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COMLEAM

COMLEAM Software

User Manual

Version 3.0

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1 Introduction

The software COMLEAM (COnstruction Materials LEAching Model) developed at HSR is developed to assess the leaching of substances potentially harmful to the environment from vertical and horizontal building components exposed to the weather. For this purpose, the runoff on vertical surfaces (e.g. façades, walls) is calculated as wind driven rain (WDR) and on horizontal components (e.g. roofs, pavements) by using the precipitation. The leaching of substances is considered by predefined emission functions or functions derived by the user individually. A system of differential equations determine the water and substance flow from a component to the target compartment (soil or receiving surface water) as well as the substance concentrations (Figure 1). The interface compartments (IC) are virtual (e.g. emission of a building) or with environmental focus (e.g. surface water).

COMLEAM consists of a calculation core programmed in Java and a browser-based user interface. The software is intended to be a platform on which leaching and environmental exposure can be assessed on the one hand by predefined scenarios and boundary conditions (e.g. substances, emission functions). On the other hand, the user can individually define and simulate parameters and requirements of interest. The web browser-based solution installs the software only once on the network and can be run through a user verification process without any additional software or installation.

This manual explains the use of the software COMLEAM, describes the input data and details of the mathematical model.

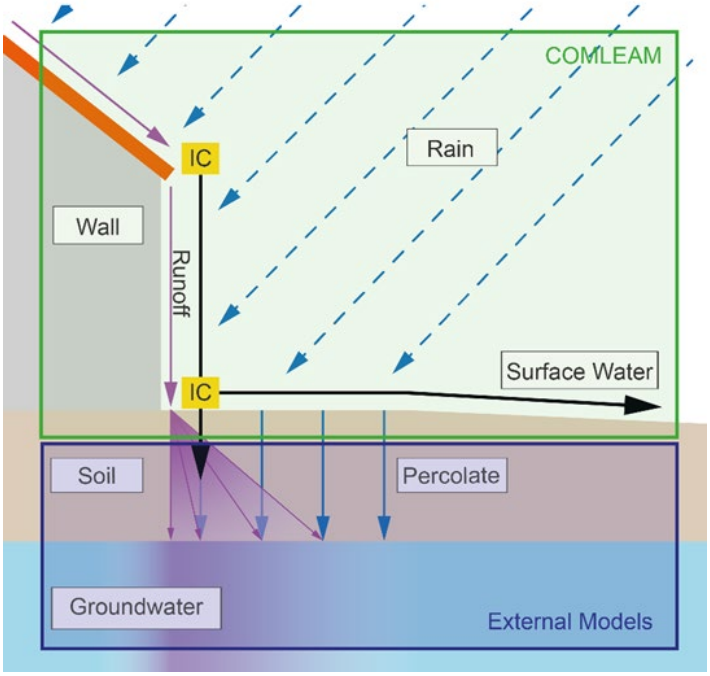


Figure 1: Schematic overview of conditions considered in COMLEAM, i.e. rundoff, leaching from vertical (facades), horizontal surfaces (roofs, pavements), and direct discharge to surface waters.

2 Get started

There are two ways for using the COMLEAM application:

- Installation on local computer (offline)
- Use of web-service (online in web-browser).

2.1 Installation on local computer

Using COMLEAM on a local computer, the installer file need to be downloaded www.comleam.com. The installer will guide the installation process. The computer needs to match certain system requirements (Tab. 1).

Table 1: System requirements for local COMLEAM installation

Requirement	Value
Operating System	Windows 10 Professional/Education 64bit
Processor (CPU)	Intel Core i3 or AMD Phenom II with virtualization enabled (VT-x/AMD-v)
Memory (RAM)	8 GB or more
Hard drive	8 GB of free space or more
Administration rights	One-time local admin rights for installation.

VT-X/AMD-v is necessary to ensure enough performance. The installer has to install programs and tools on the computer. The following programs will be added during installation:

- Google Chrome portable: For accessing the COMLEAM user interface
- Oracle Virtual Box: Software for virtualization. Within this software, the virtual machine (VM) running the COMLEAM application, is hosted.

Any other virtualization suite must be uninstalled before installing COMLEAM (e.g. VM Ware, Hyper-V).

This set-up is similar to the web application. Therefore, COMLEAM can be installed on a local server within a network to be accessible for a defined group of users.

Questions for local COMLEAM webserver applications: support@comleam.com

2.2 Use of web service

The COMLEAM application is also available on the internet. Using the link http://www.sw.comleam.ch the user access the COMLEAM frontend, as it would be shown on the local installation. The HSR University of Applied Sciences in Rapperswil hosts the online application. It is accessible from everywhere in the internet. There is no restriction in using the web app as logins. Everybody is able to see all the calculations and input data like weather, geometries, emission functions etc.

Questions for restricted COMLEAM webserver access (personal use): support@comleam.com

3 Using the Software

COMLEAM's user interface is browser-based. All operations are done in the browser. Excel is mandatorily needed for display and editing input and output data. The UI was designed for Google Chrome browser. Other browsers (e.g. Firefox, Microsoft Edge) need to be tested.

3.1 Home Screen

The home screen (Dashboard) provides direct access to the configuration of a calculation, the administration of the required input data as well as the download of calculation results (Figure 2). The dashboard gives an overview of already existing input data and stored calculations. New data can be recorded directly in the corresponding area via the "Add" buttons without having to take the detour via the detail views for the different input data. In the upper right corner (Figure 2), the notification button (red) and the help button (green) are placed.

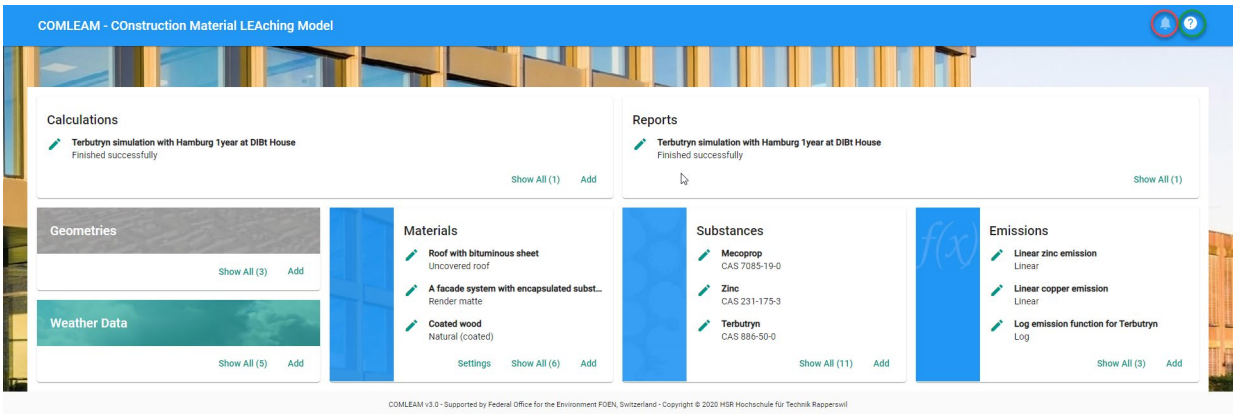


Figure 2: Dashboard of COMLEAM

3.2 Detail Views

The structure of the pages for input data (i.e. modules Geometry, Weather Data, Materials, Emission) as well as Calculations are identical. Available data are listed in the left pane and detailed information of the selected object are in the center and right side of the screen. Names and descriptions can be changed directly by clicking on the title or the description field. The workflow is processed item by item.

In each detail view, in the upper left corner, there is the navigation bar (Figure 3).

Clicking on the house icon will lead back to the home screen, whereas clicking on the left headed arrow will load the last visited page.

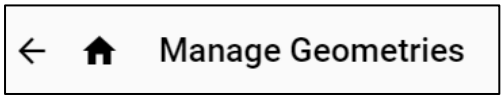


Figure 3: Navigation bar (based on the example of the geometry UI)

3.3 Manage Geometry Data

The detail view of geometry data can be accessed through the dashboard (Figure 4). For each geometry dataset, information about the content of the dataset is presented in a statistical summary on the right side.

Geometry datasets can be renamed and deleted by the user. Direct processing of individual components is possible if the corresponding file containing the data is adapted and uploaded. Information on the structure of geometry files is given in chapter 4.1.1, page 31.

