic Layer DIC
Mineral Layer
Minerla Layer Discharge
Mineral Layer SOC fast pool
Mineral Layer SOC slow pool
Mineral Layer DOC
Mineral Layer DIC
Select sub-catchment by number
Select sub-catchment by name
Parameters: bestParSet92.par
Time Series: Andoya87_And
Run 1


INCA: Andoya [2 secs] - [Time Series [x: 07/04/2006, y: 0.455]]
File Edit Run View Window Help
Andoya
Daily Phosphorus Loads (Sub-catchment 1
Inputs/Outputs
Organic layer
Mineral layer
Organic layer PDC to DOC
Organic layer DIC output
Organic layer DOC to SOC
Organic layer SOC to DOC
Organic layer SOC to DIC
Organic layer DOC to DIC
Organic layer PDC to DIC
Land Use Group Daily Loads
Use the check boxes to turn lines on/off
Bog
Organic layer PDC to SOC
kg C / ha
Select sub-catchment by number
Select sub-catchment by name
Andoya
Double-click to enlarge / reduce
Parameters: bestParSet92.par
Time Series: Andoya87_And
Run 1


INCA: Andoya [2 secs] - [Daily Loads]
File Edit Run View Window Help
Andoya
Daily Phosphorus Loads (Sub-catchment 1
Inputs/Outputs
Organic layer
Mineral layer
Mineral layer DOC input
Mineral layer DOC output
Mineral layer DIC input
Mineral layer DIC output
Mineral layer DOC to SOC
Mineral layer SOC to DOC
Mineral layer SOC to DIC
Land Use Group Daily Loads
Use the check boxes to turn lines on/off
Bog
Mineral layer DOC to DIC
kg C / ha
Select sub-catchment by number
Select sub-catchment by name
Andoya
Parameters: bestParSet92.par
Time Series: Andoya87_And
Run 1

3.2 Monte Carlo analysis

The Monte Carlo (MC) analysis is done to explore the parameter space in order to find good performing parameter sets in a number of iterations. The results can be used for uncertainty and sensitivity analyses and the best performing parameter set obtained can be used for further manual tuning.

The parameter space is explored based on credible parameter ranges that were identified from the initial manual calibration and previous model experiences (see literature and previous section describing the parameters). The starting point is the best model parameter set obtained during initial manual calibration. See parameter descriptions above and uncertainty and sensitivity analysis descriptions below for deciding parameter ranges. Ideally only parameters that have an impact in the DOC simulation (and not the flow) are varied during the MC analysis.

In order to run the MC tool, we create a new folder in our work space include the following files:

- *inca_c_cmd.exe*: file necessary to run the MC tool for INCA-C.
- *MCDemo.exe*: executable of the MC tool.
- *XXX.dat*: dat file of the catchment including daily temperature and precipitation time series (the same that has been created and used at the beginning of the calibration).
- *XXX.obs*: obs file with daily time series of flow (the same that has been created and used at the beginning of the calibration).
- *Other model input files*: abstraction, effluent, system structure, organic fertilizer, terrestrial PDC inputs, aquatic PDC inputs, land use periods, deposition and/or spatial files (optional).
- *min.par*: this is the parameter file with lower limit values of the parameters that were decided to be explored after the manual calibration. It is created manually by using the model interface and introducing those lower limit values manually for those parameters (using the best model parameter set obtained during initial manual calibration and saving a new .par file always as *min.par*).
- *max.par*: this is the parameter file with upper limit values of the parameters that were decided to be explored after the manual calibration. It is created manually by using the model interface and introducing those upper limit values manually for those parameters (using the best model parameter set obtained during initial manual calibration and saving a new .par file always as *max.par*).
- *mc.par*: a parameter file used by the MC tool. It can just be a copy of any of the other *min.par* or *max.par* files, but always need to be renamed as *mc.par*.

With these 7 mandatory (+ optional) files it is now possible to run the MC tool by opening the *MCDemo.exe* file within the folder. Here:

Please enter 1 for PERSiST
2 for INCA-C
3 for INCA-C4P
4 for INCA-P
5 for INCA-Tox
6 for INCA-Path: we type **2** (as we are using INCA-C) and press enter (in all other options after typing we also press enter for the next menu to appear).

Please enter the number of parameter sets you would like in the final ensemble: here we specify the number of iterations (loops) in our parameter space exploration. From each of these, we will obtain a parameter set (the best performing within each iteration). Usually **100**.

