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MULTIMEDIA STOCK POLLUTION TOOL - MUST 1.0

Assessing the fate of persistent chemicals in the environment

MUST 1.0

Implementation of a stock pollution model based on Mackay IV (VB.Net)

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Content

1 Summary

MUST (multimedia stock pollution tool) is a user-friendly implementation calculating the stock pollution in the environment for the assessment of long term behaviour of chemicals. The basic fugacity model is based on Mackay III and Mackay IV (Mackay and Paterson 1982). Additionally emission entries can be modified using a sewage treatment plant (STP, SimpleTreat).

Capability
The program MUST is able to calculate the steady state distribution of chemical in environment (Mackay III) as well as the change of stock pollution in time (Mackay IV). It is possible to enter time-dependent emission data. Furthermore, additional endpoints for evaluation as global half-life (Mackay III) or area under the curve (Mackay IV) are provided. In addition to that the program provides a graphical representation of the results (e.g. pie chart of distribution, line chart of time path of mass/concentration, line chart of time path of dissipation/degradation/export).

Documentation
The implementation of the stock pollution model is described. A "Working with…" section guides through the software MUST. The performance of MUST is tested using a case study of MUST as benchmark data set. Detailed output of the program is given in the appendix.

Compatibility
The program is available for major operating systems (like Windows 7-10).

Availability
The program MUST is currently available free-of-charge at the software website of the Fraunhofer Institute for Molecular Biology and Applied Ecology IME. Permanently, the program and associated material is linked to the download area http://software.ime.fraunhofer.de/MUST/. Earlier versions are available upon request. Here, the user can also obtain support from the developers of the software.

User interface
The user interface of MUST is graphical implemented in VB.Net. No further programming skills are needed for the use of the software.

Thematic Background
The aim is to assess the time path of pollution of persistent chemicals in the environment.

2 Model description

The software MUST calculates the mass/concentration of chemicals in environmental media and biota. The calculation is based on a Mackay III and Mackay IV model (Mackay and Paterson 1982) and a sewage treatment plant model (meta model based on STP, SimpleTreat). The Mackay III model is used to describe the log-term distribution of mass in the environment. In addition to that, the Mackay IV model describes the response of the considered system to emissions that change with time. It is possible to consider time-variable emission data. The STP model reduces the emission in water and increases the emission in soil (sludge on soil) simulating a sewage treatment plant. Using the STP model enables the consideration of a realistic emission scenario.

In MUST, two environmental scenarios are implemented "EU regional" and "EU continental freshwater" determining relevant environmental parameters such as environmental mass and volume values. The substance specific input data are physical chemical data as molar mass, logKow, DT50 of each compartment. Endpoints of the calculation are the time path of stock pollution (Figure 1).

With MUST it is possible to determine the time to steady state or the recovery time needed for the environment to recover.

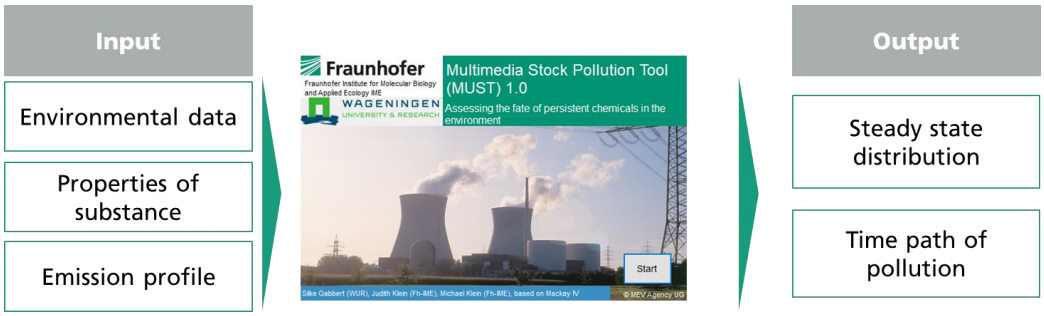

Figure 1: Input and output of the program MUST

Currently a selection of 17 substances is available for calculation:

- HBCDD
- DecaBDE
- Dechlorane Plus
- Anthracene
- Benzo[a]pyrene (BaP)
- Pyrene
- DDT
- Lindane
- PFOS
- PFOA
- PFNA
- PFDA
- D4
- D5
- Bisphenol A
- Nonylphenol
- Dimethylpropylphenol

The substance are similar to the substances described in thhe EU report "Approach for evaluation of PBTs subject to authorisation and restriction procedures in context of socio-economic analysis" (Gabbert et al. 2018 Annex 2 Table S1.1-S1.17).

2.1 Model procedure

The following procedure is implemented in MUST for the calculation of the mass/concentration in environmental media and biota. The index $i = 1, \cdots, 6$ corresponds to the considered environmental compartment: air ($i = 1$), water ($i = 2$), soil ($i = 3$), sediment ($i = 4$), suspended sediment ($i = 5$) and biota ($i = 6$).

1. Load the environmental data, the properties of the substance as well as the emission profile
2. Transform emission profile from kg per year to mole per hour
3. Set constants (transfer coefficients)
4. Calculate degradation constants in per hour for each compartment

$$k_i = \frac{1}{24} \cdot \frac{\log(2)}{DT50_i} \text{ for } i = 1, \cdots, 6$$

k_i Degradation constants in 1/h for each compartment ($i = 1, \cdots, 6$)

$DT50_i$ Degradation half-life in d for each compartment ($i = 1, \cdots, 6$) (substance specific)

5. Calculate additional transfer rates for air, water and suspended sediment k_i^*, $i = 1,2,5$, based on residence time τ_i in 1/h

$$k_i^* = \frac{1}{\tau_i \cdot 24} \text{ for } i = 1,2,5$$

k_i^* additional transfer rates in 1/h for air, water and susp. sediment ($i = 1,2,5$)

τ_i residence time in 1/h

6. Calculate the "fugacity capacity" Z in mol/(m³ Pa) (quantifies the capacity of a phase to dissolve or sorb a chemical):

$$Z_1 = \frac{1}{R \cdot T},$$
$$Z_2 = \frac{1}{H},$$
$$Z_i = Z_2 \cdot K_{oc} \cdot \frac{f_{oc_i}}{100} \cdot \rho_i \text{ for } i = 3,4,5\ ,$$
$$Z_6 = Z_2 \cdot BCF \cdot \rho_6$$

Z_i fugacity capacity in mol/(m³ Pa) for each compartment ($i = 1, \cdots, 6$)

R Gas constant 8.314 J/(mol*K)

H Henry constant (substance specific)

K_{oc} organic carbon to water partition coefficient (substance specific)

f_{oc_i}	fraction of organic carbon in soil ($i = 3$), sediment ($i = 4$), susp. sediment ($i = 5$) in %
ρ_i	Density in kg/L of soil ($i = 3$), sediment ($i = 4$), susp. sediment ($i = 5$) and biota ($i = 6$)
BCF	Bioconcentration factor (substance specific)

7. Calculate of the volume V of compartments in m³ (quantifies the capacity of a phase to dissolve or sorb a chemical):

$$V_1 = 1000000 \cdot A \cdot h \cdot 1000, V_2 = 1000000 \cdot A \cdot d_2 \cdot \frac{p_2}{100},$$
$$V_3 = 1000000 \cdot A \cdot \frac{d_3}{100} \cdot \left(\frac{100-p_2}{100}\right),$$
$$V_4 = 1000000 \cdot A \cdot \frac{d_4}{100} \cdot \frac{p_2}{100}$$
$$V_i = V_2 \cdot \frac{p_i}{1000000} \text{for } i = 5{,}6$$

V_i	Volume in m³ of each compartment ($i = 1, \cdots, 6$)
A	Area in km² (location specific)
H	Height of atmosphere in km
d_i	Depth of water in m ($i = 2$), soil in cm ($i = 3$), sediment in cm ($i = 4$)
p_i	Fraction of water ($i = 2$), susp. sediment ($i = 5$) and biota ($i = 6$) in %

8. Calculate of areas between compartments in m²

a) Air and water	$A_{12} = A_{21} = 1000000 \cdot A \cdot \frac{p_2}{100}$
b) Air and soil	$A_{13} = A_{31} = 1000000 \cdot A \cdot \left(\frac{100-p_2}{100}\right)$
c) Water and sediment	$A_{24} = A_{42} = 1000000 \cdot A \cdot \frac{p_2}{100}$
d) Water and susp. sediment (assumed diameter of susp. particle: 0.1 mm)	$A_{25} = A_{52} = 6 \cdot \frac{V_5}{0.0001}$
e) Water and biota (assumed diameter of biota: 1 cm)	$A_{26} = A_{62} = 6 \cdot \frac{V_5}{0.01}$

V_i Volume in m³ of each compartment ($i = 1, \cdots, 6$)

A Area in km² (location specific)

p_i Fraction of water ($i = 2$), susp. sediment ($i = 5$) and biota ($i = 6$) in %

9. Interpolate linearly the emission for each time point and for each compartment
10. Calculate modified emission values for water and soil (sewage treatment plant)

$$E_2(t) = \overline{E_2}(t) - E_2(t) \cdot \frac{f_{STP}}{100} \cdot \frac{f_{sl}}{100},$$

$$E_3(t) = \overline{E_3}(t) - E_2(t) \cdot \frac{f_{STP}}{100} \cdot \frac{f_{sl}}{100},$$

t Time (hour)

f_{STP} average connection fraction to sewage treatment plant (STP) (location specific) in %

f_{sl} Fraction of sludge (substance specific, calculated via SimpleTreat model) in %

$E_i(t)$ Emission in mole per hour to compartment ($i = 1, \cdots, 6$)

11. Calculate diffusion coefficients in matrix D in mol /(h Pa), $i, j = 1, \cdots, 6$

$$D_{ij} = \frac{A_{ij}}{\frac{1}{kt_{ij} Z_i} + \frac{1}{kt_{ij} Z_j}}$$

Structure of matrix $D = \begin{pmatrix} x & * & * & 0 & 0 & 0 \\ * & x & 0 & * & * & * \\ * & 0 & x & 0 & 0 & 0 \\ 0 & * & 0 & x & 0 & 0 \\ 0 & * & 0 & 0 & x & 0 \\ 0 & * & 0 & 0 & 0 & x \end{pmatrix}$

12. Calculate Mackay III (steady state solution) by solving the linear equation system $D \cdot f = E$
13. Calculate Mackay IV (solving for each compartment the following differential equation)

$$\frac{d}{dt}(V_i \cdot Z_i \cdot f_i) = E_i(t) + \sum_j f_j \cdot D_{ji} - \sum_j f_i \cdot D_{ij} - f_i \cdot \sum_i D_i$$

14. Retransform results from mole to kg
15. Transform result

$C_i = f_i \cdot Z_i$ Concentration in (kg/m³) in each compartment ($i = 1, \cdots, 6$)

$M_i = C_i \cdot V_i$ Mass in kg in each compartment ($i = 1, \cdots, 6$)

$Dis = V_i \cdot C_i \cdot \left(k_i + k_{export_i}\right)$	Disappearance in kg of each compartment ($i = 1, \cdots, 6$)
$Deg = V_i \cdot C_i \cdot k_i$	Degradation in kg of each compartment ($i = 1, \cdots, 6$)
$Exp = V_i \cdot C_i \cdot k_{export_i}$	Export in kg of each compartment ($i = 1, \cdots, 6$)

In Table 1, and overview of the model parameters and constants is given. It contains a description of parameter/constant is given.

Table 1: Overview of the model parameters and description

Parameter	Unit	Description
A	km²	Area (location specific)
BCF	-	Bioconcentration factor (substance specific)
d_i	m resp. cm	Depth of water in m ($i = 2$), soil in cm ($i = 3$), sediment in cm ($i = 4$)
$DT50_i$	d	Degradation half-life for each compartment ($i = 1, \cdots, 6$) (substance specific)
$E_i(t)$	Kg	Emission in time to compartment ($i = 1, \cdots, 6$)
f_{STP}	%	Average connection fraction to sewage treatment plant (STP) (location specific)
f_{sl}	%	Fraction of sludge (substance specific, calculated via SimpleTreat model)
f_{oc_i}	%	Fraction of organic carbon in soil ($i = 3$), sediment ($i = 4$), susp. sediment ($i = 5$)
h	km	Height of atmosphere
H	Pa m³/mol	Henry constant (substance specific)
k_i	1/h	Degradation constants for each compartment ($i = 1, \cdots, 6$)
k_i^*	1/h	Additional transfer rates for air, water and susp. sediment ($i = 1,2,5$)
kt_i	1/h	Transfer coefficients in 1/h used for the simulations of interphase transfer
K_{oc}	L/kg	Organic carbon to water partition coefficient (substance specific)
p_i	%	Fraction of water ($i = 2$), susp. sediment ($i = 5$) and biota ($i = 6$)
R	J/(mol*K)	Gas constant 8.314 J/(mol*K)
ρ_i	kg/L	Density of soil ($i = 3$), sediment ($i = 4$), susp. sediment ($i = 5$) and biota ($i = 6$)
τ_i	d	residence time
t		time
V_i	m³	Volume of each compartment ($i = 1, \cdots, 6$)
Z_i	mol/(m³ Pa)	fugacity capacity for each compartment ($i = 1, \cdots, 6$)

2.2 Model parametrization

There are three different kind of parameters: substance specific parameters, environmental parameters and fix constants.

