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GREAT-ER

GREAT-ER Sediment Exposure Module Manual

Geo-referenced Regional Exposure Assessment Tool for European Rivers

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1 GREAT-ER Sediment Extension

The GREAT-ER Sediment Extension development is a CEFIC LRI project. Its focus is to add sediment as an additional compartment to GREAT-ER. This covers:

- Make the water column concentrations for sorbed/dissolved fractions available to the GUI.
- Derive per stretch sediment concentrations based on equilibrium partitioning.
- Various modes to specify the most important parameter for fractioning: Suspended solids concentration.
- Include diffuse inputs as provided by the TERRACE[1] project.

1.1 Model basics

The core of the GREAT-ER river model is the analytical steady-state surface water model WATER (Trapp and Matthies, 1998). The chemical elimination is described by first order instream removal:

$$\frac{dC(t)}{dt} = -kC(t) \tag{1}$$

which results in:

$$C_{River} = C_0 \cdot e^{-HRT \cdot k} \tag{2}$$

The elimination rate coefficient (k) is calculated as follows:

$$k = k_{deg} + f_s k_{sed} + f_d k_{vol} \tag{3}$$

with

$$f_d = \frac{1}{1 + 10^{-6} \cdot K_{d,River} \cdot SSC} \tag{4}$$

$$f_s = 1 - f_d \tag{5}$$

1.1.1 Fractional concentrations and Sediment

Based on partitioning the three concentrations for the water column can be calculated:

[1]**TE**rrestrial **R**unoff Modelling for **R**isk **A**ssessment of **C**hemical **E**xposure

$$C_{total} = C_{total,0} \cdot e^{-HRT \cdot k} \quad (6)$$
$$C_{dissolved} = f_d \cdot C_{total} \quad (7)$$
$$C_{sorbed} = f_s \cdot C_{total} \quad (8)$$

The WATER model also covers an equilibrium based sediment model component:

$$C_{Sediment} = f_d \cdot C_{total} \cdot K_{SW} = C_{dissolved} \cdot \left(K_{d,River} \cdot \frac{\rho_{Sediment,dry}}{\rho_{Water}} + \theta \right) \quad (9)$$

where:

K_{SW} : Partitioning coefficient bulk sediment to external water
$\rho_{Sediment,dry}$: Dry sediment density $[kg_{dwt}/m^3]$
ρ_{Water} : Water density (1 $[kg/m^3]$)
θ : Volume fraction water of sediment ($[m^3/m^3]$)

1.1.2 Diffuse Input

Considering diffuse input equation (1) is extended with an input term:

$$\frac{dC(t)}{dt} = -k \cdot C(t) + \frac{I(t)}{V} \quad (10)$$

With constant and continous input I the solution of the inhomogeneous linear differential equation of the first order is:

$$C(t) = C_0 \cdot e^{-k \cdot t} + \frac{I}{V \cdot k}(1 - e^{-k \cdot t}) \quad (11)$$

The special case $k = 0$ must be considered seperately:

$$C(t) = C_0 + \frac{I}{V} \cdot t \quad (12)$$

I : Diffuse input ($[kg/d]$)
V : Stretch volumn ($[m^3]$)
k : Combined elimination rate ($[1/d]$).

1.2 Model Implementation

The model as described above is implemented by the GREAT-ER II river model modes 2 and 3.

1.2.1 Model Input

The following parameters are added to the GREAT-ER II user interface to control the model (default values are taken from the TGD):

Table 1: Sediment extension - default values

Parameter	Unit	Default Value	Warning Range	Error Range
SSC	$[g/m^3]$	15	]0;3000]	]0;25000000]
The *suspended solids concentration* can be entered either as (distributed) environmental parameter or can be taken from SSC band statistics or TERRACE input files. See sections A and B below.				
$f_{OC,River}$	$[kg/kg]$	0.1		[0;1]
The *weight fraction of organic carbon in suspended solids* is not directly considered by the model but can be used to estimate the partitioning coefficient suspended solids to water: $K_{d,River} = f_{OC,River} \cdot K_{OC}$				
$\rho_{Sediment,wet}$	$[kg/m^3]$	1300	[500;1800]	[0;10000]
To be consistent with the TGD the *bulk density of wet sediment* is used as parameter for sediment density. Based on the sediment porosity (θ) the parameter is transformed to the dry sediment density internally				
θ	$[m^3/m^3]$	0.8		[0;1]
The *volume fraction of water in sediment (porosity)* is an average depending on the assumed sediment height. The default from the TGD is based on a 3 cm sediment.				