Please enter the number of runs used for the identification of each candidate parameter set: here we specify the number of model runs as part of each iteration. Depending on time constrains, size of the parameter ranges, how thorough we want to explore the parameter space, etc. this number can be around **500-1000**. Example: it takes around 30 hours to run 100 loops of 300 runs each in a simple 1 reach type of system structure with 15 years simulation.

Please enter the maximum number of unsuccessful jumps: random starting points are drawn from the parameter space and compared to the best model performance. When the random starting point is better than the best model performance, a predefined jump is applied to randomly perturb the parameter values and repeated until no further improvement in model performance is obtained. Here we specify the number of unsuccessful jumps (no improvement) before a new starting point is set. Usually **5-10**.

Please enter the number of files to use for model output: in a very complex system we can have a large generation of data and may want to split the output files (results0.txt) in several. But usually **1**.

Please enter the name of the Parameter File: here we type **mc.par**.

Please enter the name of the Data File: the name of the .dat file **XXX.dat**.

Please enter the name of the Observed Data File: the name of the .obs file **XXX.obs**.

Please enter the name of the Abstraction Time Series File: name of the .abs file if any.

Please enter the name of the Effluent Time Series File: name of the .ets file if any.

Please enter the name of the System structure file: name of the .ssf file if any.

Please enter the name of the Organic Fertiliser Time Series File: name of the .ofd file if any.

Please enter the name of the Terrestrial PDC inputs: name of the .tpi file if any.

Please enter the name of the Aquatic PDC inputs: name of the .api file if any.

Please enter the name of the Land Use Periods: name of the .lup file if any.

Please enter the name of the Deposition Time Series File: name of the .dts file if any.

Please enter the name of the Spatial Time Series: name of the .sts file if any.

Please enter the number of Land uses <6 for standard INCA>: we specify the number of land use in which we have divided the catchment. For INCA-C always type **6** (even if we have less land use types).

Please enter the number of reaches: specify the number of reaches in which we have divided the catchment and that are going to be calibrated. For simple applications **1**.

Please enter the number of buckets <use a value of 3 for INCA>: **3** in INCA-C (surface runoff, organic/upper layer, mineral/lower layer).

1: we type **1**.

, R?, N-S, RMSE, RE: just press **enter**. Different likelihood measures (metrics for assessing model performance). *R?* is the coefficient of determination (0-1, higher values better). *N-S* is the Nash Sutcliffe and determines the relative magnitude of the residual variance compared to the measured data variance and it is good to fit high values as it is sensitive to those (-∞-1, higher values better). *RMSE* is the root mean square error and represents the sample standard deviation of the differences between predicted values and observed values. *RE* is the residual.

Flow, XXXX: we specify the relative importance we want to give to fit the flow (versus fitting DOC, DIC, and PDC). Usually **1**.

Open water DOC XXX: we specify the relative importance we want to give to fit the DOC (versus fitting flow, DIC, and PDC). Usually **1**.