The diffusion fluxes are constants that are independent of the chosen scenario and of the considered substance. The following diffusion fluxes are considered in the model:

- Air and water
- Air and soil
- Water and sediment
- Water and suspended Sediment
- Water and biota

The fluxes are graphically represented in Figure 2.

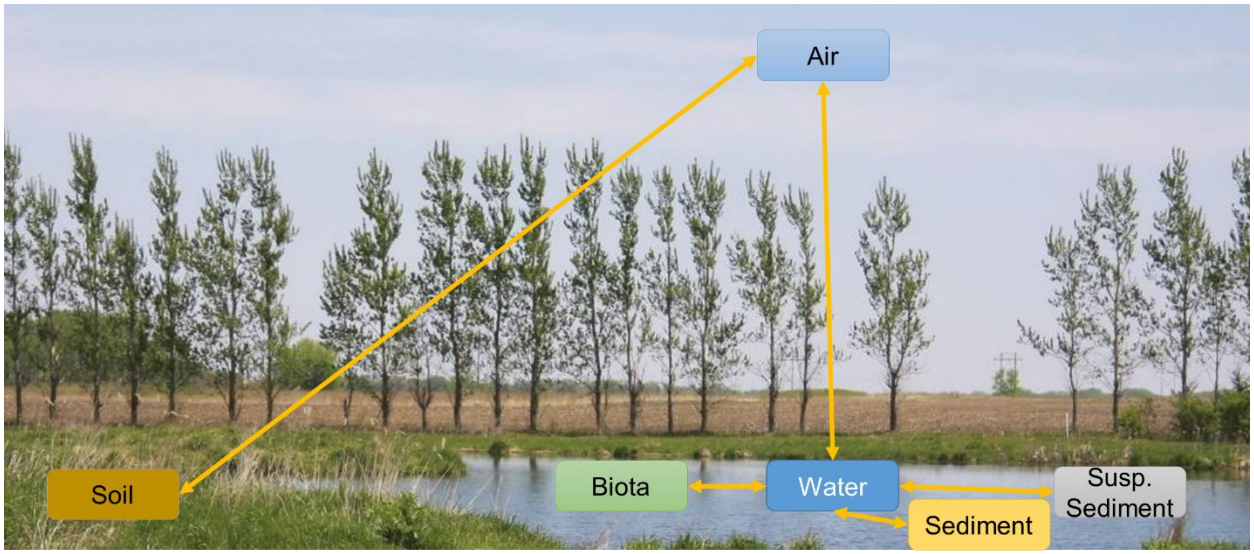

Figure 2: Considered diffusion processes in model, © iStock Photo modified by Fh-IME

Transfer coefficients simulate the interphase transfer and are used to calculate the diffusion matrix.

Table 2: Transfer coefficients in 1/h used for the simulations of interphase transfer

Source compartment i	Target compartment j	kt_{ij}
Air (i=1)	Water (j=2)	10
Water (i=2)	Air (j=1)	0.05
Air (i=1)	Soil (j=3)	2
Soil (i=3)	Air (j=1)	0.01
Water (i=2)	Sediment (j=4)	0.001
Sediment (i=4)	Water (j=2)	0.0001
Water (i=2)	Susp. Sediment (j=5)	0.001
Susp. Sediment (i=5)	Water (j=2)	0.0001
Water (i=2)	Biota (j=6)	0.01
Biota (i=6)	Water (j=2)	0.0001

In MUST, two environmental scenarios are implemented: "EU continental water" and "EU regional". The parameters needed for calculation are presented in Table 3. The values of these environmental scenarios are

based on EUSES and its regional and continental scale. The area of EU regional scenario is smaller than EU continental water as marine freshwater is not considered. The data is taken from Gabbert et al. 2018 (Annex 2 Table S2.4, and p.25).

Table 3: Parameters of environmental scenarios.

Parameter	Unit	EU continental water	EU regional
Height of the atmosphere	km	1	1
Area	km²	3560000	40400
Water fraction	%	3	4
Water depth	m	3	4.75
Soil depth	cm	10	10
Sediment depth	cm	3	3
Fraction of susp. sediment	ppm	15	15
Fraction of biota	ppm	100	100
Soil density	kg/L	1.7	1.7
Soil org. carbon content	%	2	2
Sediment org. carbon content	%	5	5
Susp. sediment org. carbon content	%	10	10
Temperature	K	285	285
Residence time air	d	9.05	0.7
Residence time water	d	172	40
Average connection percentage to STP	%	80	80

The residence time in air and water are used to include time of water in certain water body. The values differ within continental and regional scale. These parameter are used to calculated additional export coefficients for air, water and suspended sediment.

Currently a selection of 17 substances is available for calculation. The properties of substance are listed in Table 4. The values are taken from the EU report "Approach for evaluation of PBTs subject to authorisation and restriction procedures in context of socio-economic analysis" (Gabbert et al. 2018 Annex 2 Table S1.1-S1.17).

Table 4: Properties of substances implemented in MUST.

Substance	Molar mass	LogKow	LogKaw	Henry	KOC	BCF	DT50 (air)	DT50 (water)	DT50 (soil)	DT50 (sed.)	DT50 (susp. Sed.)	DT50 (biota)
	g/mol	-	-	Pa m³/mol	L/kg	-	d	d	d	d	d	d
HBCDD	641.7	5.63	-3.6	0.75	175000	18100	3.2	1E+06	120	214	1E+06	1E+06
DecaBDE	959.2	6.27		44	1590000	2000	94	1E+06	360	1E+06	1E+06	1E+06
Dechlorane Plus	653.73	9	1.75	1.30E+05	1.00E+08	5500	0.7	1E+06	350000	1E+06	1E+06	1E+06
Anthracene	178.24	4.68	-2.84	3.56	29500	6760	0.14	23	229	708	1E+06	1E+06
Benzo[a]pyrene (BaP)	252.31	6.13	-4.34	0.0463	832000	72190	0.32	71	708	2292	1E+06	1E+06
Pyrene	202.3	4.98	-99	1.4	58900	11300	0.44	71	708	2292	1E+06	1E+06
DDT	354.49	6.91	-99	0.84	220000	56000	7.08	229	708	2292	1E+06	1E+06
Lindane	290.83	3.5	-99	0.15	1271	1400	2.3	21	913	135	1E+06	1E+06
PFOS	500.13	-99	-4.7	-99	372	2796	114	1E+06	1E+06	1E+06	1E+06	1E+06
PFOA	414.07	-99	-2.99	-99	115	2000	130	33603	1E+06	1E+06	1E+06	1E+06
PFNA	464.08	-99	-2.99	-99	115	2000	130	2477	4954	1E+06	1E+06	1E+06
PFDA	514.08	-99	-2.99	-99	115	1575	130	4722	9444	1E+06	1E+06	1E+06
D4	296.62	6.49	2.69	1.21E+06	1270000	11495	14	16.7	180	315	1E+06	1E+06
D5	370.77	8.02	3.13	3.34E+06	43000000	10000	10.4	315	180	1950	1E+06	1E+06
Bisphenol A	228.29	3.4	-99	3.12E-07	796	36	0.13	15	3	30	1E+06	1E+06
Nonylphenol	220.34	4.48	-2.33	1.10E+01	5360	1300	0.3	150	300	300	1E+06	1E+06
Dimethylpropylphenol	164.24	3.6	-99	1.02E+00	2300	501	0.4	50	90	900	1E+06	1E+06

3 Evaluation

The program provides a visual evaluation. It shows the entered emission data in time using the absolute and relative data. The result of Mackay III is presented as pie chart and table showing the respective distribution in the environmental compartments. The result of Mackay IV, the time path of pollution, is presented in mass in kg and in concentration in kg/m³. Furthermore, the change of disappearance of substance (sum of export and of degradation), export and degradation is presented in time.
A text report contains:

Input:

- Information on program's version
- Name of the study
- Details on the chosen environmental scenario
- Details on the chosen substance
- The by user entered emission profile in kg
- The modified emission profile after SPT in%
- The volume of the compartments

Output:

- Mackay level III steady state distribution for each compartment in %, as well as the half live and persistency
- The area under curve (AUC) calculated using the trapezoidal rule
- The level IV change of mass in time in kg
- The level IV change of concentration in time in kg/m³
- The level IV change of disappearance (export + degradation) in time in kg
- The level IV change of degradation in time in kg
- The level IV change of export in time in kg
- Check of mass balance of the system

A global transfer rate per hour can be calculated as follows:

$$k_{global} = \frac{\sum_{i=1}^{6} V_i \cdot f_i \cdot Z_i \cdot (k_i + k_i^*)}{\sum_{i=1}^{6} V_i \cdot f_i \cdot Z_i}$$

which can be translated into a half-live value in years $DT50_{global}$.

$$DT50_{global} = \frac{\log(2)}{365 \cdot 24 \cdot k_{global}}$$

Using the Mackay IV result, the change of mass in time for each compartment, the area under the curve (kg a) can be calculated. In MUST; the trapezoid rule is used for its calculation summing up the mass in the environment for each time point.

$$AUC_i = \sum_{l=1}^{n-1} 0.5 \cdot (t_{l+1} - t_l) \cdot (V_l \cdot f_l \cdot Z_l + V_{l+1} \cdot f_{l+1} \cdot Z_{l+1})$$

4 Working with MUST 1.0

4.1 Installing MUST 1.0

The program MUST is available at the software website of the Fraunhofer Institute for Molecular Biology and Applied Ecology IME. Permanently, the program and associated material is linked to the download area http://software.ime.fraunhofer.de/MUST.

Please download the installer "MUST_setup_xxxxxxxx.exe" and follow the instructions. After installing MUST successfully, the start form of the program appears.

4.2 Working with MUST

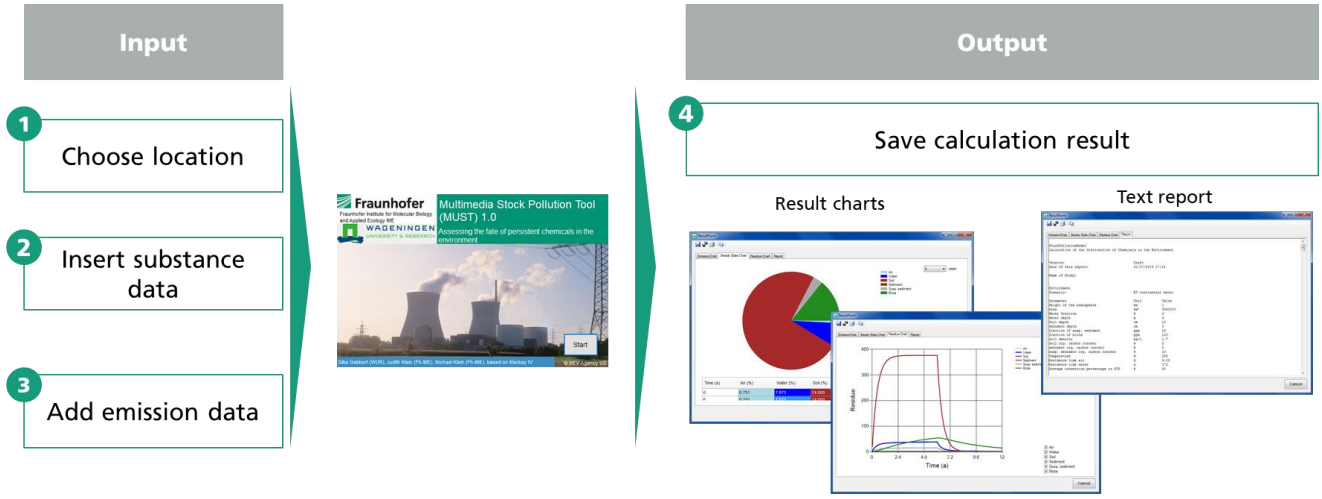

Figure 3: Procedure- The user has to fulfill four steps for the calculation of chemical stock pollution in the environment.

Procedure:

1. Choose environmental scenario
    a. EU continental water
    b. EU regional
2. Choose substance
3. Add emission data (in kg per year)
4. Start calculation
5. Save the calculation results

By starting the program MUST, a start screen appears (Figure 4). Clicking at start the proper program is started.

Figure 4: Start screen of the program MUST

The main form of the program includes a tab control containing the environment specific data, as well as substance specific data and emission data (Figure 3).

The user can decide between two environmental scenarios, EU regional and EU continental freshwater (Figure 5, left figure). The substance specific data can be entered in the tab page "Substance" as presented in Figure 5, right figure. Emission data (Figure 6) can be entered manually or by copy paste (CTRL-C,CTRL-V) from EXCEL. Calculation is only possible if emission data is entered.