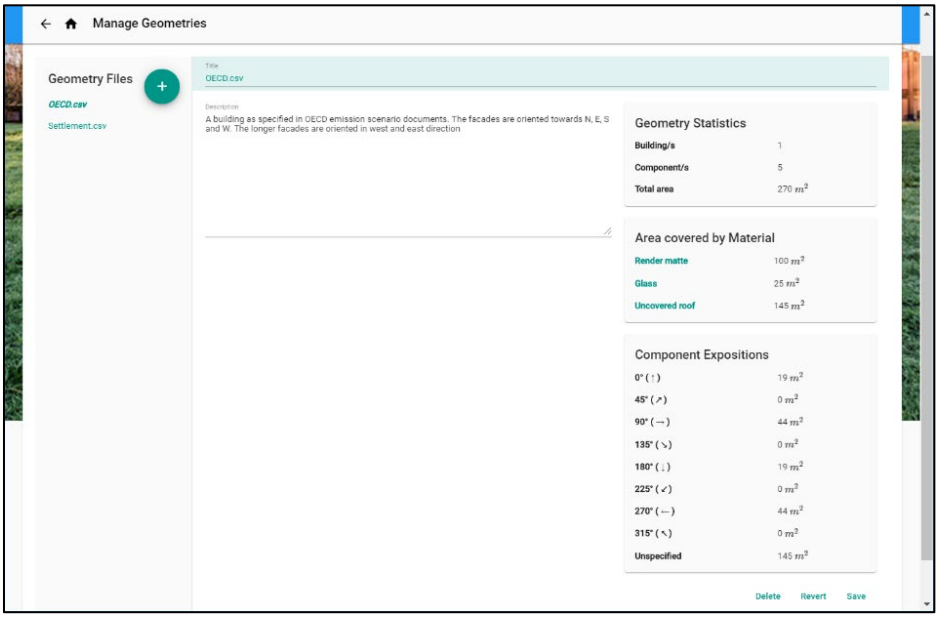


Figure 4: Detail view geometry data including the statistical summary in the right hand

3.3.1 Adding Geometry Data

The sequence for the upload of new geometric data is as follows:

1. Click “+” icon in the detail page or "Add" button in the geometry area on the dashboard.
2. Select a file and upload.

Should the geometry file be corrupt or incorrectly formatted, a note is given that the error can be located and corrected in the respective file.

3.3.2 Editing Geometry Data

Click on "Title" and "Description" to edit the data. Press the "Save" button to save changes. Press "Delete" button to delete a geometry. Clicking the "Revert" button will undo the last change.

Geometries used in previous calculations are stored in the database e.g. to check the validity or process the results later. These geometries are hidden from the actual workflow.

3.4 Manage Weather Data

Similar to geometric data, weather data are managed in the corresponding detail view (Figure 5). The information area provides statistical information of the weather file automatically. The period of the data set, the rainfall quantity (total, annual, monthly) and the main weather direction are displayed.

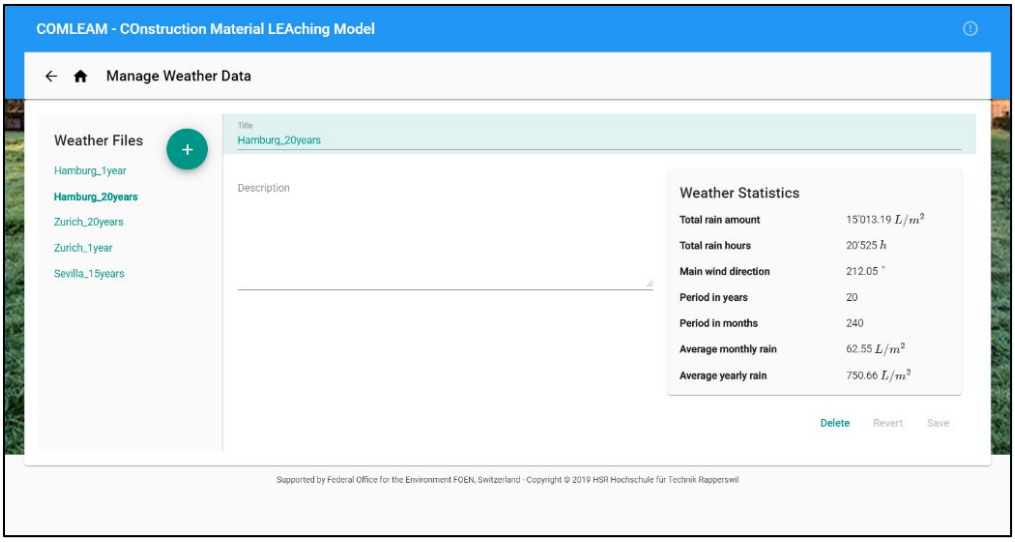


Figure 5: Detail view for managing weather data

3.4.1 Adding Weather Data

The sequence for the upload of new weather data is as follows:

1. Click “+” icon in the detail page or the "Add" button in the weather area on the dashboard.
2. Select a file and upload.

3.4.2 Editing Weather Data

Click "Title" and "Description" to edit the data directly. Press "Save" button to save the changes.

Press "Delete" button to delete a weather dataset. Clicking the "Revert" button will undo the last change.

Weather data used in previous calculations are stored in the database like geometry data to ensure access to the results later.

3.5 Manage Emissions

Emissions represent a relationship between the accumulated amount of runoff ($q_{c,cum}$) and the resulting cumulative emission of a substance (E_{cum}). Typically, such data are collected in field studies or laboratory tests with specific building products. For calculating the emission of a substance, COMLEAM needs these data in form of an emission function (see chapter 3.5.1).

The detail view for emission functions shows existing functions with their parameters and the assigned substance (Figure 6). The substance is linked to the substance database (see chapter 3.7).

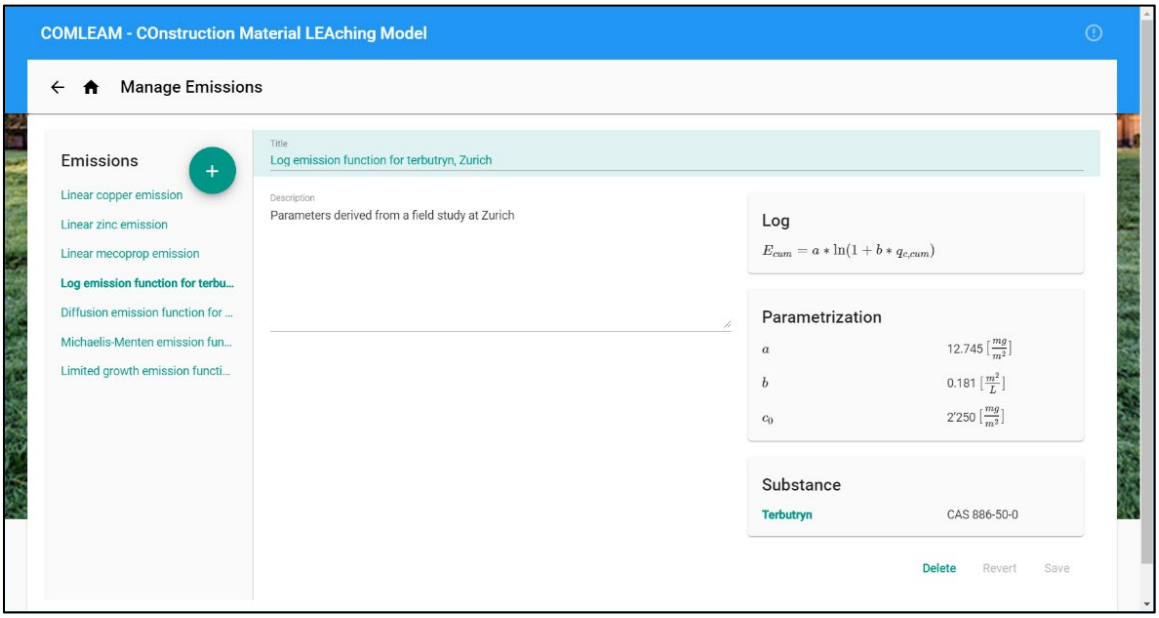


Figure 6: Detail view for managing emission functions

3.5.1 Adding Emission Data and Functions

A dialog box guides the process of adding new emission data. To add new emission data, click the “+” icon in the detail page or the "Add" button in the Emission area on the dashboard. The Dialog shows several possibilities to add new data (Figure 7).

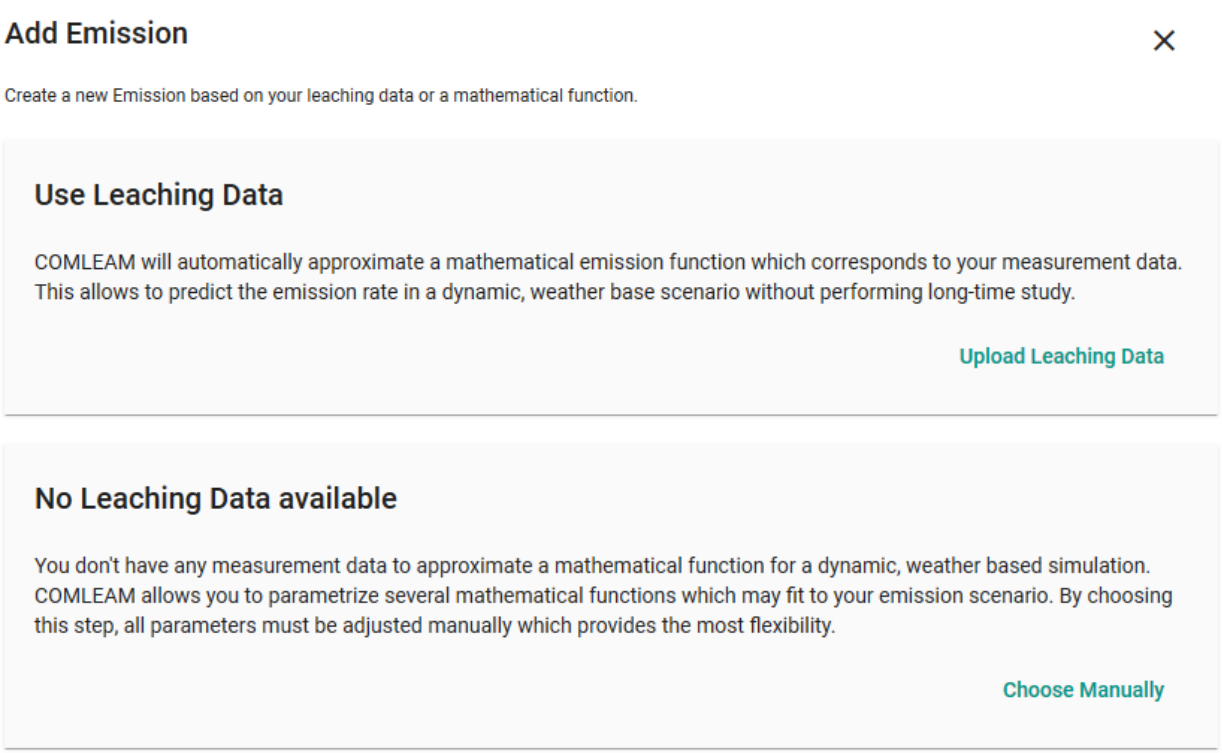


Figure 7: Dialog for adding new emission data

Use Leaching Data

Choose leaching data (file structure: see chapter 4.3, page 32) to generate an emission function. The approximation is done automatically by non-linear regression ("nls": non-linear least squares).