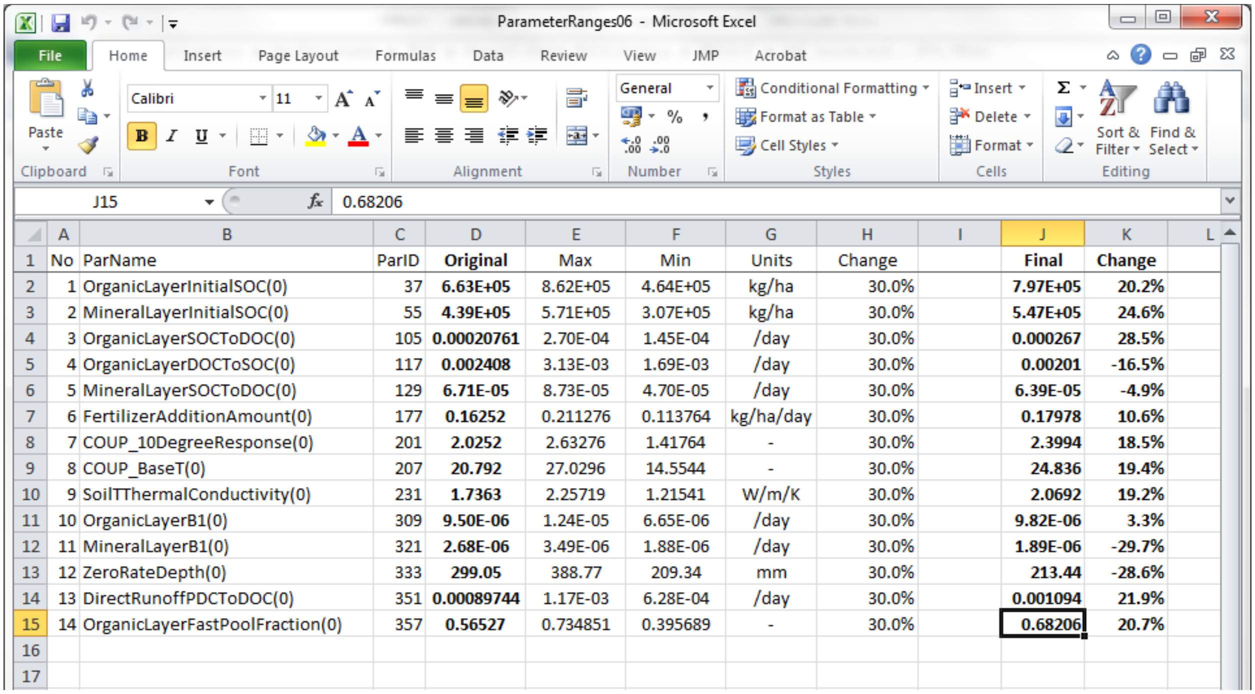
Open water DIC: XXX: we specify the relative importance we want to give to fit the DIC (versus fitting flow, DOC, and PDC). Usually **0** unless we are also calibrating it.

Open water PDC: XXX: we specify the relative importance we want to give to fit the PDC (versus fitting flow, DOC, and DIC). Usually **0** unless we are also calibrating it.

In the last line where there is just a ":" we type 1 and press enter to start running the analysis. If everything goes OK, something like in the screen picture should start appearing (one line at a time, the first two numbers corresponding to the number of loop and number of run).

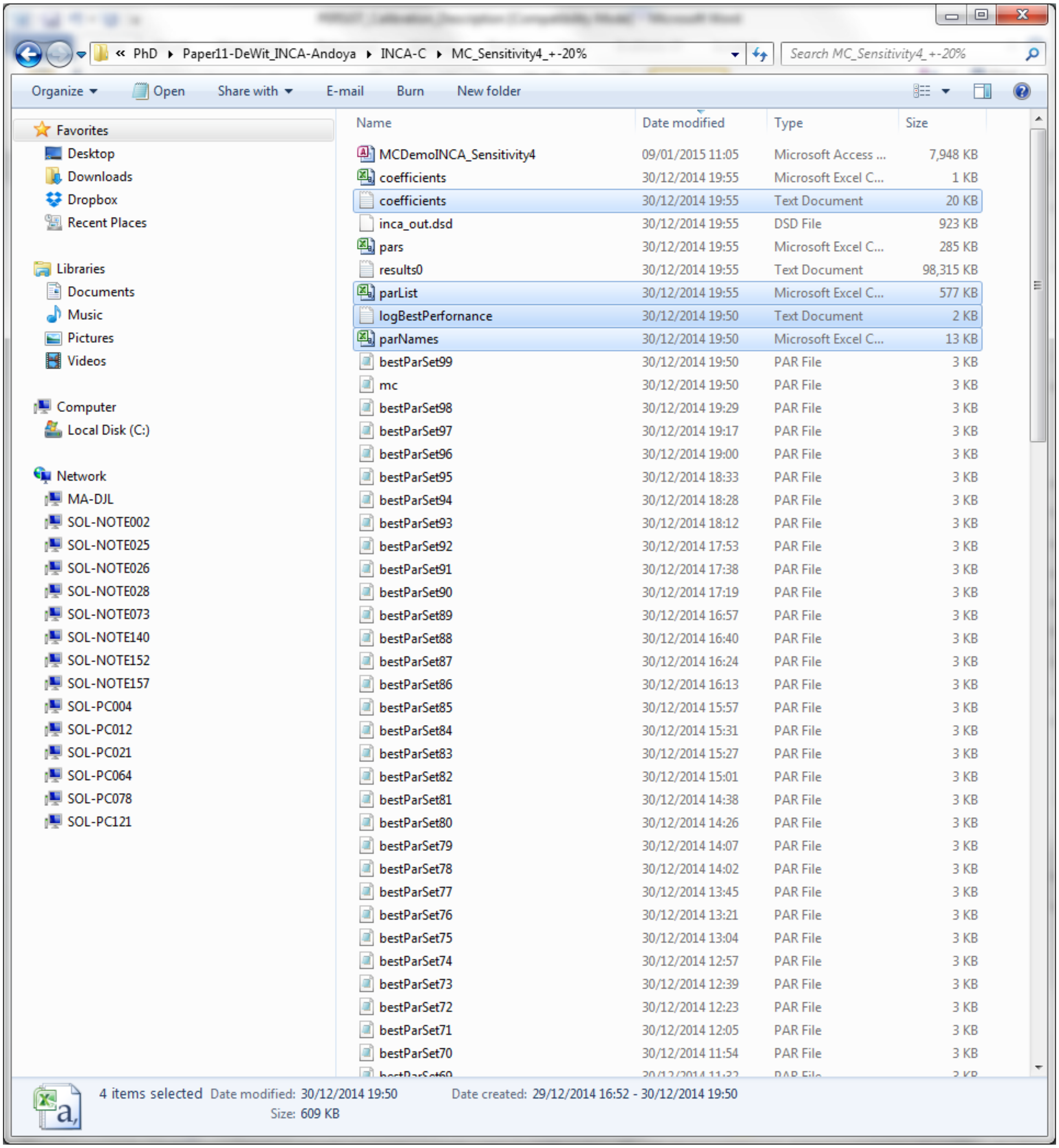
The process can of course be repeated several times as we may need to explore a different portion of the parameter space or test different model structures.