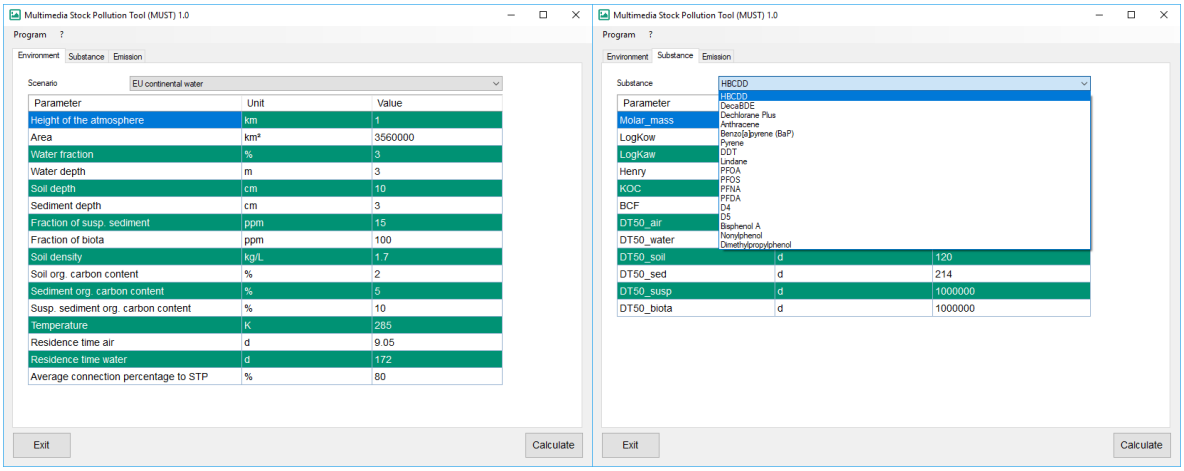

Figure 5: Main form of MUST – on the left tab page "Environment"; on the right tab page "Substance"

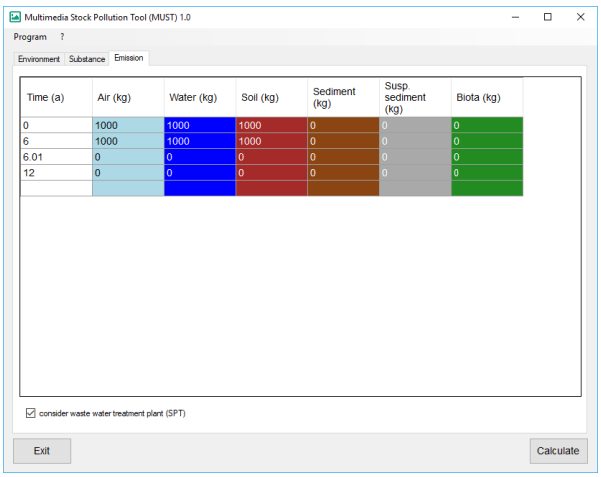

Figure 6: Main form of MUST – Tab page "Emission"

The result of the calculation is represented as

1. Input Chart (Figure 7): Visual representation of by user entered emission data, the change of emission to each compartment in time
2. Steady State Chart (Figure 9): Result of Mackay III -Steady state distribution of mass in the environment
3. Result Chart : Result of Mackay IV – Change of chemical mass/concentration in time in the environment
4. Disappearance Chart: Result of Mackay IV – Change of disappearance/export/degradation in time
5. Report (Figure 11): Text file containing input data and result of calculation

The program enables the user to save, copy into clipboard and print the results by clicking at the menu items "Save", "Save All", "Print" and "Copy".

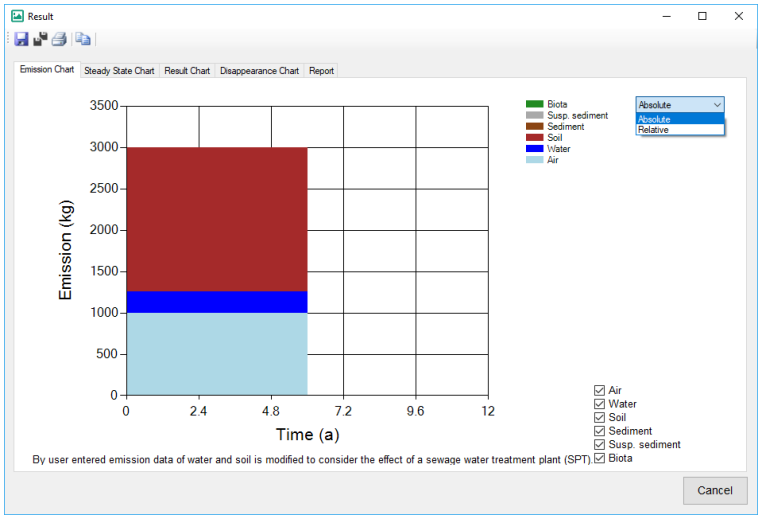

Figure 7: Input chart: emission data after sewage water treatment plant (SPT)

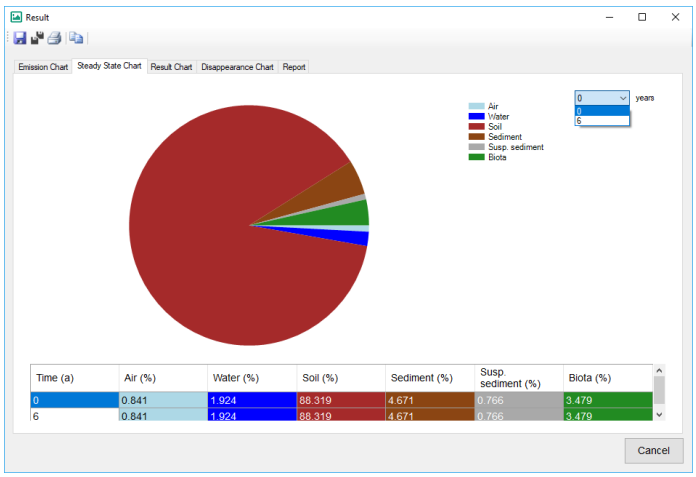

Figure 8: Steady state chart. Result of Mackay III calculation, distribution of mass in the environment in long term perspective

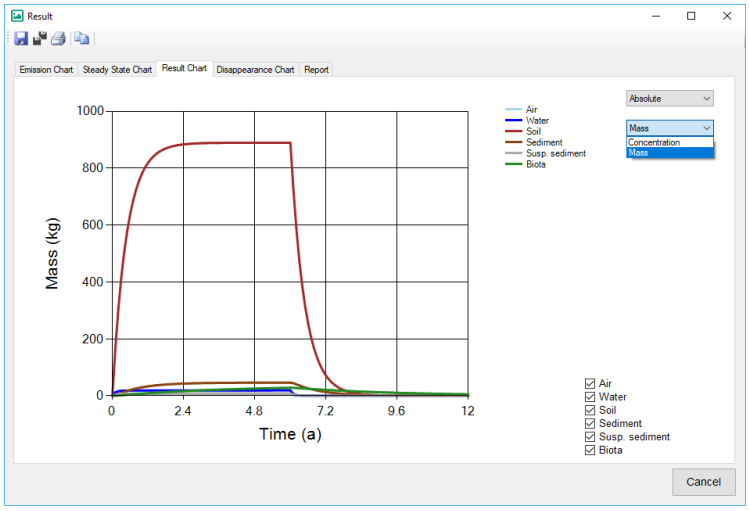

Figure 9: Result chart: Change of mass in the environmental compartments in time

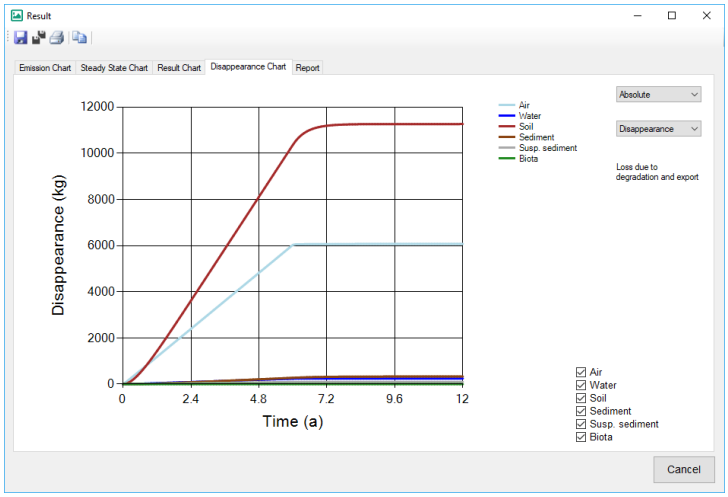

Figure 10: Disappearance chart: Change of degradation in the environmental compartments in time

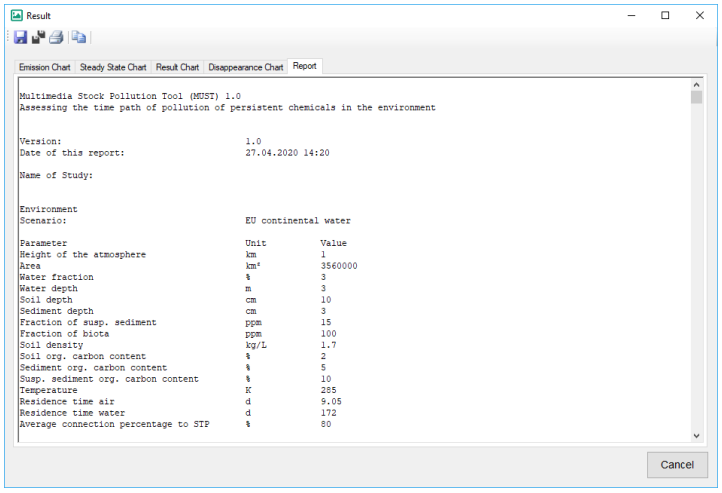

Figure 11: Text report file containing the input data as well as the calculation result

5 Result of test simulation using MUST 1.0

The aim of this chapter is to show the performance of the software MUST 1.0. For testing, we consider as test data set the substance HBCDD (Table 5).

5.1 Input Data

We use HBCDD as case study. The properties of HBCDD are given in Table 5. As environmental scenario, we choose "EU continental water".

Table 5: Substance specific parameter values: HBCDD

Parameter	Unit	Value
Molar_mass	g/mol	641.7
LogKow	-	5.63
LogKaw	-	-3.6
Henry	Pa m³/mol	0.75
KOC	kg/L	175000
BCF	-	18100
DT50_air	d	3.2
DT50_water	d	1000000
DT50_soil	d	120
DT50_sed	d	214
DT50_susp	d	1000000
DT50_biota	d	1000000

For emission, we choose an equal distribution for air, water and soil. No emission to sediment, suspended sediment and biota is assumed. We consider a time period of 12 years, where emission is set to zero after six years (Table 6). In addition to that we allow the program to redefine the emission data using sewage treatment plant (SPT).

Table 6: Emission data

Time (a)	Air (kg/a)	Water (kg/a)	Soil (kg/a)	Sediment (kg/a)	Susp. Sediment (kg/a)	Biota (kg/a)
0	1000	1000	1000	0	0	0
6	1000	1000	1000	0	0	0
6.01	0	0	0	0	0	0
12	0	0	0	0	0	0

5.2 Results

In Table 7, the steady state solution is given, namely the distribution for each compartment. The results are obtained choosing above described options as well as substance specific parameter data and emission data given in Table 5 and Table 6. The Mackay III calculation is performed for each emission data point if the sum of emission of all compartments for the time point is greater than zero. Here, the steady state distribution is calculated for year 0 and 6. The steady state distribution is the same for both time points as we consider a constant emission in the years 0 to 6.

Table 7: Result of test simulation using the input data given in Table 5 and Table 6

Time (a)	Air (%)	Water (%)	Soil (%)	Sediment (%)	Susp. sediment (%)	Biota (%)
0	0.841	1.924	88.319	4.671	0.766	3.479
6	0.841	1.924	88.319	4.671	0.766	3.479

The result is presented graphically as pie chart in Figure 12. Additionally the time path of stock pollution (Mackay IV) is shown.

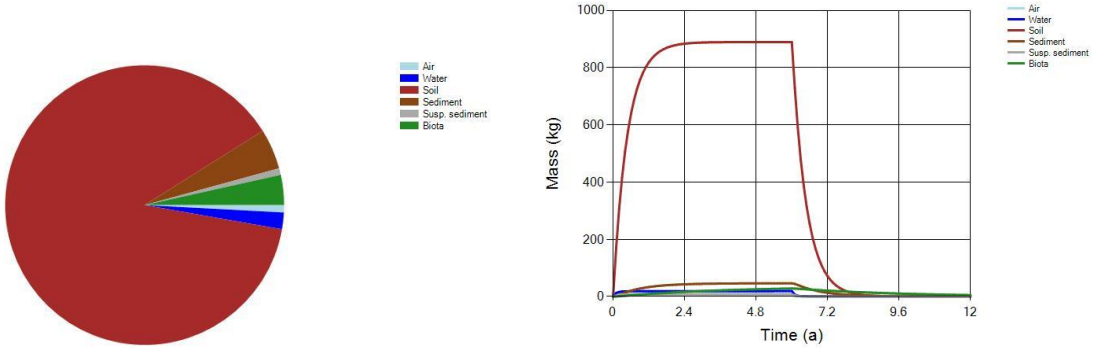

Figure 12: Result. Left: Steady state solution (Mackay III); right: time path of pollution (Mackay IV)

Detailed output (text report) by MUST is given in appendix A.