First, select the data file (Figure 8).

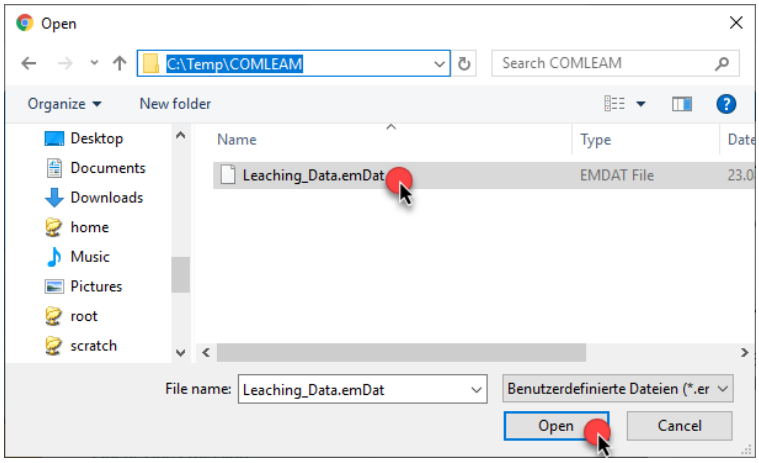


Figure 8: Dialog during emission data upload

Second, COMLEAM calculates the emission function. COMLEAM parametrize the logarithmic emission function as a default but other emission functions are provided additionally. By expanding the dropdown menu 'Override Emission Function' (Figure 10, lower end) the user can choose following functions: Limited Growth, Diffusion controlled or Michaelis-Menten (more details see chapter 5.6). A file name is required with optional description of data information (Figure 9).

In case your file is corrupt or the nls algorithm could not find an appropriate emission function, COMLEAM provides an error note.

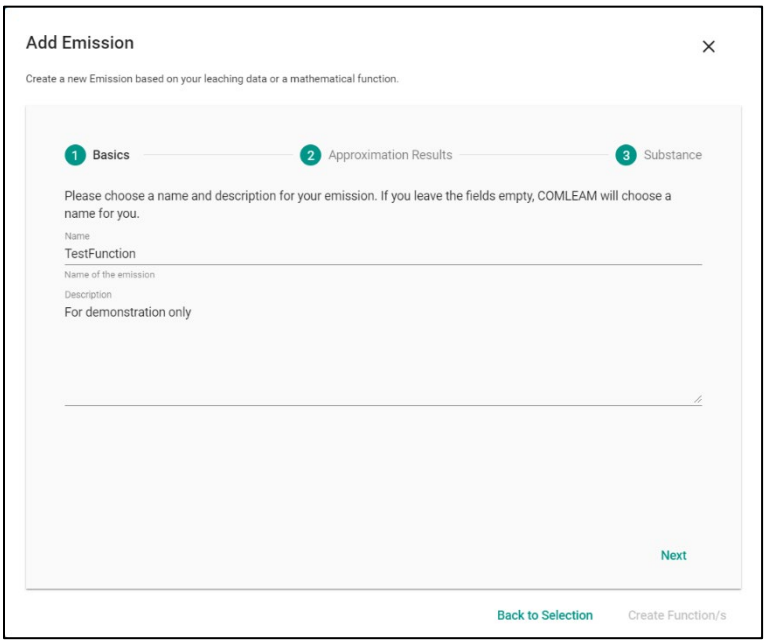


Figure 9: Input of Emission name after file upload in emissions dialog

Third, the user has to specify the initial content (c0) of the substance analyzed in this emission data to normalize the emission function. The parameters approximated by nls are displayed (see Figure 10). The parameters can be modified.

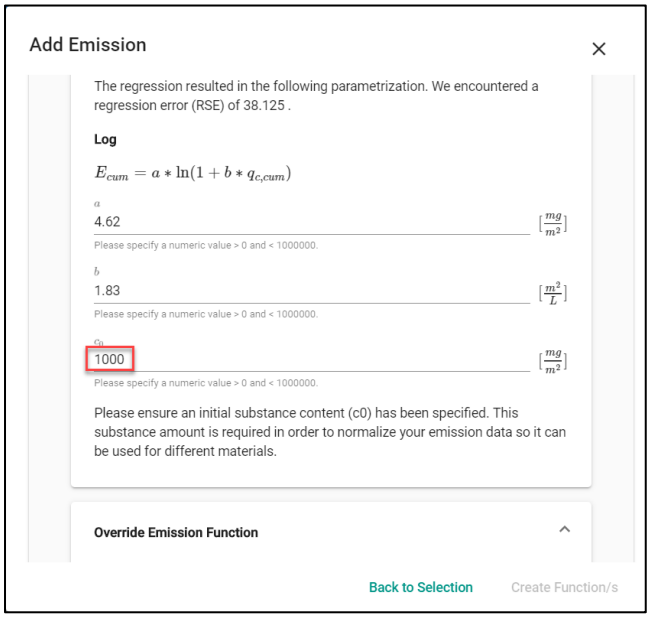


Figure 10: Input of initial concentration in emission dialog

Finally, a substance is selected for the emission function (Figure 11). This link is used for the assignment of building materials in the configuration of a calculation later.

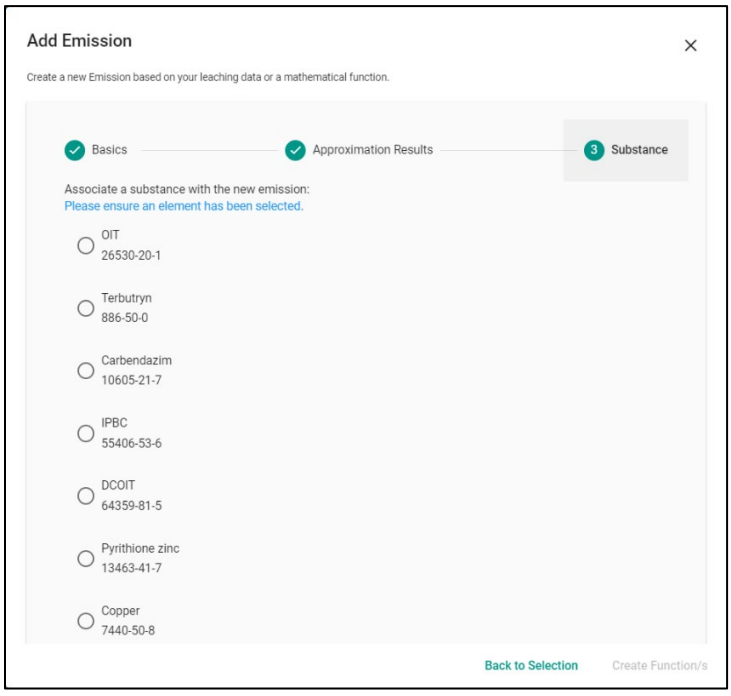


Figure 11: Selection of associated substance in emission dialog

Leaching Data are not available

Emission data with individual parameters is possible with 'Choose manually' (Figure 7). This option is recommended for users experienced in emission functions and their origin.

1. Set a name for the emission (Figure 8).
2. Choose the emission function as showed in Figure 12 (chapter 5.6, page 38).
3. Set the parameters individually (depending on the emission function) (Figure 13).
4. Define a substance to the emission function (Figure 11).