It could be a good idea to keep a record of the parameter ranges used, original and final values (from best performing parameter set), sensitive parameters (see below), etc. Example:



No	ParName	ParID	Original	Max	Min	Units	Change		Final	Change
1	OrganicLayerInitialSOC(0)	37	**6.63E+05**	8.62E+05	4.64E+05	kg/ha	30.0%		**7.97E+05**	**20.2%**
2	MineralLayerInitialSOC(0)	55	**4.39E+05**	5.71E+05	3.07E+05	kg/ha	30.0%		**5.47E+05**	**24.6%**
3	OrganicLayerSOCToDOC(0)	105	**0.00020761**	2.70E-04	1.45E-04	/day	30.0%		**0.000267**	**28.5%**
4	OrganicLayerDOCToSOC(0)	117	**0.002408**	3.13E-03	1.69E-03	/day	30.0%		**0.00201**	**-16.5%**
5	MineralLayerSOCToDOC(0)	129	**6.71E-05**	8.73E-05	4.70E-05	/day	30.0%		**6.39E-05**	**-4.9%**
6	FertilizerAdditionAmount(0)	177	**0.16252**	0.211276	0.113764	kg/ha/day	30.0%		**0.17978**	**10.6%**
7	COUP_10DegreeResponse(0)	201	**2.0252**	2.63276	1.41764	-	30.0%		**2.3994**	**18.5%**
8	COUP_BaseT(0)	207	**20.792**	27.0296	14.5544	-	30.0%		**24.836**	**19.4%**
9	SoilTThermalConductivity(0)	231	**1.7363**	2.25719	1.21541	W/m/K	30.0%		**2.0692**	**19.2%**
10	OrganicLayerB1(0)	309	**9.50E-06**	1.24E-05	6.65E-06	/day	30.0%		**9.82E-06**	**3.3%**
11	MineralLayerB1(0)	321	**2.68E-06**	3.49E-06	1.88E-06	/day	30.0%		**1.89E-06**	**-29.7%**
12	ZeroRateDepth(0)	333	**299.05**	388.77	209.34	mm	30.0%		**213.44**	**-28.6%**
13	DirectRunoffPDCToDOC(0)	351	**0.00089744**	1.17E-03	6.28E-04	/day	30.0%		**0.001094**	**21.9%**
14	OrganicLayerFastPoolFraction(0)	357	**0.56527**	0.734851	0.395689	-	30.0%		**0.68206**	**20.7%**

When the MC analysis is done, we will have in the folder a number of files including all the 100 best performing parameter sets (one from each iteration), and the most important is *results0.txt*. With the files created we can do sensitivity and uncertainty analyses.