The diffuse input information can be read from a TERRACE file (see section B for details).

1.2.2 Model Output

The model calculates the total mass of chemical per unit mass of dry solids (unit: $[g/kg_{dwt}]$) in equivalence to the $C_{Sim,Start}$, $C_{Sim,Internal}$ and $C_{Sim,End}$. Concentrations are assumed to be logarithmic normal distributed, the descriptive values are returned by the model and available for further analysis by the user (section 1.4).

1.3 Sediment Modes

The ruling parameter (apart from substance specific values) for the partitioning and sedimentation is the suspended solids concentration (SSC). To reflect different scenarios of parameter availability the GREAT-ER Sediment Extension provides four options for the SSC parameter:

- A single SSC as fixed value for all river stretches,
- a single distributed SSC (considered as lognormal) for all river stretches,
- a SSC based on catchment characteristics (optionally catchment specific) and
- a per stretch SSC derived from TERRACE and provided as CSV file uploaded to the database.

1.3.1 Per catchment suspended solids

The first two options are implemented by the environmental parameter for suspended solids concentration (see Fig. 1): The user can either specify a fixed value or a distribution for the SS on the card 'River' which will be applied on the entire river network. The use of these two variants is straight forward and analog to all other parameters editable through the GREAT-ER desktop client.

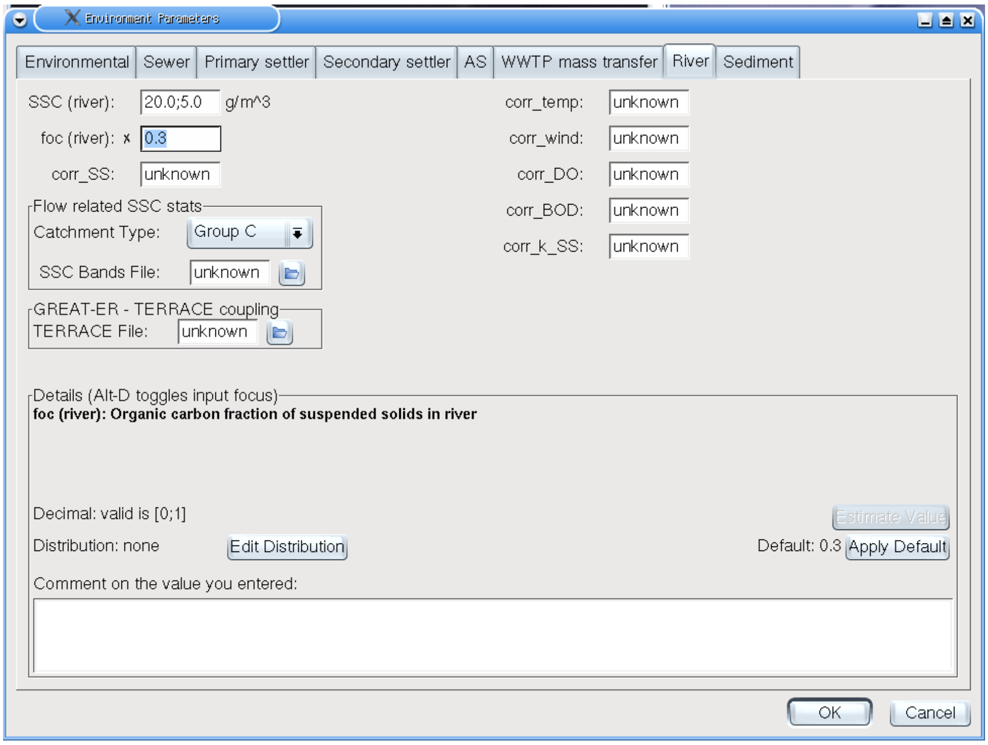

Figure 1: Edit Environment Dialog - page River

The dialog (Fig. 1) provides also access to the third option: The studies conducted by the University of Cranfield, UK (White et. al (2005)) within this project identified three different groups of catchment types. For each group a collection of bands related to river flow exceedance has been identified, each band is related to a distributed SSC, with minimum and maximum concentration:

- Group A: Rivers which are predominantly groundwater fed, with low topography and/or frequent lakes

  Examples: Danish rivers, Somme (France), Pang (UK)

- Group B: Rivers draining high mountain areas with glacial activity and or high snow cover in winter. Strong relief. Not impacted by major lakes.