A Supplementary Material

A.1 Documentation of model output: MUST 1.0

```
Multimedia Stock Pollution Tool (MUST) 1.0
Assessing the time path of pollution of persistent chemicals in the environment


Version:                                1.0
Date of this report:                    29.04.2020 14:50

Name of Study:


Environment
Scenario:                               EU continental water

Parameter                               Unit          Value
Height of the atmosphere                km            1
Area                                    km²           3560000
Water fraction                          %             3
Water depth                             m             3
Soil depth                              cm            10
Sediment depth                          cm            3
Fraction of susp. sediment              ppm           15
Fraction of biota                       ppm           100
Soil density                            kg/L          1.7
Soil org. carbon content                %             2
Sediment org. carbon content            %             5
Susp. sediment org. carbon content      %             10
Temperature                             K             285
Residence time air                      d             9.05
Residence time water                    d             172
Average connection percentage to STP    %             80
```

Substance HBCDD

Parameter	Unit	Value
Molar_mass	g/mol	641.7
LogKow	-	5.63
LogKaw	-	-3.6
Henry	Pa m³/mol	0.75
KOC	L/kg	175000
BCF	-	18100
DT50_air	d	3.2
DT50_water	d	1000000
DT50_soil	d	120
DT50_sed	d	214
DT50_susp	d	1000000
DT50_biota	d	1000000

Emission (kg)

Time (a)	Air	Water	Soil	Sediment	Susp. sediment	Biota
0	1000	1000	1000	0	0	0
6	1000	1000	1000	0	0	0
6.01	0	0	0	0	0	0
12	0	0	0	0	0	0

By user entered emission data of water and soil is modified to consider the effect of a sewage water treatment plant (SPT).

rel. Emission after SPT (%)

Time (a)	Air	Water	Soil	Sediment	Susp. sediment	Biota
0.000	33.333	8.685	57.981	0.000	0.000	0.000
6.000	33.333	8.685	57.981	0.000	0.000	0.000
6.010	0.000	0.000	0.000	0.000	0.000	0.000
12.000	0.000	0.000	0.000	0.000	0.000	0.000

Volume of Compartments

Air	Water	Soil	Sediment	Susp. sediment	Biota
3.56E+15	320400000000	345320000000	3204000000	4806000	32040000

Results

Level III steady state distributions (%)

Time (a)	Air	Water	Soil	Sediment	Susp. sediment	Biota
0	0.841	1.924	88.319	4.671	0.766	3.479
6	0.841	1.924	88.319	4.671	0.766	3.479

Time (a)	half life (a)	Persistency (a)
0	0.23	0.27
6	0.23	0.27

Level IV area under the curve (trapezoidal rule) (kg a)

Air	Water	Soil	Sediment	Susp. sediment	Biota
50.781	115.239	5339.805	278.867	45.914	158.034

Level IV change of mass in time (kg)

Time (a)	Air	Water	Soil	Sediment	Susp. sediment	Biota
0	0	0	0	0	0	0
0.1	7.982367	12.757411	167.795066	2.230636	3.357829	0.415287
0.2	8.233231	16.327793	305.002564	6.065843	5.737446	1.171757
0.3	8.334358	17.725061	416.26748	10.092521	6.745203	2.025242
0.4	8.379072	18.302622	506.399614	13.915578	7.16043	2.902135
0.5	8.400509	18.549957	579.376168	17.411497	7.334137	3.773978
0.6	8.412013	18.663033	638.447961	20.557983	7.409752	4.629665
0.7	8.419073	18.72114	686.258669	23.370417	7.4454	5.465071
0.8	8.423988	18.756418	724.952905	25.876671	7.46463	6.27889
0.9	8.427749	18.781922	756.268287	28.107239	7.476993	7.070948
1	8.430809	18.802978	781.611815	30.091507	7.486372	7.841519
1.1	8.433391	18.821777	802.122432	31.856497	7.494354	8.591054
1.2	8.435621	18.83924	818.721948	33.426568	7.501596	9.320066
1.3	8.437575	18.855768	832.156381	34.823491	7.508375	10.029085
1.4	8.439307	18.87155	843.029458	36.066648	7.514815	10.718639
1.5	8.440857	18.886686	851.829747	37.173263	7.520976	11.389252
1.6	8.442256	18.901237	858.952617	38.158632	7.526891	12.041432
1.7	8.443528	18.915247	864.718018	39.036331	7.532582	12.675679

1.8	8.444694	18.92875	869.384866	39.818409	7.538063	13.29248
1.9	8.445769	18.941777	873.162686	40.515562	7.543349	13.892308
2	8.446766	18.954353	876.221035	41.137279	7.54845	14.475625
2.1	8.447698	18.966502	878.697126	41.691984	7.553376	15.042882
2.2	8.448571	18.978246	880.701997	42.187152	7.558136	15.594516
2.3	8.449394	18.989603	882.325504	42.629415	7.562738	16.130954
2.4	8.450174	19.000593	883.640366	43.024663	7.567191	16.652612
2.5	8.450914	19.011231	884.705428	43.378121	7.571499	17.159895
2.6	8.451619	19.021534	885.568313	43.694426	7.575671	17.653195
2.7	8.452293	19.031514	886.267557	43.977698	7.579712	18.132898
2.8	8.452938	19.041186	886.834349	44.231589	7.583627	18.599375
2.9	8.453558	19.050562	887.293928	44.459344	7.587422	19.052989
3	8.454153	19.059653	887.66672	44.663844	7.591101	19.494094
3.1	8.454727	19.06847	887.969253	44.847645	7.594669	19.923034
3.2	8.455281	19.077024	888.214905	45.013018	7.59813	20.340142
3.3	8.455815	19.085324	888.414504	45.161978	7.601487	20.745745
3.4	8.456331	19.093379	888.57681	45.296316	7.604746	21.140158
3.5	8.456831	19.101198	888.708915	45.417622	7.607908	21.52369
3.6	8.457314	19.108788	888.816558	45.527307	7.610978	21.89664
3.7	8.457782	19.116158	888.904384	45.626626	7.613958	22.2593
3.8	8.458236	19.123315	888.976152	45.716694	7.616852	22.611952
3.9	8.458676	19.130265	889.034907	45.7985	7.619663	22.954873
4	8.459103	19.137017	889.083111	45.872925	7.622392	23.288331
4.1	8.459517	19.143575	889.122758	45.94075	7.625044	23.612586
4.2	8.459919	19.149946	889.155463	46.002671	7.62762	23.927892
4.3	8.460309	19.156135	889.182531	46.059306	7.630122	24.234496
4.4	8.460688	19.16215	889.205021	46.111204	7.632553	24.532637
4.5	8.461056	19.167994	889.223791	46.158854	7.634916	24.822549
4.6	8.461413	19.173673	889.239533	46.202691	7.637211	25.10446
4.7	8.46176	19.179192	889.252809	46.243103	7.639442	25.378589
4.8	8.462097	19.184555	889.264075	46.280434	7.64161	25.645151
4.9	8.462425	19.189769	889.2737	46.314991	7.643717	25.904355
5	8.462743	19.194835	889.281982	46.347047	7.645765	26.156404
5.1	8.463053	19.19976	889.289164	46.376845	7.647756	26.401496
5.2	8.463353	19.204548	889.295443	46.404604	7.649691	26.639821
5.3	8.463646	19.209201	889.300976	46.430517	7.651572	26.871568
5.4	8.46393	19.213725	889.305895	46.454756	7.6534	27.096917
5.5	8.464206	19.218122	889.310304	46.477476	7.655177	27.316045
5.6	8.464474	19.222397	889.314288	46.498816	7.656905	27.529124
5.7	8.464735	19.226553	889.317917	46.518897	7.658584	27.736321
5.8	8.464989	19.230593	889.321247	46.53783	7.660217	27.937797
5.9	8.465236	19.234521	889.324324	46.555714	7.661805	28.133712
6	8.465475	19.23834	889.327186	46.572638	7.663348	28.324218
6.1	0.504071	6.779324	729.099862	44.526621	4.479335	28.126222

6.2	0.240378	3.026052	590.470297	40.737298	2.00615	27.558404
6.3	0.135083	1.568183	478.043521	36.721949	0.954378	26.882597
6.4	0.088807	0.968478	386.967284	32.898499	0.521862	26.176313
6.5	0.066832	0.714098	313.225358	29.398569	0.341916	25.469499
6.6	0.055206	0.600021	253.533829	26.247561	0.264523	24.773933
6.7	0.048192	0.54331	205.221634	23.431229	0.228882	24.094083
6.8	0.043392	0.510349	166.121762	20.92205	0.210363	23.431466
6.9	0.039773	0.487489	134.478367	18.689581	0.198977	22.786412
7	0.036866	0.469163	108.869658	16.704369	0.190663	22.158775
7.1	0.034439	0.453083	88.144712	14.939293	0.183765	21.548223
7.2	0.032365	0.438292	71.372014	13.369886	0.177597	20.954355
7.3	0.030565	0.424373	57.79769	11.974279	0.171869	20.376748
7.4	0.028985	0.411134	46.811657	10.732996	0.166455	19.814976
7.5	0.027584	0.398473	37.920202	9.628733	0.161294	19.268618
7.6	0.026331	0.386331	30.723792	8.646122	0.156352	18.73726
7.7	0.025202	0.374665	24.899109	7.771521	0.151608	18.220499
7.8	0.024176	0.363441	20.18451	6.992825	0.147048	17.717941
7.9	0.023237	0.352631	16.368264	6.29929	0.142658	17.229201
8	0.022373	0.342211	13.279029	5.681381	0.138428	16.753905
8.1	0.021571	0.33216	10.77815	5.130638	0.13435	16.291687
8.2	0.020824	0.322456	8.753418	4.639553	0.130414	15.842191
8.3	0.020124	0.313082	7.114031	4.201462	0.126613	15.40507
8.4	0.019465	0.304021	5.786507	3.810453	0.12294	14.979988
8.5	0.018842	0.29526	4.711382	3.461276	0.11939	14.566614
8.6	0.018251	0.286782	3.840531	3.149275	0.115955	14.16463
8.7	0.017688	0.278576	3.135013	2.870316	0.112631	13.773723
8.8	0.017151	0.27063	2.563312	2.62073	0.109413	13.393589
8.9	0.016636	0.262933	2.099924	2.397259	0.106297	13.023934
9	0.016143	0.255473	1.72421	2.197015	0.103277	12.66447
9.1	0.015668	0.248243	1.419466	2.017429	0.100351	12.314918
9.2	0.015212	0.241233	1.172174	1.856224	0.097514	11.975005
9.3	0.014771	0.234434	0.971396	1.711379	0.094763	11.644466
9.4	0.014346	0.227839	0.808277	1.581096	0.092094	11.323044
9.5	0.013936	0.221439	0.675652	1.463783	0.089505	11.010488
9.6	0.013539	0.215229	0.567723	1.358022	0.086993	10.706555
9.7	0.013155	0.209201	0.479797	1.262557	0.084555	10.411007
9.8	0.012783	0.20335	0.408074	1.176271	0.082189	10.123612
9.9	0.012423	0.197668	0.349479	1.098172	0.079891	9.844148
10	0.012073	0.192151	0.301525	1.027378	0.07766	9.572395
10.1	0.011734	0.186794	0.262198	0.963108	0.075493	9.308141
10.2	0.011406	0.18159	0.229865	0.904664	0.073389	9.051179
10.3	0.011087	0.176535	0.203209	0.85143	0.071346	8.801308
10.4	0.010777	0.171624	0.181159	0.802855	0.06936	8.558334
10.5	0.010477	0.166853	0.16285	0.75845	0.067431	8.322066

10.6	0.010185	0.162217	0.147583	0.717781	0.065557	8.092318
10.7	0.009902	0.157713	0.134789	0.680462	0.063737	7.868912
10.8	0.009626	0.153336	0.12401	0.646149	0.061967	7.651672
10.9	0.009359	0.149083	0.114873	0.614536	0.060248	7.440428
11	0.009099	0.144949	0.107076	0.58535	0.058577	7.235015
11.1	0.008847	0.140931	0.100375	0.558349	0.056953	7.035273
11.2	0.008601	0.137026	0.094572	0.533317	0.055375	6.841044
11.3	0.008363	0.13323	0.089506	0.510062	0.05384	6.652176
11.4	0.008131	0.129541	0.085048	0.488412	0.052349	6.468523
11.5	0.007906	0.125955	0.08109	0.468213	0.0509	6.289939
11.6	0.007687	0.122468	0.077548	0.449331	0.049491	6.116285
11.7	0.007474	0.119079	0.074352	0.431641	0.048121	5.947424
11.8	0.007267	0.115785	0.071444	0.415037	0.04679	5.783226
11.9	0.007066	0.112582	0.068779	0.39942	0.045495	5.62356
12	0.006871	0.109468	0.06632	0.384703	0.044237	5.468302

Level IV change of concentration in time (kg/m³)