Sensitivity analysis using Access query

Parameter sensitivity is assessed by comparing the ensemble of values from the 100 parameter sets (or the specified number of model iterations) identified during the MC analysis to a rectangular distribution based on the hypothesis that sensitive parameters show non-rectangular posterior distribution as some regions of parameter space are more conducive to good model performance than others. It is quantified using a Kolmogorov-Smirnov (KS) test to compare the posterior to a rectangular prior. A significant KS statistic implies that variation of parameters within an a priori interval (range) had significant effects on DOC simulated flow.

To test for sensitivity it is therefore important how wide or narrow are the ranges of the parameters that are varied. There are three main approaches on how to set parameter ranges:

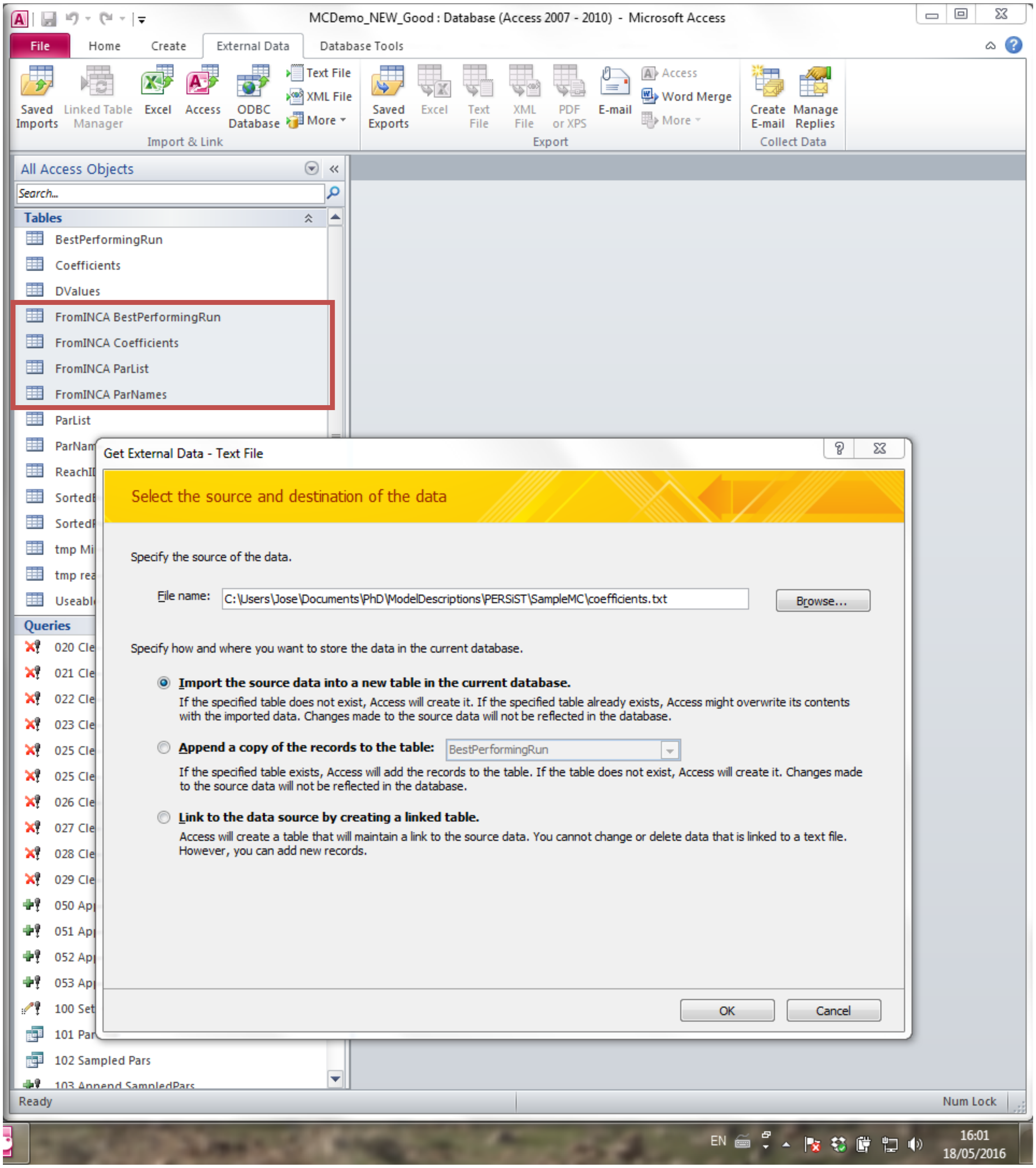
- Decide absolute sensible values for upper and lower limits for each parameter individually through expert judgment and/or previous model experiences.
- Choose some percentage for varying the best parameter set values from, something like ±10% to ±50%.
- Manually find the lower and upper values for each parameter individually that result in a model performance of NS=0.