  Examples: Upper reaches (within Switzerland) of Rhine and Rhone, Reuss, Lonza

- Group C: All rivers not included in Groups A or B

  Examples: Ebro + Jucar (Spain), Rhine, Rhone, Meuse, Moselle, Ouse system + Tees

In addition, users can upload a catchment specific collection of bands for a session, if data is available (file format described below). If the corresponding option from the catchment type list is selected, the file is used for the modelling.

An uploaded bands collection is listed under the session related tables and can be opened from the selection list as usual.

1.3.2 Per stretch suspended solids

The per stretch suspended solids concentration implements a link to the TERRACE project (also a CEFIC LRI project): In addition to diffuse inputs calculated by the TERRACE model the suspended solid concentrations are provided by a simple comma seperated value (CSV) table (see format and processing below).

After a successful upload and join the stretch specific data is available as a set of river network attributes. The user can investigate the data with the ’Identify’-Tool or via the Layer table.

1.3.3 File management

The management of bands collection and TERRACE file is similar, a click on the folder button near the entry opens a file selection dialog.

The files can be overwritten by loading a new file into the session. Setting the edit field to an empty (or unknown) value removes a file from a session. The user will be asked for confirmation before these actions are executed.

Before uploading the files are checked if they match the catchment.

The desktop client considers the files as part of a session and therewith it will be copied, saved or deleted together with the related session. Moreover the data is stronlgy related to the selected catchment. If a new catchment is selected for a session, the files are also removed from the current session.

1.3.4 Sediment specific parameters

The sediment specific parameters described above (Sec. 1.2.1) are on the ‘Sediment‘ page of the ‘Environment Parameters‘ dialog (Fig. 2).

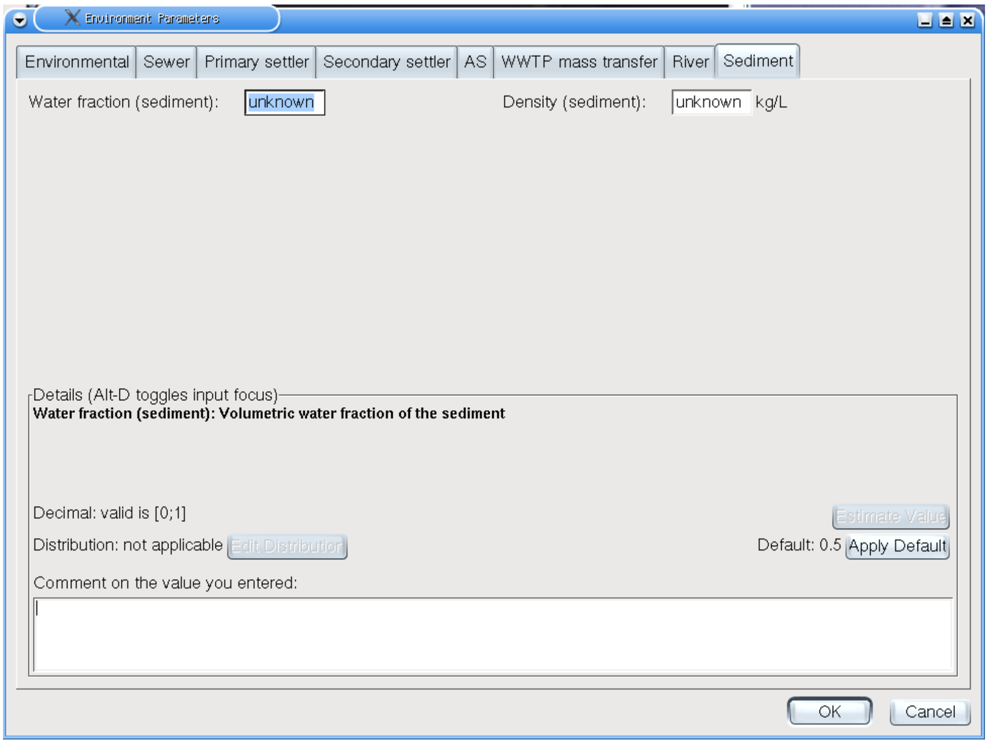

Figure 2: Edit Environment Dialog - page Sediment

1.3.5 Mode Selection

The mode selection is available through the 'Edit Model Parameters' dialog (Fig. 3) on the card 'Sediment'. First the sediment module can be switched on and off in general. The 'Data' item offers a selection between 'generic data', 'SSConc bands file', 'per stretch data' and 'class data'.:

generic data : Use the SSC value from the environmental parameters, either deterministic or distributed.