Time (a)	Air	Water	Soil	Sediment	Susp. sediment	Biota
0	0	0	0	0	0	0
0.1	7.982367	12.757411	167.795066	2.230636	3.357829	0.415287
0.2	8.233231	16.327793	305.002564	6.065843	5.737446	1.171757
0.3	8.334358	17.725061	416.26748	10.092521	6.745203	2.025242
0.4	8.379072	18.302622	506.399614	13.915578	7.16043	2.902135
0.5	8.400509	18.549957	579.376168	17.411497	7.334137	3.773978
0.6	8.412013	18.663033	638.447961	20.557983	7.409752	4.629665
0.7	8.419073	18.72114	686.258669	23.370417	7.4454	5.465071
0.8	8.423988	18.756418	724.952905	25.876671	7.46463	6.27889
0.9	8.427749	18.781922	756.268287	28.107239	7.476993	7.070948
1	8.430809	18.802978	781.611815	30.091507	7.486372	7.841519
1.1	8.433391	18.821777	802.122432	31.856497	7.494354	8.591054
1.2	8.435621	18.83924	818.721948	33.426568	7.501596	9.320066
1.3	8.437575	18.855768	832.156381	34.823491	7.508375	10.029085
1.4	8.439307	18.87155	843.029458	36.066648	7.514815	10.718639
1.5	8.440857	18.886686	851.829747	37.173263	7.520976	11.389252
1.6	8.442256	18.901237	858.952617	38.158632	7.526891	12.041432
1.7	8.443528	18.915247	864.718018	39.036331	7.532582	12.675679
1.8	8.444694	18.92875	869.384866	39.818409	7.538063	13.29248
1.9	8.445769	18.941777	873.162686	40.515562	7.543349	13.892308
2	8.446766	18.954353	876.221035	41.137279	7.54845	14.475625
2.1	8.447698	18.966502	878.697126	41.691984	7.553376	15.042882
2.2	8.448571	18.978246	880.701997	42.187152	7.558136	15.594516
2.3	8.449394	18.989603	882.325504	42.629415	7.562738	16.130954

2.4	8.450174	19.000593	883.640366	43.024663	7.567191	16.652612
2.5	8.450914	19.011231	884.705428	43.378121	7.571499	17.159895
2.6	8.451619	19.021534	885.568313	43.694426	7.575671	17.653195
2.7	8.452293	19.031514	886.267557	43.977698	7.579712	18.132898
2.8	8.452938	19.041186	886.834349	44.231589	7.583627	18.599375
2.9	8.453558	19.050562	887.293928	44.459344	7.587422	19.052989
3	8.454153	19.059653	887.66672	44.663844	7.591101	19.494094
3.1	8.454727	19.06847	887.969253	44.847645	7.594669	19.923034
3.2	8.455281	19.077024	888.214905	45.013018	7.59813	20.340142
3.3	8.455815	19.085324	888.414504	45.161978	7.601487	20.745745
3.4	8.456331	19.093379	888.57681	45.296316	7.604746	21.140158
3.5	8.456831	19.101198	888.708915	45.417622	7.607908	21.52369
3.6	8.457314	19.108788	888.816558	45.527307	7.610978	21.89664
3.7	8.457782	19.116158	888.904384	45.626626	7.613958	22.2593
3.8	8.458236	19.123315	888.976152	45.716694	7.616852	22.611952
3.9	8.458676	19.130265	889.034907	45.7985	7.619663	22.954873
4	8.459103	19.137017	889.083111	45.872925	7.622392	23.288331
4.1	8.459517	19.143575	889.122758	45.94075	7.625044	23.612586
4.2	8.459919	19.149946	889.155463	46.002671	7.62762	23.927892
4.3	8.460309	19.156135	889.182531	46.059306	7.630122	24.234496
4.4	8.460688	19.16215	889.205021	46.111204	7.632553	24.532637
4.5	8.461056	19.167994	889.223791	46.158854	7.634916	24.822549
4.6	8.461413	19.173673	889.239533	46.202691	7.637211	25.10446
4.7	8.46176	19.179192	889.252809	46.243103	7.639442	25.378589
4.8	8.462097	19.184555	889.264075	46.280434	7.64161	25.645151
4.9	8.462425	19.189769	889.2737	46.314991	7.643717	25.904355
5	8.462743	19.194835	889.281982	46.347047	7.645765	26.156404
5.1	8.463053	19.19976	889.289164	46.376845	7.647756	26.401496
5.2	8.463353	19.204548	889.295443	46.404604	7.649691	26.639821
5.3	8.463646	19.209201	889.300976	46.430517	7.651572	26.871568
5.4	8.46393	19.213725	889.305895	46.454756	7.6534	27.096917
5.5	8.464206	19.218122	889.310304	46.477476	7.655177	27.316045
5.6	8.464474	19.222397	889.314288	46.498816	7.656905	27.529124
5.7	8.464735	19.226553	889.317917	46.518897	7.658584	27.736321
5.8	8.464989	19.230593	889.321247	46.53783	7.660217	27.937797
5.9	8.465236	19.234521	889.324324	46.555714	7.661805	28.133712
6	8.465475	19.23834	889.327186	46.572638	7.663348	28.324218
6.1	0.504071	6.779324	729.099862	44.526621	4.479335	28.126222
6.2	0.240378	3.026052	590.470297	40.737298	2.00615	27.558404
6.3	0.135083	1.568183	478.043521	36.721949	0.954378	26.882597
6.4	0.088807	0.968478	386.967284	32.898499	0.521862	26.176313
6.5	0.066832	0.714098	313.225358	29.398569	0.341916	25.469499
6.6	0.055206	0.600021	253.533829	26.247561	0.264523	24.773933
6.7	0.048192	0.54331	205.221634	23.431229	0.228882	24.094083

6.8	0.043392	0.510349	166.121762	20.92205	0.210363	23.431466
6.9	0.039773	0.487489	134.478367	18.689581	0.198977	22.786412
7	0.036866	0.469163	108.869658	16.704369	0.190663	22.158775
7.1	0.034439	0.453083	88.144712	14.939293	0.183765	21.548223
7.2	0.032365	0.438292	71.372014	13.369886	0.177597	20.954355
7.3	0.030565	0.424373	57.79769	11.974279	0.171869	20.376748
7.4	0.028985	0.411134	46.811657	10.732996	0.166455	19.814976
7.5	0.027584	0.398473	37.920202	9.628733	0.161294	19.268618
7.6	0.026331	0.386331	30.723792	8.646122	0.156352	18.73726
7.7	0.025202	0.374665	24.899109	7.771521	0.151608	18.220499
7.8	0.024176	0.363441	20.18451	6.992825	0.147048	17.717941
7.9	0.023237	0.352631	16.368264	6.29929	0.142658	17.229201
8	0.022373	0.342211	13.279029	5.681381	0.138428	16.753905
8.1	0.021571	0.33216	10.77815	5.130638	0.13435	16.291687
8.2	0.020824	0.322456	8.753418	4.639553	0.130414	15.842191
8.3	0.020124	0.313082	7.114031	4.201462	0.126613	15.40507
8.4	0.019465	0.304021	5.786507	3.810453	0.12294	14.979988
8.5	0.018842	0.29526	4.711382	3.461276	0.11939	14.566614
8.6	0.018251	0.286782	3.840531	3.149275	0.115955	14.16463
8.7	0.017688	0.278576	3.135013	2.870316	0.112631	13.773723
8.8	0.017151	0.27063	2.563312	2.62073	0.109413	13.393589
8.9	0.016636	0.262933	2.099924	2.397259	0.106297	13.023934
9	0.016143	0.255473	1.72421	2.197015	0.103277	12.66447
9.1	0.015668	0.248243	1.419466	2.017429	0.100351	12.314918
9.2	0.015212	0.241233	1.172174	1.856224	0.097514	11.975005
9.3	0.014771	0.234434	0.971396	1.711379	0.094763	11.644466
9.4	0.014346	0.227839	0.808277	1.581096	0.092094	11.323044
9.5	0.013936	0.221439	0.675652	1.463783	0.089505	11.010488
9.6	0.013539	0.215229	0.567723	1.358022	0.086993	10.706555
9.7	0.013155	0.209201	0.479797	1.262557	0.084555	10.411007
9.8	0.012783	0.20335	0.408074	1.176271	0.082189	10.123612
9.9	0.012423	0.197668	0.349479	1.098172	0.079891	9.844148
10	0.012073	0.192151	0.301525	1.027378	0.07766	9.572395
10.1	0.011734	0.186794	0.262198	0.963108	0.075493	9.308141
10.2	0.011406	0.18159	0.229865	0.904664	0.073389	9.051179
10.3	0.011087	0.176535	0.203209	0.85143	0.071346	8.801308
10.4	0.010777	0.171624	0.181159	0.802855	0.06936	8.558334
10.5	0.010477	0.166853	0.16285	0.75845	0.067431	8.322066
10.6	0.010185	0.162217	0.147583	0.717781	0.065557	8.092318
10.7	0.009902	0.157713	0.134789	0.680462	0.063737	7.868912
10.8	0.009626	0.153336	0.12401	0.646149	0.061967	7.651672
10.9	0.009359	0.149083	0.114873	0.614536	0.060248	7.440428
11	0.009099	0.144949	0.107076	0.58535	0.058577	7.235015
11.1	0.008847	0.140931	0.100375	0.558349	0.056953	7.035273

11.2	0.008601	0.137026	0.094572	0.533317	0.055375	6.841044
11.3	0.008363	0.13323	0.089506	0.510062	0.05384	6.652176
11.4	0.008131	0.129541	0.085048	0.488412	0.052349	6.468523
11.5	0.007906	0.125955	0.08109	0.468213	0.0509	6.289939
11.6	0.007687	0.122468	0.077548	0.449331	0.049491	6.116285
11.7	0.007474	0.119079	0.074352	0.431641	0.048121	5.947424
11.8	0.007267	0.115785	0.071444	0.415037	0.04679	5.783226
11.9	0.007066	0.112582	0.068779	0.39942	0.045495	5.62356
12	0.006871	0.109468	0.06632	0.384703	0.044237	5.468302

Level IV change of disappearance in time (kg)

Time (a)	Air	Water	Soil	Sediment	Susp. sediment	Biota
0	0	0	0	0	0	0
0.1	85.160094	1.69608	18.190099	0.09967	0.315459	0.000004
0.2	182.202054	4.843847	68.51694	0.584324	1.314178	0.000024
0.3	281.188825	8.479155	144.947787	1.540014	2.654292	0.000064
0.4	380.996598	12.310996	242.534754	2.961808	4.136265	0.000126
0.5	481.179586	16.225213	357.254969	4.816811	5.676965	0.000211
0.6	581.551171	20.175589	485.845473	7.064449	7.242594	0.000317
0.7	682.030243	24.143287	625.662733	9.664112	8.81941	0.000445
0.8	782.579385	28.120552	774.566272	12.577896	10.401799	0.000593
0.9	883.179692	32.104127	930.823441	15.771401	11.987438	0.000762
1	983.82042	36.092586	1093.031907	19.213792	13.575343	0.000951
1.1	1084.494675	40.08525	1260.056767	22.877569	15.165074	0.001159
1.2	1185.197565	44.081752	1430.979571	26.738275	16.756413	0.001386
1.3	1285.925368	48.081857	1605.057059	30.774174	18.349236	0.00163
1.4	1386.675133	52.085389	1781.687742	34.965964	19.943461	0.001893
1.5	1487.444458	56.0922	1960.384863	39.296502	21.539023	0.002172
1.6	1588.23136	60.10216	2140.754511	43.750568	23.135865	0.002469
1.7	1689.034188	64.115151	2322.477911	48.314645	24.733939	0.002782
1.8	1789.851551	68.131061	2505.297088	52.976729	26.333198	0.00311
1.9	1890.682277	72.149786	2689.003274	57.72616	27.9336	0.003454
2	1991.525364	76.171227	2873.427516	62.553468	29.535103	0.003813
2.1	2092.379956	80.195292	3058.433085	67.450243	31.13767	0.004186
2.2	2193.245314	84.221891	3243.909325	72.409013	32.741266	0.004574
2.3	2294.120796	88.250942	3429.766684	77.423139	34.345854	0.004975
2.4	2395.005838	92.282364	3615.932686	82.48672	35.951403	0.00539
2.5	2495.899946	96.316081	3802.348673	87.594512	37.557882	0.005818
2.6	2596.802678	100.35202	3988.96717	92.741855	39.165261	0.006258
2.7	2697.713639	104.390111	4175.749752	97.924604	40.773511	0.006711
2.8	2798.632473	108.430288	4362.66532	103.139074	42.382606	0.007176
2.9	2899.558856	112.472485	4549.688699	108.381986	43.992518	0.007652