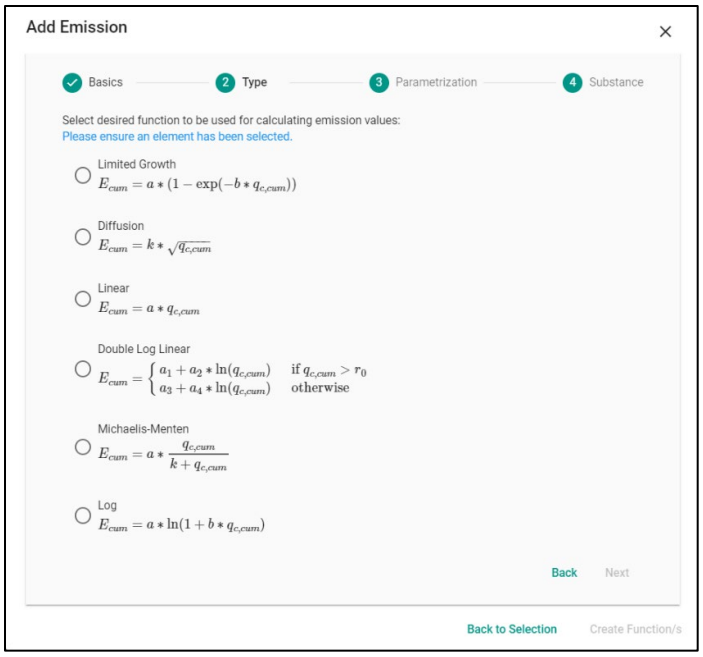


Figure 12: Manual selection of emission function in emission dialog

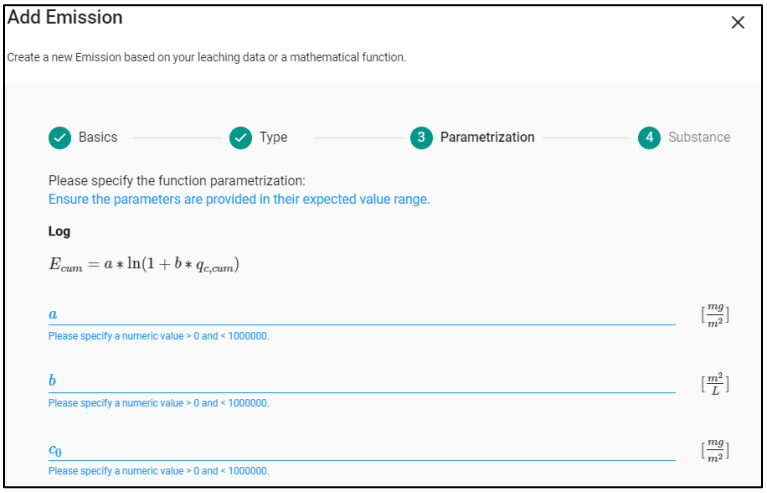


Figure 13: Definition of parameters in emission dialog

3.6 Manage Materials

Building materials (e.g. glass, render, wood) are linking geometries and emission functions (Figure 14) (see chapter 4.4, p. 33). The material subtype is connecting geometry and building material. This setup is flexible for geometries and emission functions in individual scenarios for specific building materials.

If a user is not familiar with the implementation of building materials, it is recommended to go to the chapter 4.4 before implementing "new building materials".

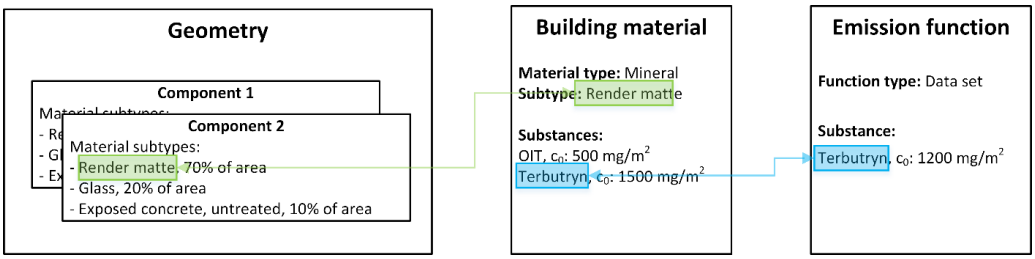


Figure 14: Relationship between the modules geometry, building material and emission function

3.6.1 Manage Material types

Material types are managed by 'Settings' in the Material UI on the home screen (Figure 15).

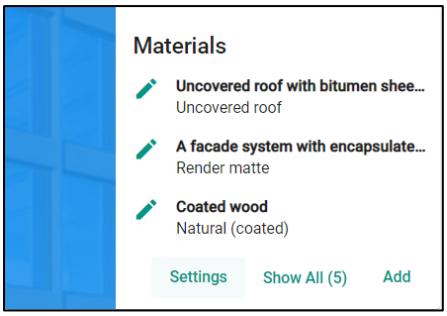


Figure 15: Manage material types and subtypes in homescreen

Figure 16 shows the UI for managing material types and subtypes. On the left-hand side, the existing material types are shown. The default material types are Mineral, Wood, Metal, Plastic, Glass and Special form.

A new Material type is added by the "+" Button on the left hand side. A name must be specified with optional description of the material type. default material types are not allowed to be deleted.

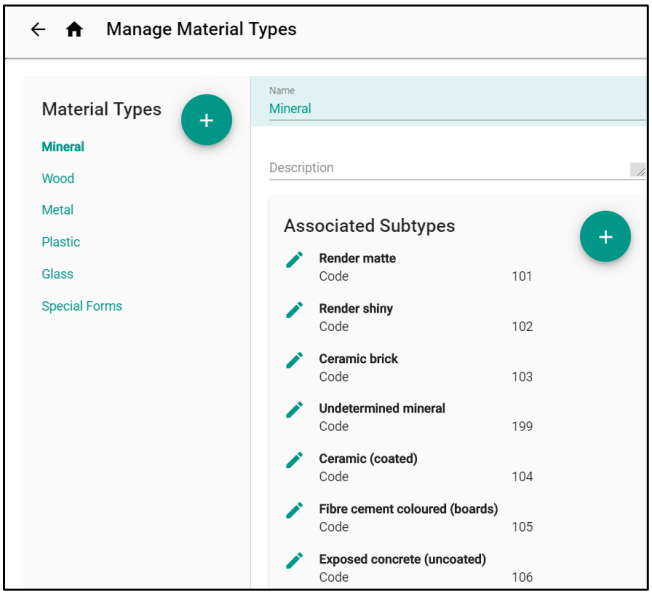


Figure 16: Manage material types and subtypes UI

3.6.2 Manage material subtypes and runoff coefficients

For material subtypes, the material types UI has to be opened (Figure 19) (see chapter 3.6.1). When a material type on the left-hand side is selected, the associated subtypes are shown on the right hand (Figure 19, right). For each subtype, the specific material code is noted (chapter 4.1.1 for more details).

Create new Subtypes
After clicking "+" on the right hand side, the new material subtype has to be defined with a name and a runoff coefficient and optional description. For example, a new type of render with different runoff coefficient can be defined different to the predefined render (Figure 17).

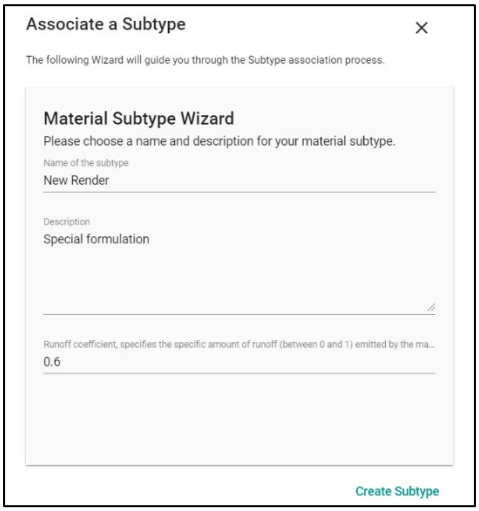


Figure 17: Example of adding a new material subtype

Runoff coefficients of existing subtypes

Clicking on a subtype, the parameters can be varied (Figure 18). The user sets the new runoff coefficient and optional a new name for the material subtype confirmed by 'update subtype'.

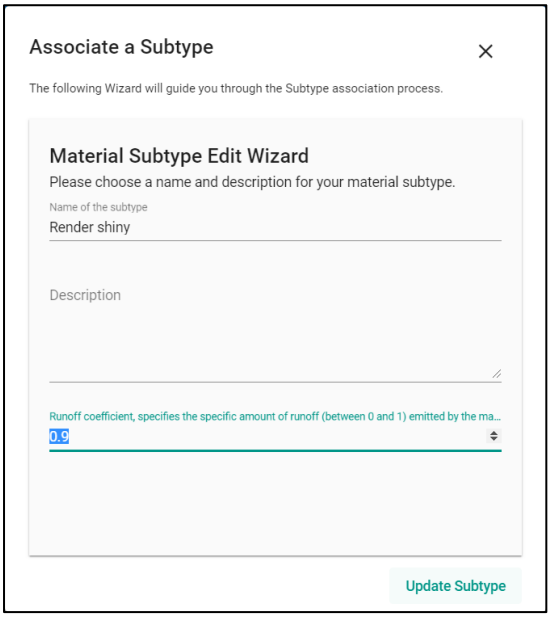


Figure 18: Change of runoff coefficient of existing material subtype

3.6.3 Manage building materials

Building materials are managed in the detail view of the Material UI (Figure 19). Material types and subtypes are displayed with a runoff coefficient and a substance. Both the Material type and material subtype are directly linked to the UI for material types and subtypes (Figure 16).