SSC bands file : Use a SSC bands collection. The 'Information' box on the right hand shows if a file is loaded.

per stretch data : Use the data from a TERRACE file. The 'Information' box on the right hand shows if a file is loaded.

class data : Use the data from the classes generated during preprocessing[2].

[2]This mode refers to an alternative concept of GREAT-ER 1.0 / 2.0: Classes are defined for stretches/discharges by the preprocessing, the user has no direct way to edit or query these settings. However, the concept provides a method to use 'typical' values for a class of discharges (e.g. trickling filter, activated sludge) or stretches (brook, main stream) for parameters where per object values are not available.

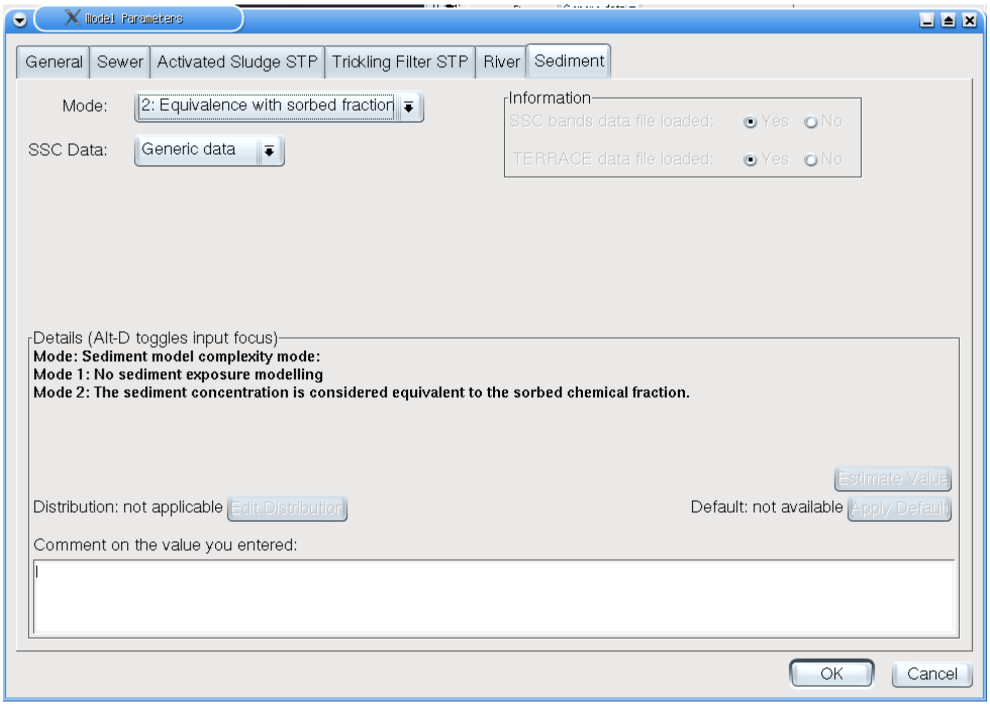

Figure 3: Edit Model Parameters - page Sediment

In addition to the suspended sediment concentration handling the 'Edit Model Parameters' dialog page 'River' (Fig. 4) offers the control over the diffuse input data provided through the TERRACE file: The 'diffuse input' switch activates/deactivates the diffuse input.