3	3000.492493	116.516642	4736.799511	113.650425	45.603223	0.00814
3.1	3101.43311	120.5627	4923.981262	118.941795	47.214698	0.008638
3.2	3202.380454	124.6106	5111.220596	124.253785	48.826918	0.009148
3.3	3303.33429	128.660289	5298.506701	129.584338	50.439862	0.009667
3.4	3404.294396	132.711713	5485.830824	134.931622	52.053508	0.010197
3.5	3505.260566	136.764822	5673.185874	140.294004	53.667835	0.010737
3.6	3606.232604	140.819565	5860.566109	145.670027	55.282823	0.011286
3.7	3707.210322	144.875896	6047.96688	151.058395	56.898453	0.011845
3.8	3808.193545	148.933769	6235.384417	156.457947	58.514707	0.012412
3.9	3909.182104	152.993138	6422.815667	161.867651	60.131566	0.012989
4	4010.175836	157.053962	6610.258154	167.286583	61.749013	0.013574
4.1	4111.174587	161.116197	6797.709872	172.713916	63.367031	0.014167
4.2	4212.178209	165.179805	6985.169193	178.148912	64.985603	0.014768
4.3	4313.186558	169.244745	7172.634794	183.590912	66.604714	0.015378
4.4	4414.199497	173.31098	7360.105604	189.039322	68.224349	0.015995
4.5	4515.216893	177.378474	7547.58075	194.493612	69.844493	0.016619
4.6	4616.238618	181.44719	7735.059523	199.953307	71.465131	0.017251
4.7	4717.264547	185.517095	7922.541347	205.417978	73.086249	0.017889
4.8	4818.294561	189.588154	8110.025751	210.887242	74.707834	0.018535
4.9	4919.328544	193.660336	8297.512352	216.360752	76.329872	0.019187
5	5020.366384	197.733609	8485.000836	221.838198	77.952352	0.019845
5.1	5121.40797	201.807941	8672.490946	227.319298	79.57526	0.02051
5.2	5222.453199	205.883305	8859.982473	232.803798	81.198584	0.021181
5.3	5323.501968	209.95967	9047.475242	238.29147	82.822313	0.021858
5.4	5424.554177	214.037009	9234.969111	243.782104	84.446436	0.022541
5.5	5525.60973	218.115294	9422.463961	249.275513	86.070942	0.023229
5.6	5626.668533	222.1945	9609.959696	254.771525	87.695819	0.023923
5.7	5727.730496	226.2746	9797.456231	260.269985	89.321058	0.024622
5.8	5828.795531	230.35557	9984.953499	265.77075	90.946649	0.025326
5.9	5929.863553	234.437386	10172.451442	271.27369	92.572581	0.026036
6	6030.934477	238.520024	10359.950011	276.778687	94.198846	0.02675
6.1	6051.550836	241.03913	10530.954073	282.198323	95.543974	0.027465
6.2	6055.738615	242.014353	10669.566964	287.244756	96.197799	0.02817
6.3	6057.892437	242.479129	10781.804154	291.823159	96.495787	0.028859
6.4	6059.193515	242.739231	10872.663928	295.935984	96.645805	0.02953
6.5	6060.10775	242.914101	10946.210862	299.615293	96.734774	0.030184
6.6	6060.829809	243.052053	11005.742005	302.901445	96.798033	0.030819
6.7	6061.444074	243.172765	11053.928618	305.835067	96.849946	0.031437
6.8	6061.989289	243.28432	11092.933669	308.454165	96.896373	0.032038
6.9	6062.4849	243.390097	11124.50803	310.793255	96.939734	0.032623
7	6062.94186	243.491563	11150.068788	312.883293	96.981047	0.033192
7.1	6063.36714	243.589402	11170.762787	314.751884	97.020764	0.033744
7.2	6063.765646	243.683976	11187.518139	316.423582	97.059102	0.034282
7.3	6064.141088	243.775508	11201.085925	317.920205	97.096181	0.034805

7.4	6064.496396	243.864161	11212.073958	319.261126	97.132079	0.035313
7.5	6064.83394	243.950066	11220.974114	320.463549	97.166855	0.035808
7.6	6065.155669	244.03334	11228.184444	321.542748	97.20056	0.036288
7.7	6065.463197	244.114088	11234.027072	322.512282	97.233237	0.036756
7.8	6065.757877	244.192407	11238.762681	323.384193	97.264927	0.03721
7.9	6066.040844	244.268389	11242.602231	324.169171	97.295667	0.037653
8	6066.313058	244.342119	11245.716445	324.876711	97.325493	0.038082
8.1	6066.575337	244.413676	11248.243486	325.515244	97.354437	0.0385
8.2	6066.828382	244.483137	11250.295166	326.092257	97.382531	0.038907
8.3	6067.072795	244.550574	11251.961973	326.614404	97.409805	0.039302
8.4	6067.3091	244.616055	11253.317142	327.087593	97.436285	0.039686
8.5	6067.537757	244.679645	11254.419939	327.517073	97.461998	0.04006
8.6	6067.759167	244.741406	11255.318333	327.907511	97.486971	0.040424
8.7	6067.97369	244.801397	11256.051146	328.263053	97.511226	0.040777
8.8	6068.181646	244.859673	11256.649801	328.587383	97.534788	0.041121
8.9	6068.383324	244.91629	11257.139729	328.883778	97.557677	0.041455
9	6068.578985	244.971299	11257.541518	329.155152	97.579915	0.04178
9.1	6068.76887	245.024749	11257.871829	329.404096	97.601522	0.042096
9.2	6068.953198	245.076688	11258.144154	329.632915	97.622518	0.042403
9.3	6069.132173	245.127161	11258.369411	329.84366	97.642921	0.042702
9.4	6069.305984	245.176214	11258.556443	330.038158	97.662748	0.042992
9.5	6069.47481	245.223887	11258.712409	330.218034	97.682018	0.043275
9.6	6069.638816	245.270223	11258.843104	330.384736	97.700746	0.04355
9.7	6069.79816	245.31526	11258.953225	330.539554	97.71895	0.043817
9.8	6069.952991	245.359036	11259.046573	330.683638	97.736643	0.044076
9.9	6070.103451	245.401589	11259.126232	330.818014	97.753842	0.044329
10	6070.249674	245.442953	11259.194696	330.943596	97.77056	0.044575
10.1	6070.39179	245.483164	11259.25399	331.061201	97.786811	0.044813
10.2	6070.529922	245.522254	11259.305755	331.171558	97.802609	0.045046
10.3	6070.664189	245.560255	11259.351322	331.275319	97.817967	0.045271
10.4	6070.794704	245.597198	11259.39177	331.373067	97.832898	0.045491
10.5	6070.921578	245.633115	11259.427977	331.465322	97.847413	0.045705
10.6	6071.044915	245.668033	11259.460656	331.552553	97.861525	0.045912
10.7	6071.16482	245.701982	11259.490385	331.635177	97.875244	0.046114
10.8	6071.281389	245.734988	11259.517636	331.71357	97.888583	0.04631
10.9	6071.394719	245.767078	11259.542793	331.788068	97.901551	0.046501
11	6071.504901	245.798278	11259.56617	331.858975	97.91416	0.046687
11.1	6071.612025	245.828613	11259.588022	331.926563	97.926419	0.046867
11.2	6071.716177	245.858108	11259.608559	331.991076	97.938338	0.047043
11.3	6071.817442	245.886785	11259.627952	332.052737	97.949927	0.047214
11.4	6071.9159	245.914668	11259.646344	332.111745	97.961195	0.04738
11.5	6072.011631	245.941779	11259.66385	332.168281	97.972151	0.047541
11.6	6072.10471	245.96814	11259.680567	332.222508	97.982804	0.047698
11.7	6072.195212	245.993771	11259.696575	332.274574	97.993162	0.047851

11.8	6072.28321	246.018693	11259.71194	332.324613	98.003233	0.047999
11.9	6072.368772	246.042926	11259.726718	332.372749	98.013026	0.048143
12	6072.451968	246.066488	11259.740956	332.419092	98.022547	0.048284

Level IV change of degradation in time (kg)

Time (a)	Air	Water	Soil	Sediment	Susp. sediment	Biota
0	0	0	0	0	0	0
0.1	56.392774	0.000202	18.190099	0.09967	0.000038	0.000004
0.2	120.653687	0.000577	68.51694	0.584324	0.000157	0.000024
0.3	186.202448	0.001011	144.947787	1.540014	0.000316	0.000064
0.4	252.294874	0.001468	242.534754	2.961808	0.000493	0.000126
0.5	318.635766	0.001934	357.254969	4.816811	0.000677	0.000211
0.6	385.101547	0.002405	485.845473	7.064449	0.000863	0.000317
0.7	451.638505	0.002878	625.662733	9.664112	0.001051	0.000445
0.8	518.221864	0.003352	774.566272	12.577896	0.00124	0.000593
0.9	584.839104	0.003827	930.823441	15.771401	0.001429	0.000762
1	651.483111	0.004302	1093.031907	19.213792	0.001618	0.000951
1.1	718.149319	0.004778	1260.056767	22.877569	0.001808	0.001159
1.2	784.834489	0.005255	1430.979571	26.738275	0.001997	0.001386
1.3	851.536156	0.005732	1605.057059	30.774174	0.002187	0.00163
1.4	918.252367	0.006209	1781.687742	34.965964	0.002377	0.001893
1.5	984.98153	0.006687	1960.384863	39.296502	0.002568	0.002172
1.6	1051.722333	0.007165	2140.754511	43.750568	0.002758	0.002469
1.7	1118.473681	0.007643	2322.477911	48.314645	0.002948	0.002782
1.8	1185.234655	0.008122	2505.297088	52.976729	0.003139	0.00311
1.9	1252.004478	0.008601	2689.003274	57.72616	0.00333	0.003454
2	1318.782486	0.00908	2873.427516	62.553468	0.003521	0.003813
2.1	1385.568113	0.00956	3058.433085	67.450243	0.003712	0.004186
2.2	1452.360869	0.01004	3243.909325	72.409013	0.003903	0.004574
2.3	1519.160328	0.01052	3429.766684	77.423139	0.004094	0.004975
2.4	1585.966119	0.011001	3615.932686	82.48672	0.004286	0.00539
2.5	1652.777913	0.011482	3802.348673	87.594512	0.004477	0.005818
2.6	1719.595418	0.011963	3988.96717	92.741855	0.004669	0.006258
2.7	1786.418372	0.012444	4175.749752	97.924604	0.00486	0.006711
2.8	1853.24654	0.012926	4362.66532	103.139074	0.005052	0.007176
2.9	1920.079707	0.013408	4549.688699	108.381986	0.005244	0.007652
3	1986.917676	0.01389	4736.799511	113.650425	0.005436	0.00814
3.1	2053.760268	0.014372	4923.981262	118.941795	0.005628	0.008638
3.2	2120.607315	0.014854	5111.220596	124.253785	0.005821	0.009148
3.3	2187.458661	0.015337	5298.506701	129.584338	0.006013	0.009667
3.4	2254.314159	0.01582	5485.830824	134.931622	0.006205	0.010197
3.5	2321.173673	0.016303	5673.185874	140.294004	0.006398	0.010737

3.6	2388.037071	0.016787	5860.566109	145.670027	0.00659	0.011286
3.7	2454.904232	0.01727	6047.96688	151.058395	0.006783	0.011845
3.8	2521.775038	0.017754	6235.384417	156.457947	0.006975	0.012412
3.9	2588.649377	0.018238	6422.815667	161.867651	0.007168	0.012989
4	2655.527142	0.018722	6610.258154	167.286583	0.007361	0.013574
4.1	2722.40823	0.019206	6797.709872	172.713916	0.007554	0.014167
4.2	2789.292544	0.019691	6985.169193	178.148912	0.007747	0.014768
4.3	2856.179988	0.020175	7172.634794	183.590912	0.00794	0.015378
4.4	2923.070472	0.02066	7360.105604	189.039322	0.008133	0.015995
4.5	2989.963907	0.021145	7547.58075	194.493612	0.008326	0.016619
4.6	3056.860209	0.02163	7735.059523	199.953307	0.008519	0.017251
4.7	3123.759294	0.022115	7922.541347	205.417978	0.008712	0.017889
4.8	3190.661085	0.0226	8110.025751	210.887242	0.008906	0.018535
4.9	3257.565504	0.023086	8297.512352	216.360752	0.009099	0.019187
5	3324.472477	0.023571	8485.000836	221.838198	0.009292	0.019845
5.1	3391.381931	0.024057	8672.490946	227.319298	0.009486	0.02051
5.2	3458.293797	0.024543	8859.982473	232.803798	0.009679	0.021181
5.3	3525.208007	0.025029	9047.475242	238.29147	0.009873	0.021858
5.4	3592.124495	0.025515	9234.969111	243.782104	0.010067	0.022541
5.5	3659.043197	0.026001	9422.463961	249.275513	0.01026	0.023229
5.6	3725.964052	0.026487	9609.959696	254.771525	0.010454	0.023923
5.7	3792.886999	0.026974	9797.456231	260.269985	0.010648	0.024622
5.8	3859.811981	0.02746	9984.953499	265.77075	0.010841	0.025326
5.9	3926.73894	0.027947	10172.451442	271.27369	0.011035	0.026036
6	3993.667821	0.028433	10359.950011	276.778687	0.011229	0.02675
6.1	4007.319916	0.028734	10530.954073	282.198323	0.01139	0.027465
6.2	4010.093051	0.02885	10669.566964	287.244756	0.011467	0.02817
6.3	4011.519307	0.028905	10781.804154	291.823159	0.011503	0.028859
6.4	4012.380877	0.028936	10872.663928	295.935984	0.011521	0.02953
6.5	4012.98628	0.028957	10946.210862	299.615293	0.011531	0.030184
6.6	4013.464426	0.028974	11005.742005	302.901445	0.011539	0.030819
6.7	4013.87119	0.028988	11053.928618	305.835067	0.011545	0.031437
6.8	4014.232231	0.029001	11092.933669	308.454165	0.011551	0.032038
6.9	4014.560422	0.029014	11124.50803	310.793255	0.011556	0.032623
7	4014.86302	0.029026	11150.068788	312.883293	0.011561	0.033192
7.1	4015.144639	0.029038	11170.762787	314.751884	0.011566	0.033744
7.2	4015.408529	0.029049	11187.518139	316.423582	0.01157	0.034282
7.3	4015.657146	0.02906	11201.085925	317.920205	0.011575	0.034805
7.4	4015.89243	0.02907	11212.073958	319.261126	0.011579	0.035313
7.5	4016.11595	0.029081	11220.974114	320.463549	0.011583	0.035808
7.6	4016.328998	0.029091	11228.184444	321.542748	0.011587	0.036288
7.7	4016.532642	0.0291	11234.027072	322.512282	0.011591	0.036756
7.8	4016.727779	0.029109	11238.762681	323.384193	0.011595	0.03721
7.9	4016.915158	0.029119	11242.602231	324.169171	0.011598	0.037653