A combination of the above can also be valid as the different parameters have different behaviors and significance.

The sensitivity test is run using the Access file *MCDemo_NEW_Good.accdb*. First, open the file. We need to import four files that have been created during the MC analysis, marked in the figure above (coefficients.txt, logBestPerformance.txt, parList.csv, parNames.csv).

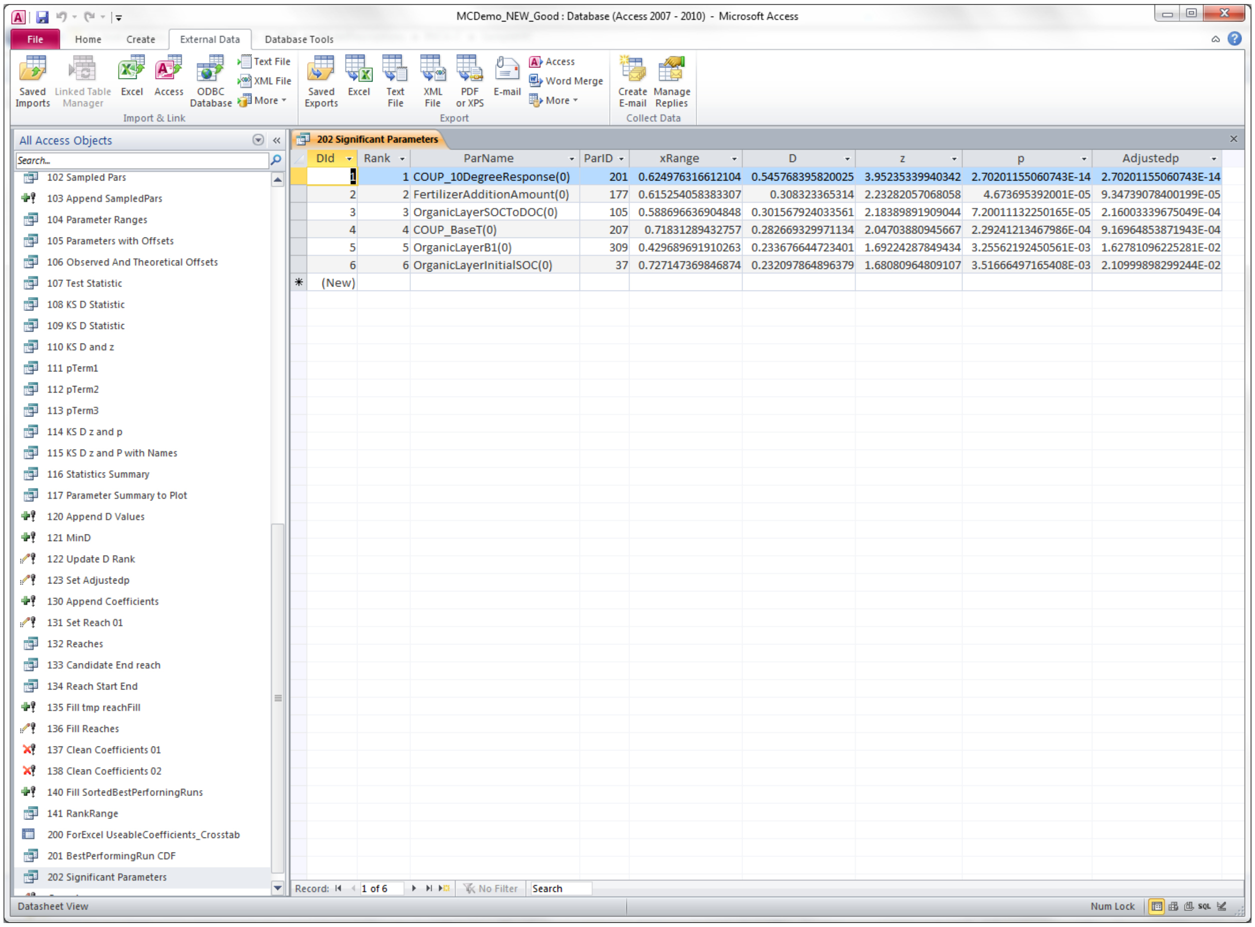
The way to import the two .txt files is: external data> text file > browse the file > Import the source data into a new table in the current database > follow the steps (OBS choose default options except that “No primary key” instead of “Let Access add primary key” in one of the menus). In the last step we rewrite the names as “FromINCA Coefficients” and “FromINCA BestPerformingRun” respectively (this will overwrite the tables.