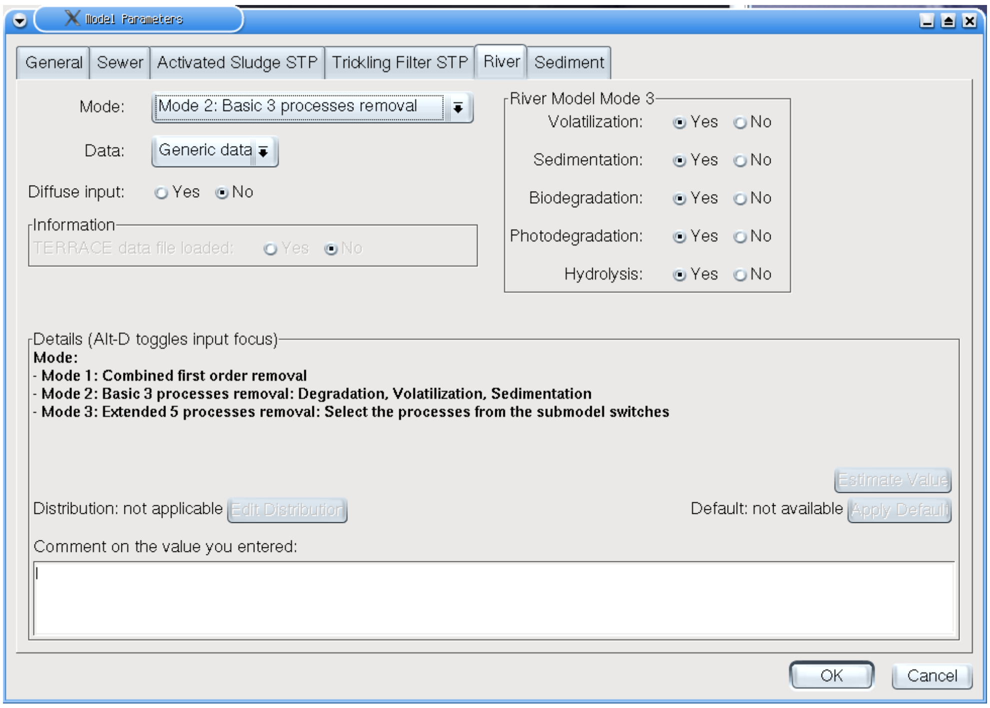

Figure 4: Edit Model Parameters - page River

1.4 Result Analysis

To provide easy access on the results calculated by the GREAT-ER Sediment Extension the features of the GREAT-ER Analysis menu have been enhanced: A new menu item Sediment Extension Results is added. The item is active if results from the sediment extension are available. A dialog is raised from which the results of interest can be selected.

For each selected result set a layer will be added to the legend. As a consequence the analysis tools now are available only if a result layer is selected in the legend. Depending on the selected result layer various tools are available (e.g. the PEC calculation or Risk Analysis are only defined for the total water column concentration).

The following functions are available per result group:

Function	C_{total}	$C_{dissolved}$	C_{sorbed}	$C_{Sediment}$
Calculate River CSim X	✓	✓	✓	✓
CSim Classes River	✓	✓	✓	✓
Combine CSim/Flow	✓	✓	✓	✓
PEC Inital	✓	-	-	-
PEC Catchment	✓	-	-	-
Risk Analysis	✓	-	-	-
Mass Flux	✓	✓	✓	-
Concentration Profile	✓	✓	✓	✓

A Suspended sediment concentration bands

The SSC bands file

The SSC bands file is a simple table of records as comma seperated values (CSV). It must define a consistent collection of flow exceedance bands (ranging from 0 to 100), without overlapping or gaps.

Each band definition requires 6 values:

Band minimum	: Lower boundary of the band range.
Band maximum	: Upper boundary of the band range.
SSC Mean	: Suspended Solids concentration, mean value $[g/m^3]$.
SSC StdDev	: Suspended Solids concentration, standard deviation.
Minimum	: Minimum SSC, during Monte Carlo simulations values cannot be below this limit $[g/m^3]$.
Maximum	: Maximum SSC, during Monte Carlo simulations values cannot be above this limit $[g/m^3]$.

Based on the mean and standard deviation suspended solids concentration and are considered as distributed parameters. It is assumed that parameters are logarithmic-normal distributed per band.