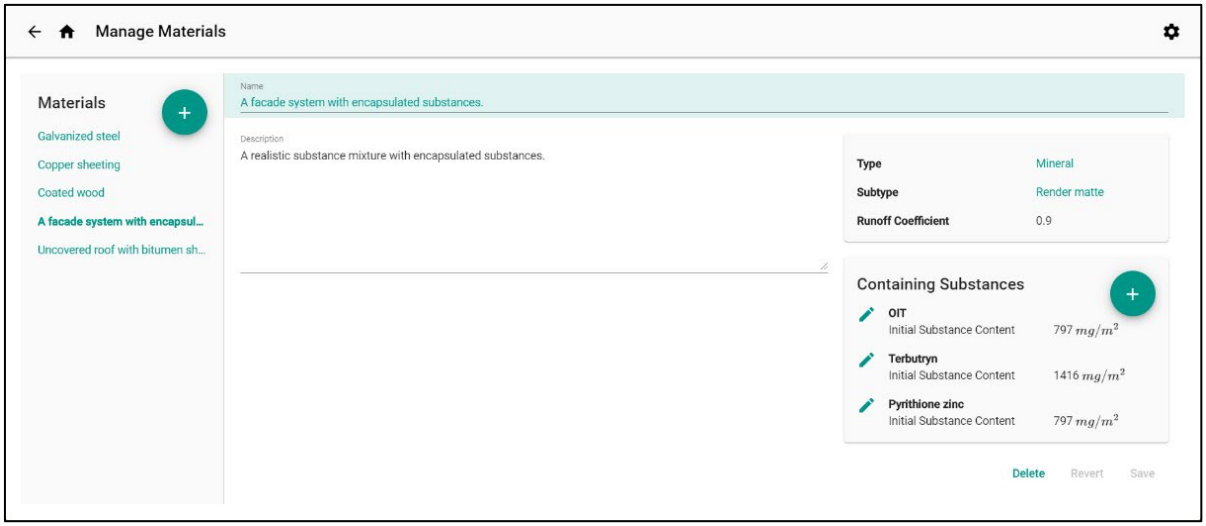


Figure 19: Detail view for managing building materials

Create a new building material

Click “+” icon in the material list on the left hand of the detail view. A name must be specified and optional a description can be added. Confirm the material by clicking 'Create Material'.

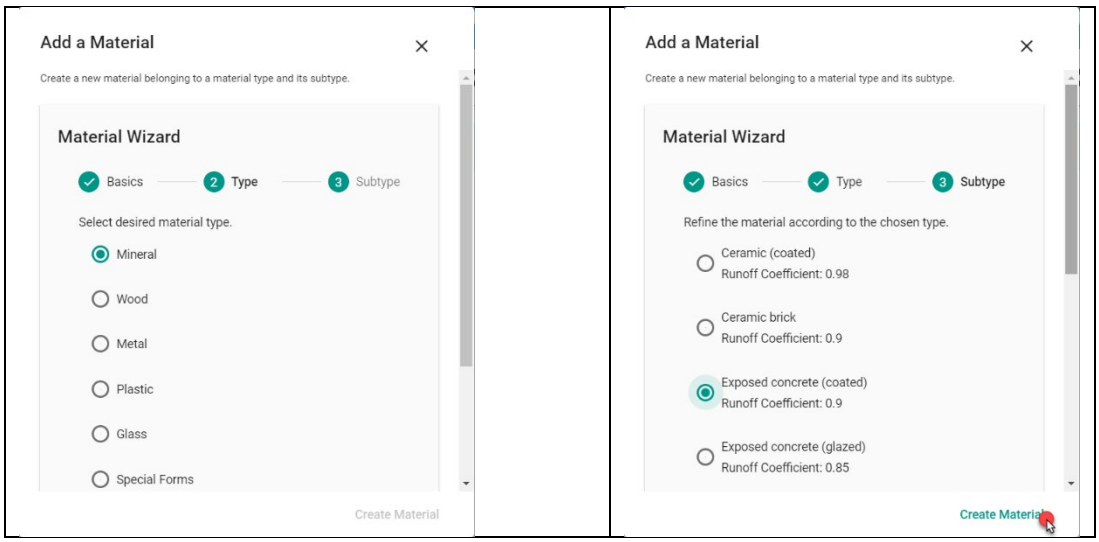


Figure 20: Add a building material in Material dialog

Add substances to the building material

One or more substances are assigned to the newly created material (Figure 21). Click on “+” icon in the detail view of the building material in the right panel.

Figure 21: Add a substance to an existing building material in Material dialog

Select a substance from the predefined list and give the initial amount [mg/m^2] (Figure 22). For other substances, the procedure is the same. Every substance can be edited and deleted.

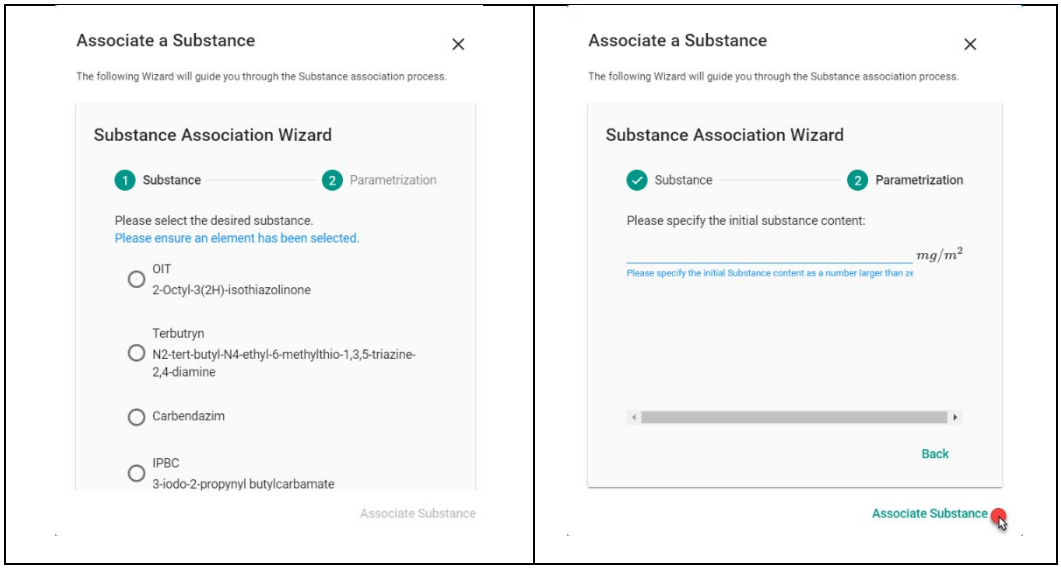


Figure 22: Substance linked to building material in Material dialog

3.7 Manage Substances

Substances are managed in the detail view of the Substance UI (Figure 23).

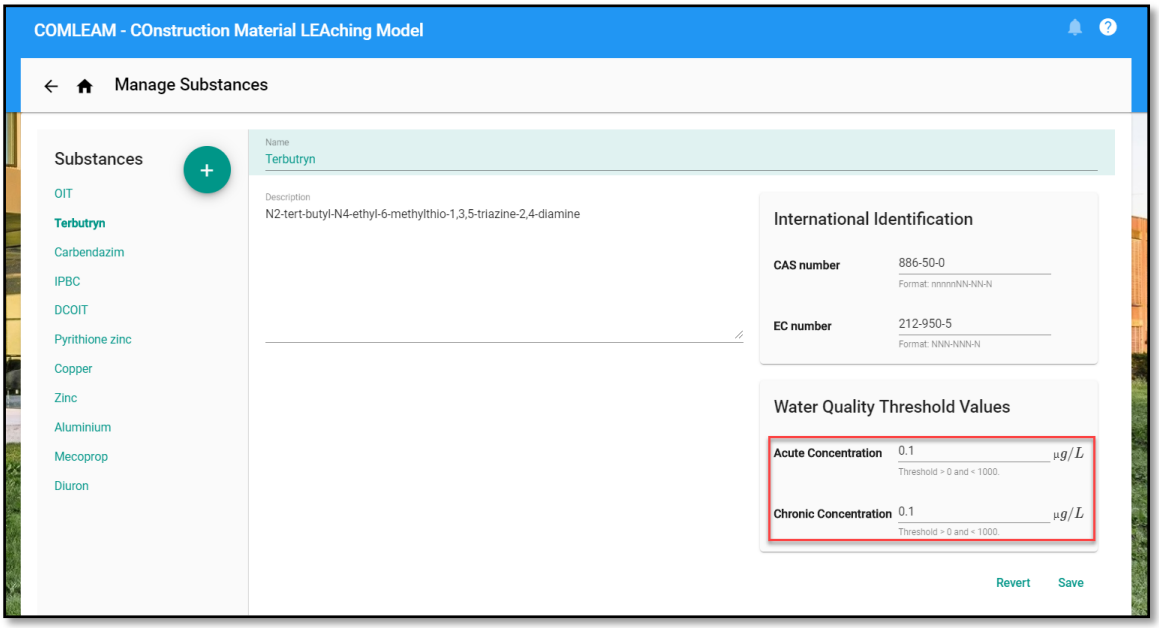


Figure 23: Substance UI to manage parameters

Change Threshold values

Clicking on a substance allows the user to alter the thresholds for acute and chronic quality standards (Figure 23, red boundary). The default value is set to 0.1 µg/L according to Swiss Water Protection Regulation (GSchV) for organic pesticides and biocidal substances.

Create new substance

Click “+” icon in the substance list on the left hand of the detail view (Figure 23). A substance is defined by a name and both acute and chronic quality values. The EC-Number and CAS-Number with a description can be added (Figure 24).