8	4017.095418	0.029127	11245.716445	324.876711	0.011602	0.038082
8.1	4017.269099	0.029136	11248.243486	325.515244	0.011605	0.0385
8.2	4017.436664	0.029144	11250.295166	326.092257	0.011609	0.038907
8.3	4017.598514	0.029152	11251.961973	326.614404	0.011612	0.039302
8.4	4017.754994	0.02916	11253.317142	327.087593	0.011615	0.039686
8.5	4017.90641	0.029168	11254.419939	327.517073	0.011618	0.04006
8.6	4018.053027	0.029175	11255.318333	327.907511	0.011621	0.040424
8.7	4018.195084	0.029182	11256.051146	328.263053	0.011624	0.040777
8.8	4018.332792	0.029189	11256.649801	328.587383	0.011627	0.041121
8.9	4018.466342	0.029196	11257.139729	328.883778	0.01163	0.041455
9	4018.595909	0.029202	11257.541518	329.155152	0.011632	0.04178
9.1	4018.72165	0.029209	11257.871829	329.404096	0.011635	0.042096
9.2	4018.843711	0.029215	11258.144154	329.632915	0.011637	0.042403
9.3	4018.962228	0.029221	11258.369411	329.84366	0.01164	0.042702
9.4	4019.077325	0.029227	11258.556443	330.038158	0.011642	0.042992
9.5	4019.189121	0.029232	11258.712409	330.218034	0.011644	0.043275
9.6	4019.297725	0.029238	11258.843104	330.384736	0.011647	0.04355
9.7	4019.403243	0.029243	11258.953225	330.539554	0.011649	0.043817
9.8	4019.505771	0.029249	11259.046573	330.683638	0.011651	0.044076
9.9	4019.605405	0.029254	11259.126232	330.818014	0.011653	0.044329
10	4019.702234	0.029259	11259.194696	330.943596	0.011655	0.044575
10.1	4019.796343	0.029263	11259.25399	331.061201	0.011657	0.044813
10.2	4019.887813	0.029268	11259.305755	331.171558	0.011659	0.045046
10.3	4019.976724	0.029273	11259.351322	331.275319	0.011661	0.045271
10.4	4020.063151	0.029277	11259.39177	331.373067	0.011662	0.045491
10.5	4020.147167	0.029281	11259.427977	331.465322	0.011664	0.045705
10.6	4020.228841	0.029285	11259.460656	331.552553	0.011666	0.045912
10.7	4020.308241	0.029289	11259.490385	331.635177	0.011667	0.046114
10.8	4020.385433	0.029293	11259.517636	331.71357	0.011669	0.04631
10.9	4020.460479	0.029297	11259.542793	331.788068	0.011671	0.046501
11	4020.533442	0.029301	11259.56617	331.858975	0.011672	0.046687
11.1	4020.604379	0.029305	11259.588022	331.926563	0.011674	0.046867
11.2	4020.673348	0.029308	11259.608559	331.991076	0.011675	0.047043
11.3	4020.740405	0.029311	11259.627952	332.052737	0.011676	0.047214
11.4	4020.805604	0.029315	11259.646344	332.111745	0.011678	0.04738
11.5	4020.868997	0.029318	11259.66385	332.168281	0.011679	0.047541
11.6	4020.930634	0.029321	11259.680567	332.222508	0.01168	0.047698
11.7	4020.990564	0.029324	11259.696575	332.274574	0.011681	0.047851
11.8	4021.048836	0.029327	11259.71194	332.324613	0.011683	0.047999
11.9	4021.105495	0.02933	11259.726718	332.372749	0.011684	0.048143
12	4021.160587	0.029333	11259.740956	332.419092	0.011685	0.048284

Level IV change of export in time (kg)

Time (a)	Air	Water	Soil	Sediment	Susp. sediment	Biota
0	0	0	0	0	0	0
0.1	28.76732	1.695878	0	0	0.315421	0
0.2	61.548367	4.84327	0	0	1.314021	0
0.3	94.986377	8.478144	0	0	2.653975	0
0.4	128.701724	12.309529	0	0	4.135772	0
0.5	162.54382	16.223279	0	0	5.676289	0
0.6	196.449624	20.173184	0	0	7.24173	0
0.7	230.391737	24.140409	0	0	8.818359	0
0.8	264.357521	28.117199	0	0	10.400559	0
0.9	298.340588	32.1003	0	0	11.986009	0
1	332.337309	36.088283	0	0	13.573725	0
1.1	366.345356	40.080472	0	0	15.163266	0
1.2	400.363076	44.076497	0	0	16.754415	0
1.3	434.389212	48.076126	0	0	18.347049	0
1.4	468.422766	52.07918	0	0	19.941084	0
1.5	502.462928	56.085513	0	0	21.536455	0
1.6	536.509028	60.094996	0	0	23.133107	0
1.7	570.560507	64.107508	0	0	24.73099	0
1.8	604.616896	68.122939	0	0	26.330059	0
1.9	638.677799	72.141185	0	0	27.93027	0
2	672.742878	76.162147	0	0	29.531582	0
2.1	706.811843	80.185732	0	0	31.133959	0
2.2	740.884446	84.211852	0	0	32.737363	0
2.3	774.960467	88.240422	0	0	34.34176	0
2.4	809.039719	92.271364	0	0	35.947118	0
2.5	843.122033	96.3046	0	0	37.553405	0
2.6	877.20726	100.340058	0	0	39.160592	0
2.7	911.295267	104.377667	0	0	40.768651	0
2.8	945.385933	108.417362	0	0	42.377553	0
2.9	979.47915	112.459078	0	0	43.987274	0
3	1013.574817	116.502753	0	0	45.597787	0
3.1	1047.672841	120.548328	0	0	47.20907	0
3.2	1081.773139	124.595746	0	0	48.821098	0
3.3	1115.875629	128.644952	0	0	50.433849	0
3.4	1149.980237	132.695893	0	0	52.047302	0
3.5	1184.086894	136.748518	0	0	53.661437	0
3.6	1218.195532	140.802779	0	0	55.276233	0
3.7	1252.30609	144.858626	0	0	56.891671	0
3.8	1286.418507	148.916015	0	0	58.507732	0
3.9	1320.532727	152.9749	0	0	60.124398	0
4	1354.648694	157.03524	0	0	61.741652	0
4.1	1388.766357	161.096991	0	0	63.359477	0

4.2	1422.885665	165.160114	0	0	64.977856	0
4.3	1457.00657	169.22457	0	0	66.596775	0
4.4	1491.129025	173.29032	0	0	68.216216	0
4.5	1525.252986	177.357329	0	0	69.836167	0
4.6	1559.378409	181.425561	0	0	71.456611	0
4.7	1593.505253	185.49498	0	0	73.077536	0
4.8	1627.633476	189.565554	0	0	74.698928	0
4.9	1661.76304	193.63725	0	0	76.320773	0
5	1695.893907	197.710037	0	0	77.943059	0
5.1	1730.02604	201.783884	0	0	79.565774	0
5.2	1764.159403	205.858762	0	0	81.188905	0
5.3	1798.293961	209.934641	0	0	82.81244	0
5.4	1832.429682	214.011494	0	0	84.43637	0
5.5	1866.566533	218.089293	0	0	86.060682	0
5.6	1900.704481	222.168013	0	0	87.685365	0
5.7	1934.843497	226.247627	0	0	89.310411	0
5.8	1968.98355	230.32811	0	0	90.935807	0
5.9	2003.124613	234.40944	0	0	92.561546	0
6	2037.266656	238.491591	0	0	94.187616	0
6.1	2044.23092	241.010396	0	0	95.532585	0
6.2	2045.645563	241.985503	0	0	96.186331	0
6.3	2046.373131	242.450223	0	0	96.484284	0
6.4	2046.812638	242.710295	0	0	96.634284	0
6.5	2047.121469	242.885144	0	0	96.723242	0
6.6	2047.365383	243.02308	0	0	96.786494	0
6.7	2047.572883	243.143777	0	0	96.8384	0
6.8	2047.757059	243.255319	0	0	96.884822	0
6.9	2047.924477	243.361083	0	0	96.928178	0
7	2048.07884	243.462537	0	0	96.969486	0
7.1	2048.2225	243.560365	0	0	97.009199	0
7.2	2048.357117	243.654927	0	0	97.047532	0
7.3	2048.483943	243.746448	0	0	97.084606	0
7.4	2048.603967	243.83509	0	0	97.1205	0
7.5	2048.71799	243.920985	0	0	97.155272	0
7.6	2048.826671	244.004249	0	0	97.188973	0
7.7	2048.930555	244.084988	0	0	97.221646	0
7.8	2049.030098	244.163298	0	0	97.253332	0
7.9	2049.125685	244.239271	0	0	97.284069	0
8	2049.21764	244.312991	0	0	97.313891	0
8.1	2049.306239	244.38454	0	0	97.342832	0
8.2	2049.391718	244.453993	0	0	97.370923	0
8.3	2049.474281	244.521422	0	0	97.398193	0
8.4	2049.554106	244.586895	0	0	97.42467	0
8.5	2049.631347	244.650478	0	0	97.45038	0

8.6	2049.70614	244.712231	0	0	97.47535	0
8.7	2049.778606	244.772215	0	0	97.499602	0
8.8	2049.848854	244.830484	0	0	97.523161	0
8.9	2049.916982	244.887094	0	0	97.546047	0
9	2049.983077	244.942096	0	0	97.568283	0
9.1	2050.04722	244.99554	0	0	97.589887	0
9.2	2050.109487	245.047473	0	0	97.610881	0
9.3	2050.169945	245.09794	0	0	97.631281	0
9.4	2050.228659	245.146987	0	0	97.651106	0
9.5	2050.285689	245.194655	0	0	97.670374	0
9.6	2050.34109	245.240985	0	0	97.6891	0
9.7	2050.394917	245.286016	0	0	97.707301	0
9.8	2050.44722	245.329788	0	0	97.724992	0
9.9	2050.498045	245.372335	0	0	97.742189	0
10	2050.54744	245.413695	0	0	97.758905	0
10.1	2050.595447	245.4539	0	0	97.775154	0
10.2	2050.642109	245.492986	0	0	97.79095	0
10.3	2050.687464	245.530982	0	0	97.806307	0
10.4	2050.731553	245.567922	0	0	97.821235	0
10.5	2050.774411	245.603834	0	0	97.835749	0
10.6	2050.816075	245.638748	0	0	97.849859	0
10.7	2050.856579	245.672692	0	0	97.863577	0
10.8	2050.895956	245.705694	0	0	97.876914	0
10.9	2050.934239	245.737781	0	0	97.889881	0
11	2050.971459	245.768977	0	0	97.902488	0
11.1	2051.007646	245.799309	0	0	97.914746	0
11.2	2051.042829	245.8288	0	0	97.926664	0
11.3	2051.077036	245.857474	0	0	97.938251	0
11.4	2051.110296	245.885354	0	0	97.949518	0
11.5	2051.142634	245.912461	0	0	97.960472	0
11.6	2051.174076	245.938819	0	0	97.971124	0
11.7	2051.204648	245.964447	0	0	97.98148	0
11.8	2051.234374	245.989366	0	0	97.99155	0
11.9	2051.263277	246.013596	0	0	98.001342	0
12	2051.291381	246.037155	0	0	98.010862	0

Level IV change of emission in time (kg)

Time (a)	Air	Water	Soil	Sediment	Susp. sediment	Biota
0	0	0	0	0	0	0
0.1	100	26.055923	173.944077	0	0	0
0.2	100	26.055923	173.944077	0	0	0
0.3	100	26.055923	173.944077	0	0	0