A sample SSC bands file:

```
# The SSC bands file can contain comments (lines must begin with square)
# The spaces included in this example are not needed and only allow a
# better reading.
#"BAND_MIN","BAND_MAX","SSC MEAN","SSC SDEV",  "MIN",   "MAX"
          0,         5,    11.393,     2.481,  2.699,  170.034
          5,        15,    10.751,     2.394,  1.599,   98.003
         15,        50,    11.100,     2.382,  2.300,   90.017
         50,        75,    13.250,     2.033,  2.398,   71.022
         75,       100,     8.846,     1.834,  3.001,   55.980
```

Predefined SSC bands tables

The studies conducted by the University of Cranfield, UK (White et. al (2005)) as a joined action for the GREAT-ER Sediment extension identified three different groups of catchment types.

The report is available under the documentation directory of a GREAT-ER II installation with Sediment Extension.

Group A: Lowland rivers

Group A covers rivers which are predominantly groundwater fed, with low topography and/or frequent lakes.

Examples: Danish rivers, Somme (France), Pang (UK)

Table 2: Predefined SSC bands: Group A, all SSC values in $[mgl^{-1}]$

Flow percentile band	Mean	StdDev	Minimum	Maximum
0 - 5	11.393	2.482	2.699	170.034
5 - 15	10.751	2.394	1.600	98.003
15 - 20	11.101	2.382	2.300	90.017
20 - 25	13.250	2.034	2.399	71.023
25 - 30	8.846	1.835	3.001	55.980
30 - 35	8.989	2.067	0.400	43.992
35 - 40	9.984	2.197	2.801	99.983
40 - 50	9.016	1.682	2.801	42.991
50 - 60	9.244	1.902	2.000	49.009
60 - 70	7.660	1.891	1.900	51.987
70 - 80	6.760	1.988	1.000	45.015
80 - 90	4.749	2.140	1.000	43.992
90 - 100	4.660	2.330	0.500	52.985

Group B: High mountain rivers

Group B covers rivers draining high mountain areas with glacial activity and or high snow cover in winter. Strong relief. Not impacted by major lakes.

Examples: Upper reaches (within Switzerland) of Rhine and Rhone, Reuss, Lonza

Table 3: Predefined SSC bands: Group B, all SSC values in $[mgl^{-1}]$

Flow percentile band	Mean	StdDev	Minimum	Maximum
0 - 5	269,616	5,366	1,8	37197,618
5 - 15	142,025	5,355	0,4	26795,788
15 - 20	99,385	5,233	0,9	13373,093
20 - 25	77,015	5,013	0,1	17085,749
25 - 30	63,371	4,874	0,6	9265,008
30 - 35	51,111	4,468	0,3	9339,425
35 - 40	43,467	4,380	0,1	5203,049
40 - 50	34,536	4,250	0,5	11081,142
50 - 60	24,508	4,336	0,1	8586,960
60 - 70	16,627	4,802	0,2	2708,093
70 - 80	12,466	5,023	0,1	2588,930
80 - 90	10,135	4,764	0,1	3866,094
90 - 100	8,516	4,477	0,0	3748,084

Group C: All other rivers

Group C collects all other rivers not included in Groups A or B

Examples: Ebro + Jucar (Spain), Rhine, Rhone, Meuse, Moselle, Ouse system + Tees

Table 4: Predefined SSC bands: Group C, all SSC values in $[mgl^{-1}]$

Flow percentile band	Mean	StdDev	Minimum	Maximum
0 - 5	68,855	3,666	1,0	6680,847
5 - 15	34,432	3,300	0,1	3470,313
15 - 20	25,687	3,016	0,1	5218,681
20 - 25	19,298	3,228	0,1	2300,772
25 - 30	18,084	3,089	0,1	6700,919
30 - 35	15,211	3,307	0,1	1059,974
35 - 40	13,874	3,071	0,1	2499,885
40 - 50	13,531	3,287	0,1	1190,347
50 - 60	11,462	3,168	0,1	1090,073
60 - 70	11,370	3,108	0,1	6808,996
70 - 80	10,805	3,053	0,1	889,803
80 - 90	10,206	3,142	0,1	1263,954
90 - 100	10,004	3,077	0,1	758,240

B The TERRACE file

The TERRACE file is a simple table of records as comma seperated values (CSV). It must contain a record for each stretch of the river network (compare Table / Show / Join of RIVERNET and Stretch Attributes or the catchments `.rna` file from the preprocessing.