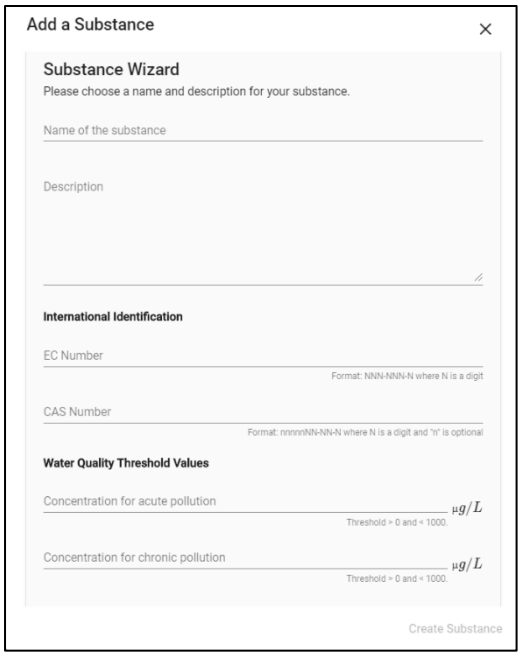


Figure 24: Add new substance in substance dialog

3.8 Simulation of Substance Emission

The simulation of a substance's emission starts with the setup of a calculation. Calculations are configured by either clicking on “+” on the dashboard icon in the *Calculations* area or in the detail view. Specific dialog boxes assist the configuration. A completed calculation can be used in a new simulation using the “copy” function for individual parameters.

Step 1: Name and description

The name of calculation and description is set. If a name is lacking, it is automatically generated.

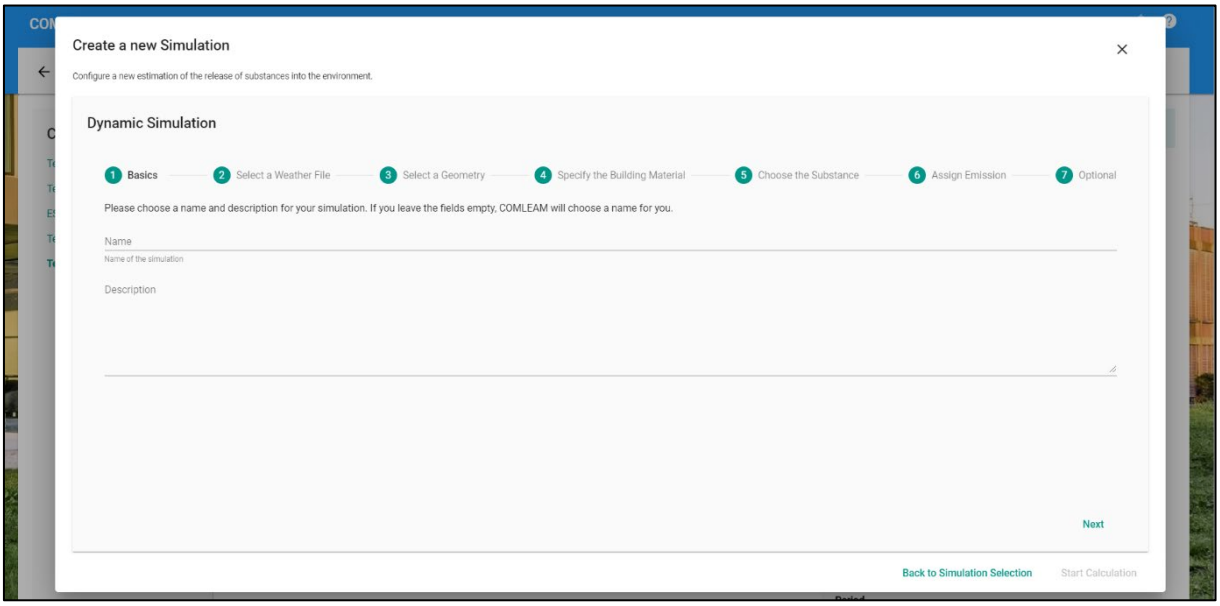


Figure 25: Dynamic calculation dialog box. In step 1 the name is defined

Step 2: Weather

The weather dataset is selected and the date range defined (Figure 26). The start and end date must be within the range available in the file.

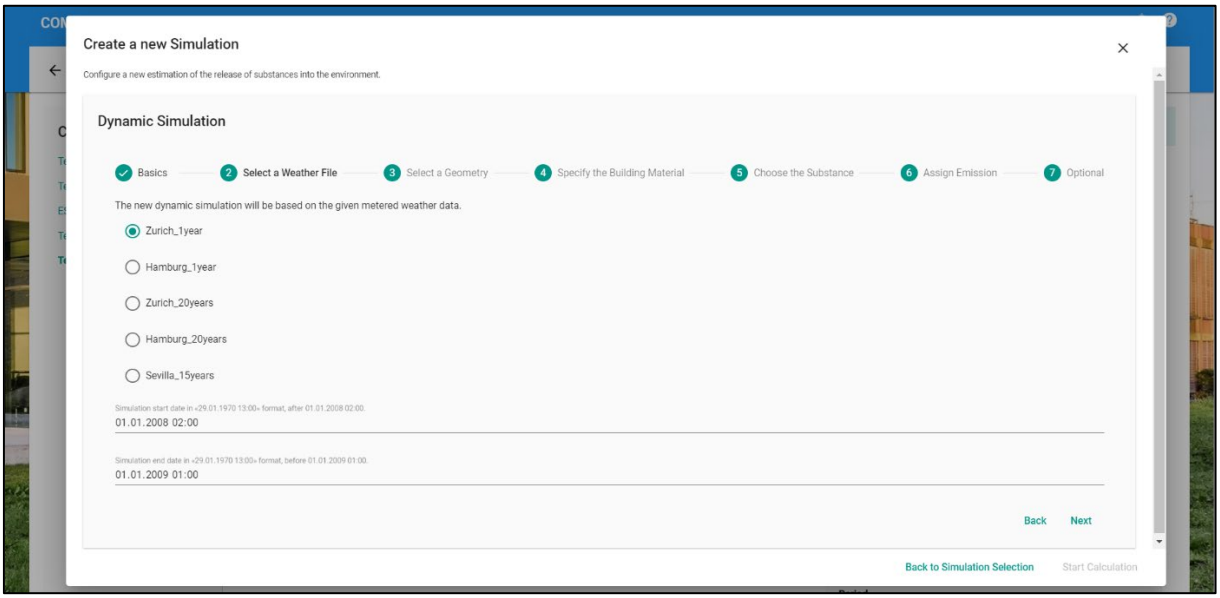


Figure 26: Dynamic calculation dialog box. In step 2 is a weather dataset selected

Step 3: Geometry

The definition of geometry affects the configuration (Figure 27). Building materials and emission functions are present for calculations with corresponding material subtype and geometry.

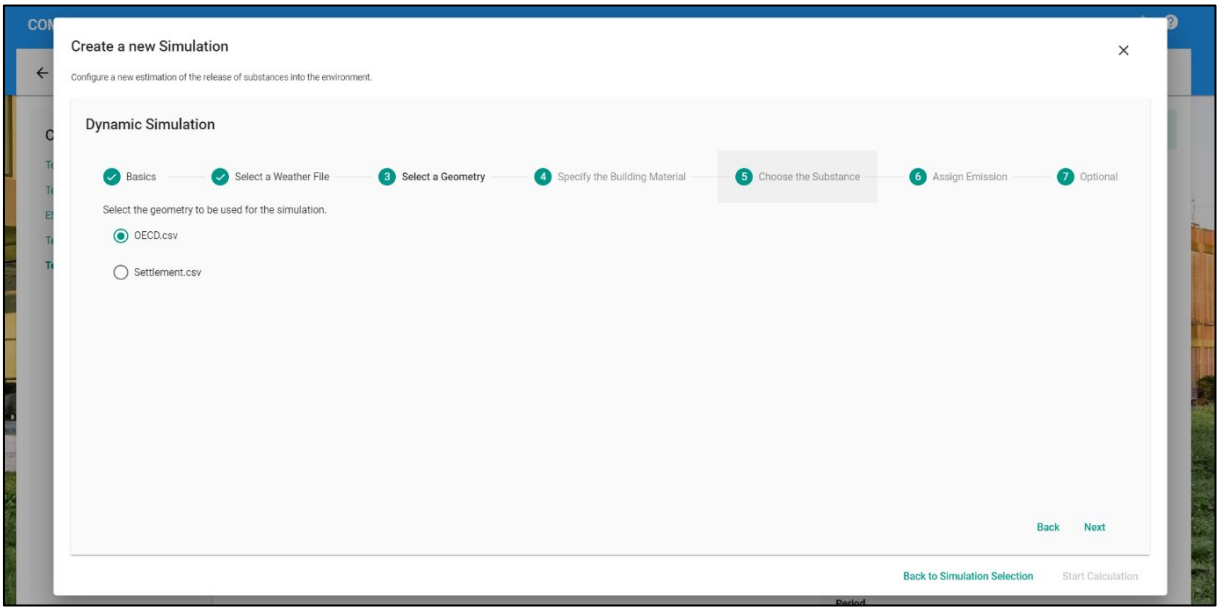


Figure 27: Dynamic calculation dialog box. In step 3 the geometry is selected

Step 4: Building material and runoff coefficient

Building materials with substances of interest belonging to a subtype are selected (Figure 28).