0.4	100	26.055923	173.944077	0	0	0
0.5	100	26.055923	173.944077	0	0	0
0.6	100	26.055923	173.944077	0	0	0
0.7	100	26.055923	173.944077	0	0	0
0.8	100	26.055923	173.944077	0	0	0
0.9	100	26.055923	173.944077	0	0	0
1	100	26.055923	173.944077	0	0	0
1.1	100	26.055923	173.944077	0	0	0
1.2	100	26.055923	173.944077	0	0	0
1.3	100	26.055923	173.944077	0	0	0
1.4	100	26.055923	173.944077	0	0	0
1.5	100	26.055923	173.944077	0	0	0
1.6	100	26.055923	173.944077	0	0	0
1.7	100	26.055923	173.944077	0	0	0
1.8	100	26.055923	173.944077	0	0	0
1.9	100	26.055923	173.944077	0	0	0
2	100	26.055923	173.944077	0	0	0
2.1	100	26.055923	173.944077	0	0	0
2.2	100	26.055923	173.944077	0	0	0
2.3	100	26.055923	173.944077	0	0	0
2.4	100	26.055923	173.944077	0	0	0
2.5	100	26.055923	173.944077	0	0	0
2.6	100	26.055923	173.944077	0	0	0
2.7	100	26.055923	173.944077	0	0	0
2.8	100	26.055923	173.944077	0	0	0
2.9	100	26.055923	173.944077	0	0	0
3	100	26.055923	173.944077	0	0	0
3.1	100	26.055923	173.944077	0	0	0
3.2	100	26.055923	173.944077	0	0	0
3.3	100	26.055923	173.944077	0	0	0
3.4	100	26.055923	173.944077	0	0	0
3.5	100	26.055923	173.944077	0	0	0
3.6	100	26.055923	173.944077	0	0	0
3.7	100	26.055923	173.944077	0	0	0
3.8	100	26.055923	173.944077	0	0	0
3.9	100	26.055923	173.944077	0	0	0
4	100	26.055923	173.944077	0	0	0
4.1	100	26.055923	173.944077	0	0	0
4.2	100	26.055923	173.944077	0	0	0
4.3	100	26.055923	173.944077	0	0	0
4.4	100	26.055923	173.944077	0	0	0
4.5	100	26.055923	173.944077	0	0	0
4.6	100	26.055923	173.944077	0	0	0
4.7	100	26.055923	173.944077	0	0	0

4.8	100	26.055923	173.944077	0	0	0
4.9	100	26.055923	173.944077	0	0	0
5	100	26.055923	173.944077	0	0	0
5.1	100	26.055923	173.944077	0	0	0
5.2	100	26.055923	173.944077	0	0	0
5.3	100	26.055923	173.944077	0	0	0
5.4	100	26.055923	173.944077	0	0	0
5.5	100	26.055923	173.944077	0	0	0
5.6	100	26.055923	173.944077	0	0	0
5.7	100	26.055923	173.944077	0	0	0
5.8	100	26.055923	173.944077	0	0	0
5.9	100	26.055923	173.944077	0	0	0
6	100	26.055923	173.944077	0	0	0
6.1	4.943079	1.287965	8.598193	0	0	0
6.2	0	0	0	0	0	0
6.3	0	0	0	0	0	0
6.4	0	0	0	0	0	0
6.5	0	0	0	0	0	0
6.6	0	0	0	0	0	0
6.7	0	0	0	0	0	0
6.8	0	0	0	0	0	0
6.9	0	0	0	0	0	0
7	0	0	0	0	0	0
7.1	0	0	0	0	0	0
7.2	0	0	0	0	0	0
7.3	0	0	0	0	0	0
7.4	0	0	0	0	0	0
7.5	0	0	0	0	0	0
7.6	0	0	0	0	0	0
7.7	0	0	0	0	0	0
7.8	0	0	0	0	0	0
7.9	0	0	0	0	0	0
8	0	0	0	0	0	0
8.1	0	0	0	0	0	0
8.2	0	0	0	0	0	0
8.3	0	0	0	0	0	0
8.4	0	0	0	0	0	0
8.5	0	0	0	0	0	0
8.6	0	0	0	0	0	0
8.7	0	0	0	0	0	0
8.8	0	0	0	0	0	0
8.9	0	0	0	0	0	0
9	0	0	0	0	0	0
9.1	0	0	0	0	0	0

9.2	0	0	0	0	0
9.3	0	0	0	0	0
9.4	0	0	0	0	0
9.5	0	0	0	0	0
9.6	0	0	0	0	0
9.7	0	0	0	0	0
9.8	0	0	0	0	0
9.9	0	0	0	0	0
10	0	0	0	0	0
10.1	0	0	0	0	0
10.2	0	0	0	0	0
10.3	0	0	0	0	0
10.4	0	0	0	0	0
10.5	0	0	0	0	0
10.6	0	0	0	0	0
10.7	0	0	0	0	0
10.8	0	0	0	0	0
10.9	0	0	0	0	0
11	0	0	0	0	0
11.1	0	0	0	0	0
11.2	0	0	0	0	0
11.3	0	0	0	0	0
11.4	0	0	0	0	0
11.5	0	0	0	0	0
11.6	0	0	0	0	0
11.7	0	0	0	0	0
11.8	0	0	0	0	0
11.9	0	0	0	0	0
12	0	0	0	0	0

Checking mass balance (kg)

Time (a)	Entry	Mass	Disappearance	Mass balance
0	0	0	0.00000	0.000000000
0.1	300	194.538595	105.46141	0.000000000
0.2	600	342.538633	257.46137	0.000000000
0.3	900	461.189864	438.81014	0.000000000
0.4	1200	557.059452	642.94055	0.000000000
0.5	1500	634.846246	865.15375	0.000000000
0.6	1800	698.120407	1101.87959	0.000000000
0.7	2100	749.679771	1350.32023	0.000000000
0.8	2400	791.753503	1608.24650	0.000000000
0.9	2700	826.133138	1873.86686	0.000000000

1	3000	854.265	2145.73500	0.000000000
1.1	3300	877.319506	2422.68049	0.000000000
1.2	3600	896.245039	2703.75496	0.000000000
1.3	3900	911.810675	2988.18933	0.000000000
1.4	4200	924.640418	3275.35958	0.000000000
1.5	4500	935.240782	3564.75922	0.000000000
1.6	4800	944.023066	3855.97693	0.000000000
1.7	5100	951.321385	4148.67862	0.000000000
1.8	5400	957.407262	4442.59274	0.000000000
1.9	5700	962.50145	4737.49855	0.000000000
2	6000	966.783509	5033.21649	0.000000000
2.1	6300	970.399567	5329.60043	0.000000000
2.2	6600	973.468616	5626.53138	0.000000000
2.3	6900	976.087609	5923.91239	0.000000000
2.4	7200	978.335598	6221.66440	0.000000000
2.5	7500	980.277088	6519.72291	0.000000000
2.6	7800	981.964758	6818.03524	0.000000000
2.7	8100	983.441671	7116.55833	0.000000000
2.8	8400	984.743064	7415.25694	0.000000000
2.9	8700	985.897803	7714.10220	0.000000000
3	9000	986.929565	8013.07043	0.000000000
3.1	9300	987.857798	8312.14220	0.000000000
3.2	9600	988.6985	8611.30150	0.000000000
3.3	9900	989.464853	8910.53515	0.000000000
3.4	10200	990.16774	9209.83226	0.000000000
3.5	10500	990.816163	9509.18384	0.000000000
3.6	10800	991.417585	9808.58242	0.000000000
3.7	11100	991.978208	10108.02179	0.000000000
3.8	11400	992.503202	10407.49680	0.000000000
3.9	11700	992.996885	10707.00311	0.000000000
4	12000	993.462879	11006.53712	0.000000000
4.1	12300	993.90423	11306.09577	0.000000000
4.2	12600	994.32351	11605.67649	0.000000000
4.3	12900	994.722899	11905.27710	0.000000000
4.4	13200	995.104253	12204.89575	0.000000000
4.5	13500	995.469159	12504.53084	0.000000000
4.6	13800	995.818981	12804.18102	0.000000000
4.7	14100	996.154895	13103.84510	0.000000000
4.8	14400	996.477923	13403.52208	0.000000000
4.9	14700	996.788957	13703.21104	0.000000000
5	15000	997.088777	14002.91122	0.000000000
5.1	15300	997.378074	14302.62193	0.000000000
5.2	15600	997.65746	14602.34254	0.000000000
5.3	15900	997.92748	14902.07252	0.000000000

5.4	16200	998.188623	15201.81138	0.000000000
5.5	16500	998.441331	15501.55867	0.000000000
5.6	16800	998.686004	15801.31400	0.000000000
5.7	17100	998.923007	16101.07699	0.000000000
5.8	17400	999.152674	16400.84733	0.000000000
5.9	17700	999.375312	16700.62469	0.000000000
6	18000	999.591206	17000.40879	0.000000000
6.1	18014.829236	813.515434	17201.31380	0.000000000
6.2	18014.829236	664.03858	17350.79066	0.000000000
6.3	18014.829236	544.305711	17470.52353	0.000000000
6.4	18014.829236	447.621242	17567.20799	0.000000000
6.5	18014.829236	369.216273	17645.61296	0.000000000
6.6	18014.829236	305.475072	17709.35416	0.000000000
6.7	18014.829236	253.567329	17761.26191	0.000000000
6.8	18014.829236	211.239382	17803.58985	0.000000000
6.9	18014.829236	176.680598	17838.14864	0.000000000
7	18014.829236	148.429494	17866.39974	0.000000000
7.1	18014.829236	125.303515	17889.52572	0.000000000
7.2	18014.829236	106.344509	17908.48473	0.000000000
7.3	18014.829236	90.775525	17924.05371	0.000000000
7.4	18014.829236	77.966203	17936.86303	0.000000000
7.5	18014.829236	67.404904	17947.42433	0.000000000
7.6	18014.829236	58.676188	17956.15305	0.000000000
7.7	18014.829236	51.442604	17963.38663	0.000000000
7.8	18014.829236	45.42994	17969.39930	0.000000000
7.9	18014.829236	40.415281	17974.41395	0.000000000
8	18014.829236	36.217328	17978.61191	0.000000000
8.1	18014.829236	32.688556	17982.14068	0.000000000
8.2	18014.829236	29.708856	17985.12038	0.000000000
8.3	18014.829236	27.180383	17987.64885	0.000000000
8.4	18014.829236	25.023375	17989.80586	0.000000000
8.5	18014.829236	23.172764	17991.65647	0.000000000
8.6	18014.829236	21.575424	17993.25381	0.000000000
8.7	18014.829236	20.187947	17994.64129	0.000000000
8.8	18014.829236	18.974825	17995.85441	0.000000000
8.9	18014.829236	17.906983	17996.92225	0.000000000
9	18014.829236	16.960588	17997.86865	0.000000000
9.1	18014.829236	16.116074	17998.71316	0.000000000
9.2	18014.829236	15.357361	17999.47188	0.000000000
9.3	18014.829236	14.671208	18000.15803	0.000000000
9.4	18014.829236	14.046696	18000.78254	0.000000000
9.5	18014.829236	13.474804	18001.35443	0.000000000
9.6	18014.829236	12.948062	18001.88117	0.000000000
9.7	18014.829236	12.460272	18002.36896	0.000000000

9.8	18014.829236	12.006278	18002.82296	0.000000000
9.9	18014.829236	11.58178	18003.24746	0.000000000
10	18014.829236	11.183183	18003.64605	0.000000000
10.1	18014.829236	10.807467	18004.02177	0.000000000
10.2	18014.829236	10.452093	18004.37714	0.000000000
10.3	18014.829236	10.114914	18004.71432	0.000000000
10.4	18014.829236	9.794109	18005.03513	0.000000000
10.5	18014.829236	9.488127	18005.34111	0.000000000
10.6	18014.829236	9.195642	18005.63359	0.000000000
10.7	18014.829236	8.915515	18005.91372	0.000000000
10.8	18014.829236	8.646761	18006.18248	0.000000000
10.9	18014.829236	8.388526	18006.44071	0.000000000
11	18014.829236	8.140066	18006.68917	0.000000000
11.1	18014.829236	7.900727	18006.92851	0.000000000
11.2	18014.829236	7.669935	18007.15930	0.000000000
11.3	18014.829236	7.447178	18007.38206	0.000000000
11.4	18014.829236	7.232003	18007.59723	0.000000000
11.5	18014.829236	7.024003	18007.80523	0.000000000
11.6	18014.829236	6.822809	18008.00643	0.000000000
11.7	18014.829236	6.628092	18008.20114	0.000000000
11.8	18014.829236	6.439549	18008.38969	0.000000000
11.9	18014.829236	6.256903	18008.57233	0.000000000
12	18014.829236	6.079901	18008.74934	0.000000000

List of abbreviations and definitions

Abbreviation	Description
BCF	Bioconcentration factor
EU	European Union
FOCUS	FOrum for the Co-ordination of pesticide fate models and their Use
MUST	MUltimedia Stock pollution Tool
STP	Sewage treatment plant

Term	Definition
Bioconcentration factor	ratio of the chemical concentration in an organism or biota to the concentration in water
diffusion	Exchange of objects in region of higher concentration to a region of lower concentration
disappearance	Mass leaving the system either due to degradation or due to export
Stock pollutant	Persistent substances accumulating over time as emission enters the environment
residence time	the time during which water remains within a water body before continuing around the hydrological cycle

References

Gabbert, S., Hahn, S., Nendza, M., Klein, M., & Oosterhuis, F. H. (2018). *Approach for Evaluation of PBTs Subject to Authorisation and Restriction Procedures in context of Socio-economic analysis: Final Report, Part 1*. Brussels: European Commission. https://doi.org/10.2873/33669

Mackay D (2001) Multimedia Environmental Models: The Fugacity Approach - Second Edition. Lewis Publishers, Boca Raton, 1-261.

Mackay D, Paterson S, Cheung B, Neely WB (1985) Evaluating the Environmental Behaviour of Chemicals with a Level III Fugacity Model. Chemosphere 14 (3/4), 335-374.

Mackay, D., Paterson, S. (1982): Fugacity revisited. Environmental Science and Technology 16(12), 654-660.

Mackay, D., Paterson, S. (1991): Evaluating the Multimedia Fate of Organic Chemicals: A Level III Fugacity Approach. Environmental Science & Technology 25, 427-436.