The way to import the two .csv files is: external data> text file > browse the file > Append a copy of the records to the table: > and choose the tables “FromINCA ParList” and “FromINCA ParNames” respectively (default options).



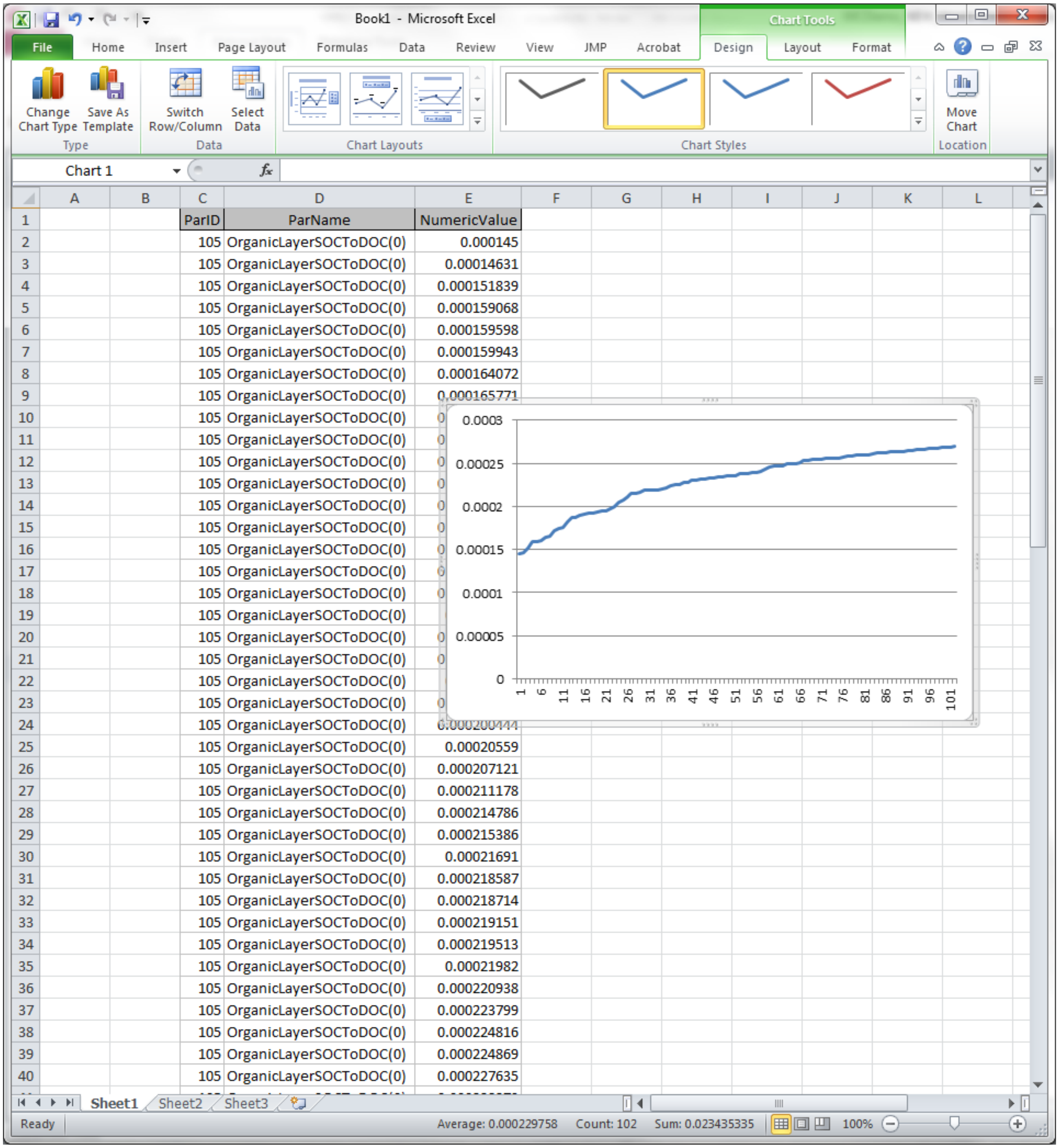
Then, under the queries list, we need to run the queries with numbers 050, 051, 052, 053, 100, 103, 120, 121, 122, 123, 130, 131, 135, 136, 137, 138, and 140 (accepting al questions asked with Yes).