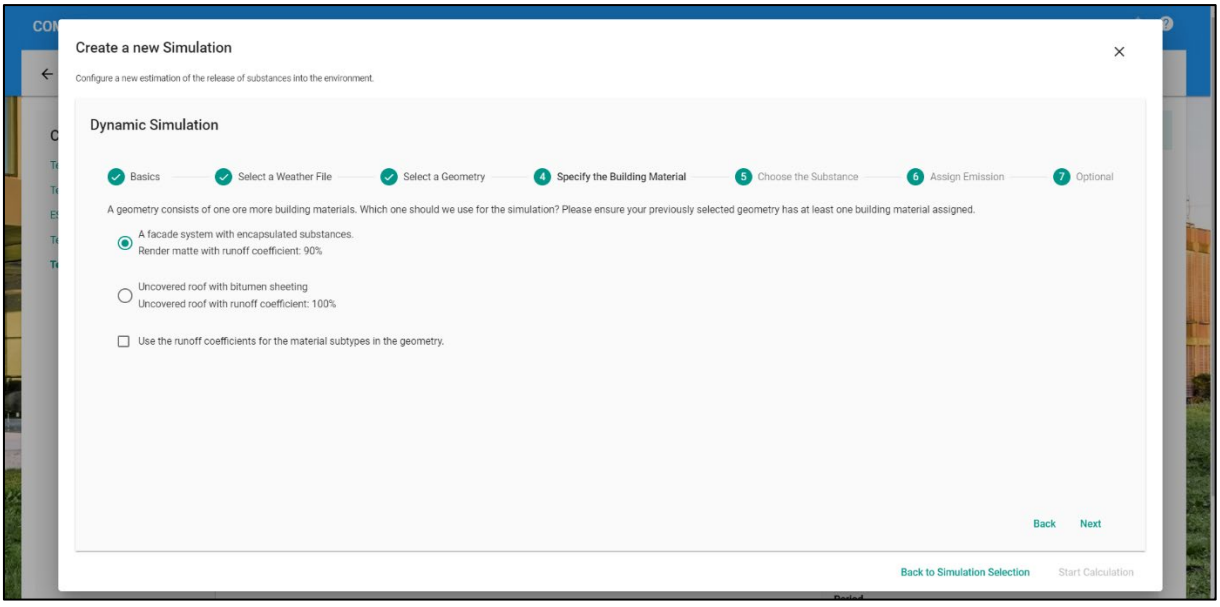
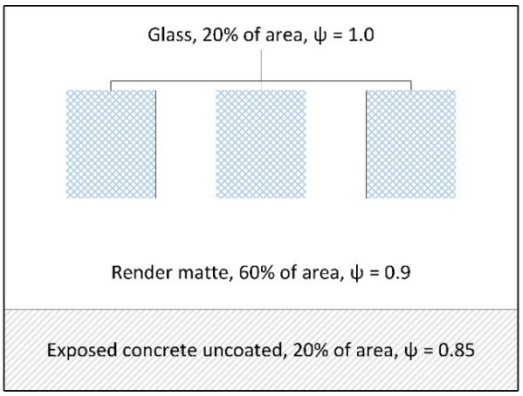


Figure 28: Dynamic calculation dialog box. In step 4, building materials are selected.

A runoff coefficient ψ of the material subtype can be considered. If the coefficient is enabled, also a combined runoff coefficient $\psi_{combined}$ for different material subtypes (Figure 29). The emission is calculated subsequently with the amount of runoff water reduced by $\psi_{combined}$.

Without definition, the total runoff calculated by WDR for vertical components or the entire precipitation for horizontal components is used for emission calculation.



$\psi_{combined} = 0.2 * 1.0 + 0.6 * 0.9 + 0.2 * 0.85 = \mathbf{0.91}$

Figure 29: Calculation of the combined runoff coefficient for a component with different material subtypes

Steps 5 and 6: Substance and emission function

All substances of the building materials can be calculated step-by-step (Figure 30). Subsequently, one of the available emission functions can be selected (Figure 31).

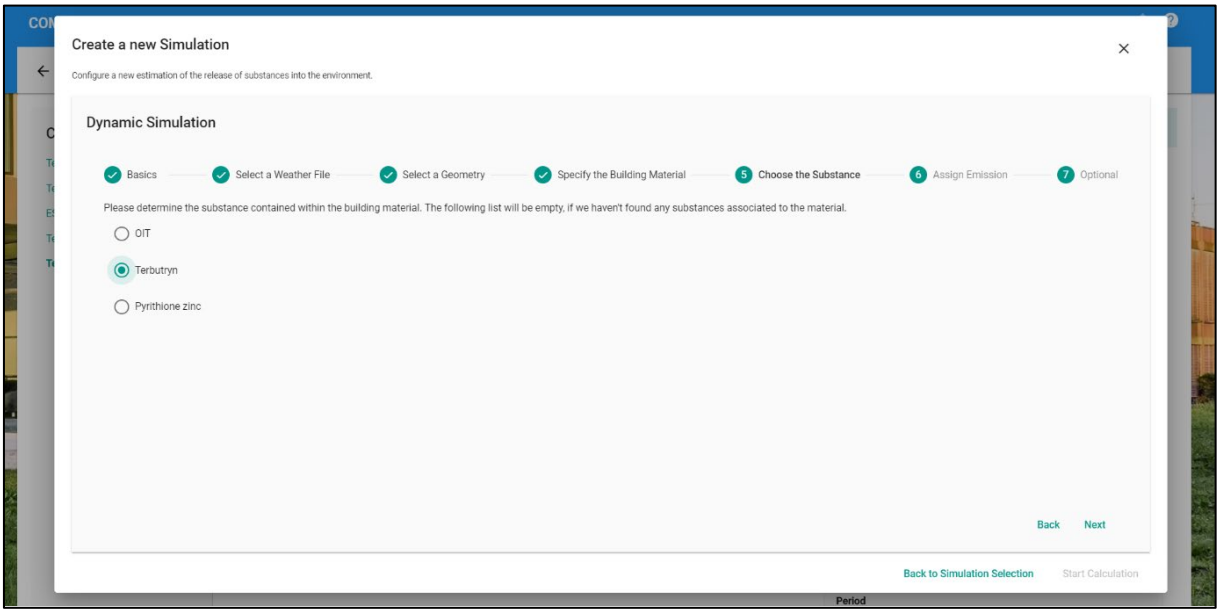


Figure 30: Dynamic calculation dialog. Step 5: selecting a substance

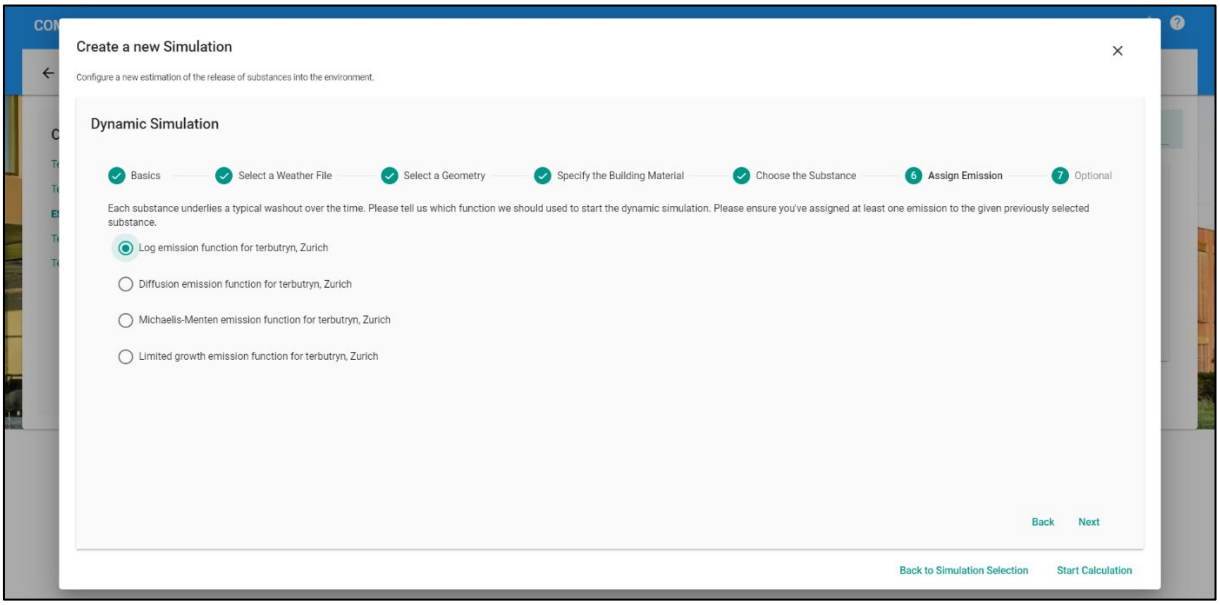


Figure 31: Dynamic calculation dialog. Step 6, selecting an emission function

Step 7: Optional settings

Optional settings are related to the size of the receiving water as well as to parameters for the calculation of WDR (Figure 32). By default, COMLEAM calculates for a small receiving water with 0.01 m^3 / s flow (10 L/s).

The WDR algorithm is preconfigured for urban areas (>15% of the catchment consists of buildings with at least 15 m height) in flat terrain with a distance in the wind direction to surrounding buildings of 15 to 25 m.