Each record consists of 6 fields:

BasinID	: ID of the TERRACE (sub) basin, for informational purposes.
StretchID	: ID of the corresponding stretch, this is the link to the river network.
SSC Mean	: Suspended Solids concentration, mean value $[g/m^3]$.
SSC StdDev	: Suspended Solids concentration, standard deviation.
Diffuse Mean	: Diffuse Input into stretch, mean value $[kg/d]$.
Diffuse StdDev	: Diffuse Input into stretch, standard deviation.

Based on the mean and standard deviation suspended solids concentration and diffuse input can be considered as distributed parameters. It is assumed that both parameters are logarithmic-normal distributed.

A sample TERRACE file for a virtual catchment:

```
# The SSC bands file can contain comments (lines must begin with square)
# The spaces included in this example are not needed and only allow a
# better reading.
#
# The sample only contains SSC values and no diffuse input.
# Nevertheless the columns must be filled!
#BASIN, STRETCH, SSC_Mean, SSC_Stdev, Diffuse_Mean, Diffuse_STDDev
     3,   12860,  8.8184,    101.601,          0.0,            0.0
     3,   14700,  8.8184,    101.601,          0.0,            0.0
     3,   15750,  8.8184,    101.601,          0.0,            0.0
     4,   13180, 66.1408,    376.668,          0.0,            0.0
     4,    8970, 66.1408,    376.668,          0.0,            0.0
     5,   10550, 22.3793,     72.886,          0.0,            0.0
     5,   13080, 22.3793,     72.886,          0.0,            0.0
     5,   14840, 22.3793,     72.886,          0.0,            0.0
     5,   15850, 22.3793,     72.886,          0.0,            0.0
     6,  191000, 23.5699,     81.858,          0.0,            0.0
[...]
```

C Derivation $C_{Sim,Internal}$

GREAT-ER defines the $C_{Sim,Internal}$ as the arithmetic mean of the substance concentration over the hydrologic retention time (HRT) in a stretch:

No diffuse input

$$\begin{aligned} C_{Sim,Internal} &= \frac{1}{HRT} \cdot \int_{t=0}^{t=HRT} C_{start} \cdot e^{-k \cdot t} dt \\ &= \frac{C_{start}}{HRT} \left[\frac{1}{-k} \cdot e^{-k \cdot t} \right]_0^{HRT} \\ &= \frac{C_{start}}{k \cdot HRT} \left(1 - e^{-k \cdot HRT} \right) \end{aligned} \tag{13}$$

In the special case $k = 0$ (no elimination) start and end concentration are equal. Therewith:

$$C_{Sim,Internal} = C_{Sim,Start} \tag{14}$$

Diffuse input

Considering constant and continous diffuse input the $C_{Sim,Internal}$ is extended to:

$$\begin{aligned} C_{Sim,Internal} &= \frac{1}{HRT} \cdot \int_{t=0}^{t=HRT} C_{start} \cdot e^{-k \cdot t} + \frac{I}{V \cdot k} \left(1 - e^{-k \cdot t} \right) dt \\ &= \frac{C_{start}}{HRT} \left[\frac{1}{-k} \cdot e^{-k \cdot t} \right]_0^{HRT} - \frac{I}{HRT \cdot V \cdot k} \left[\frac{1}{-k} \cdot e^{-k \cdot t} \right]_0^{HRT} + \frac{I}{HRT \cdot V \cdot k} [t]_0^{HRT} \\ &= \left(\frac{C_{start}}{HRT \cdot k} - \frac{I}{HRT \cdot V \cdot k^2} \right) \cdot \left(1 - e^{-k \cdot HRT} \right) + \frac{I}{V \cdot k} \end{aligned} \tag{15}$$

The special case $k = 0$ must be considered seperately:

$$
\begin{aligned}
C_{Sim,Internal} &= \frac{1}{HRT} \cdot \int\limits_{t=0}^{t=HRT} C_{start} + \frac{I}{V} \cdot t \qquad dt \\
&= \frac{C_{start}}{HRT} \cdot [t]_0^{HRT} + \frac{I}{HRT \cdot V} \cdot \left[\frac{1}{2} \cdot t^2\right]_0^{HRT} \\
&= C_{start} + \frac{1}{2} \cdot \frac{I}{V} \cdot HRT \qquad (16)
\end{aligned}
$$

References

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White, S., Fredenham, E., Worrall, F., 2005. Sediments in GREAT-ER: Estimating sediment concentration ranges for European Rivers - Final report, September 2005.