Finally, running the query “202 Significant Parameters” and setting a p-value (e.g.: 0.05) we obtain a table with statistically significant sensitive parameters according to the KS test.



Some interesting/important tables to look at are:

- "BestPerformingRun": here we find, for each iteration, the run number in which the best parameter set was obtained. If, in general, the best parameter set is obtained close to the total number of runs in each iteration it might mean that we should increase the number of runs as there is potential to find better performing parameter sets.
- "DValues": here we find the p-value for sensitivity for all the parameters that have been varied.
- "Useable Coefficients": here we find the R2, N-S, RMSE, and RE for all 100 best parameter sets so we can search for the best one of all.
- "117 Parameter Summary to Plot": here we chose a parameter from the ones that have been varied by introducing its ParID and we will obtain a table with all the 100 values (in increasing order) from the 100 best parameter sets that have been obtained for that particular parameter. We can transfer the table to Excel and simply explore visually the frequency, so it helps deciding on a new parameter range for that particular parameter in a potential new MC analysis. Also, classic dotty plots (model efficiency vs. parameter value) are helpful in this sense.



<u>Uncertainty analysis</u>

We can use the file *results0.txt*, which includes all daily simulated DOC (also flow, PDC, DIC, and SOC) for the period of simulation (i.e. every day that had temperature and precipitation values) for all 100 (or the number of iterations chosen) best performing parameter sets from the iterations.

From those results we can estimate our uncertainty boundaries. 100 parameter sets is already a conservative number, high enough to include a wide range of parameter sets that lead to a conservative (wide) uncertainty boundaries (i.e. a 1000 iterations would probably not increase uncertainty). These boundaries can be based on 95% confidence intervals (± 1.96 SD of daily simulated DOC from the 100 daily simulated values corresponding to each of the parameter sets).

A less conservative approach, also valid, is to choose a threshold for behavioral models (e.g.: only parameter sets that give a model performance based on a certain likelihood measure, let's say N-S, higher than a specified arbitrary value would be considered behavioral models) and estimate the uncertainty base only on those behavioral models (on parameter sets that give such behavioral models). Trimming the ensemble of parameter sets to use only the best performing subset will lead to more realistic uncertainty estimates as it will exclude predictions based on parameter sets that would have been rejected for poor performance during manual calibration.

3.3 Final manual tuning

The best performing parameter sets of all 100 iterations (according to our likelihood measure choice) can be retained for further improvement in model performance. This can be done by simply manually adjusting/tuning sensitive parameters. This will be our best model.

The final tuning acknowledges the role of expert judgement in model use, as an automated procedure has the potential to produce mathematically reasonable but scientifically implausible parameter values. However this potential issue could be avoided in the phase of choosing parameter range for parameter space exploration, but this might be not possible when the strategy of choosing parameter ranges is based on predefined fixed values (e.g. ± 50%) or to give N-S = 0.

Applications of INCA-C usually give model performances around N-S = 0.3-0.5 (DOC calibration) or even 0.7-0.8 and are considered good. When the number of observations is limited the performance can be higher as the potential to obtain good model fits is inversely related to the number of observations. However the longer the calibration time series the better the overall goodness of model fit.

4. References

De Wit HA, Ledesma JLJ, Futter MN. 2016. Aquatic DOC export from subarctic Atlantic blanket bog in Norway is controlled by seasalt deposition, temperature and precipitation. Biogeochemistry 127: 305-321.

Futter MN, Butterfield D, Cosby BJ, Dillon PJ, Wade AJ, Whitehead PG. 2007. Modeling the mechanisms that control in-stream dissolved organic carbon dynamics in upland and forested catchments. Water Resources Research 43.

Woo M, Heron R. 1987. Effects of forests on wetland runoff during spring. Forest Hydrology and Watershed Management. Vancouver: IAHS-AISH.