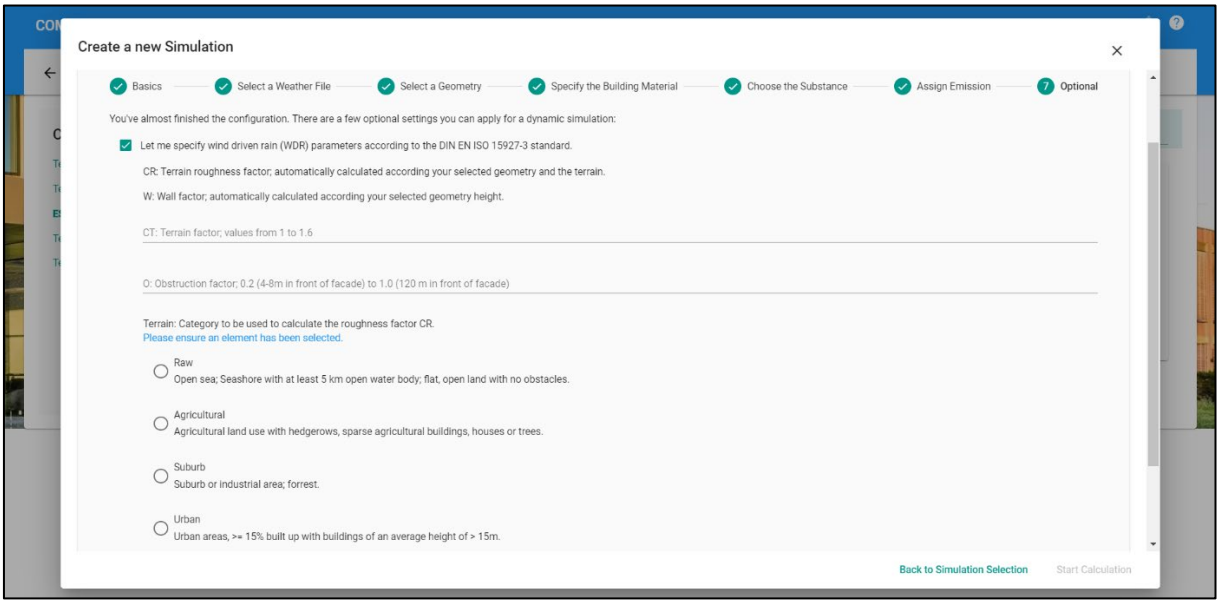


Figure 32: Dynamic calculation dialog. Step 7 for optional settings like WDR parameters

The terrain roughness Cr and wall factor w (Table 2) depend on the building height. The parameters are defined by the ISO 15927-3 except the components height z and can be varied individually for each component of the geometry. The terrain factor Kr must be chosen (Figure 32) and is the same for every component. Therefore, it is not possible for example to simulate a geometry, which is both in agricultural and urban site.

Table 2: Component heights and the corresponding wall factors

Components height	Wall factor
h > 10 m	W = 0.2
5 m < h < 10 m	W = 0.3
2m < h < 5 m	W = 0.4
h < 2 m	W = 0.55

The terrain roughness factor Cr is calculated as follows:

$$C_r(z) = K_r \times \ln\left(\frac{z}{z_0}\right) \mid z \geq z_{min} \quad \text{or} \quad C_r(z) = K_r \times \ln\left(\frac{z_{min}}{z_0}\right) \mid z < z_{min}$$

with:

z	Component height (m)
z_0	Roughness length (m)
z_{min}	Minimum height (m)
K_r	Terrain factor (-)

The receiving surface water compartment is divided in three classes: small (S), medium (M), and large (L) (Figure 33).

Figure 33: Dynamic calculation dialog. Step 7 for optional settings like surface water compartment

Runoff that is matched or surpassed on 347 days per year, averaged over 10 years, is called "Q347" (Table 3).

Table 3: Receiving surface water differentiated in three classes

Class	Q_{347_min} [m^3/s]	Q_{347_max} [m^3/s]
Small (S)	0.01	0.1
Medium (M)	0.1	1
Large (L)	1	n.A

Step 10: Finish calculation
After set all parametes, the button 'Start Calculation' becomes green and the calculation can be started. The user automatically gets back to the Calculation UI. While COMLEAM is simulating, the status (Figure 34) is reflected until reporting 'Finished successfully'. The results occur.

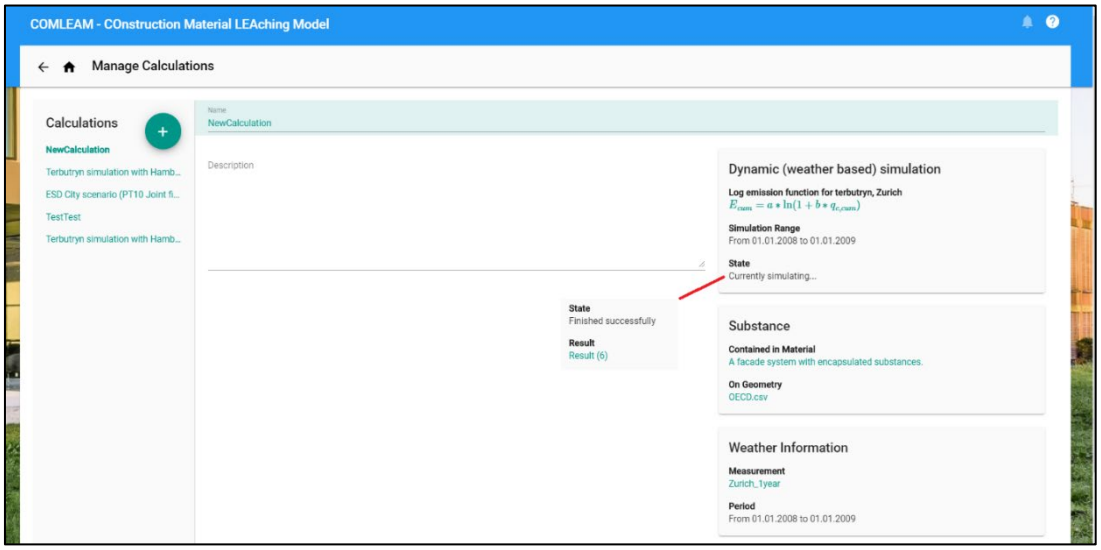


Figure 34: Dynamic calculation dialog. Step 10 is starting the calculation

3.9 Reporting of the Results and Data Export

A report in standardized ".pdf" format is automatically generated for any calculations providing an overview of setting parameters and the results (Figure 35). The process takes a few seconds to minutes depending on the complexity of the calculation. Reports can be deleted.

For individual data analyzes and processing (e.g. preparing own figures), the raw data as well as all relevant parameters are available as ".csv" files compressed in a ".zip" archive for download. Together with the raw data, a document (codebook) is delivered, which documents the structure of the individual files and provides a comprehensive list of parameters and their corresponding units.

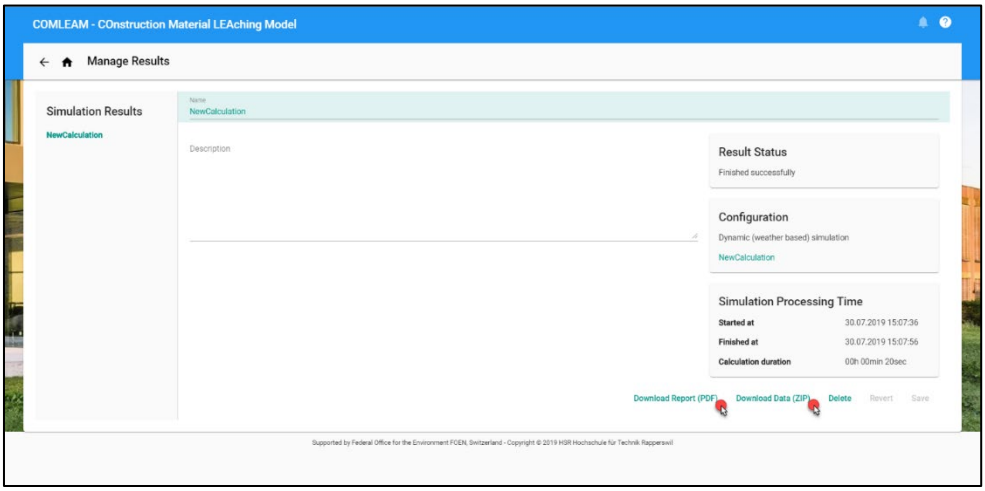


Figure 35: Detail view of reports for finished calculations.

4 Input data

To configure a calculation, information of geometry, weather, emission data, functions, and building materials are required (Figure 36). Geometries, emission data and weather data can be imported as "*.csv*" files. Building materials are created directly by the user in the application. The building materials link the geometry and emission or functions to be used and specify the substances contained with the respective initial substance amount.

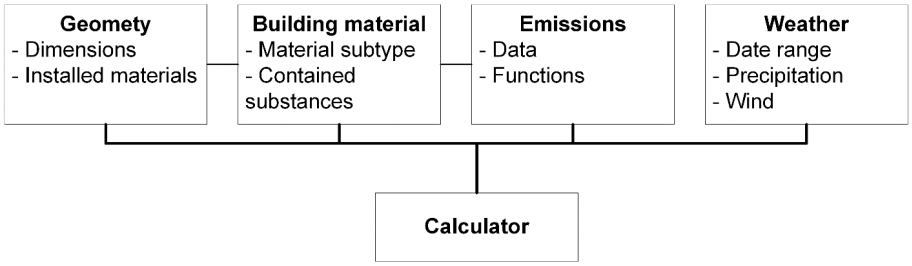


Figure 36: Module structure of COMLEAM

4.1 Module Geometry

A geometry describes the size, orientation, and material properties of one or more building components. Several components represents a building using a *buildingID*.

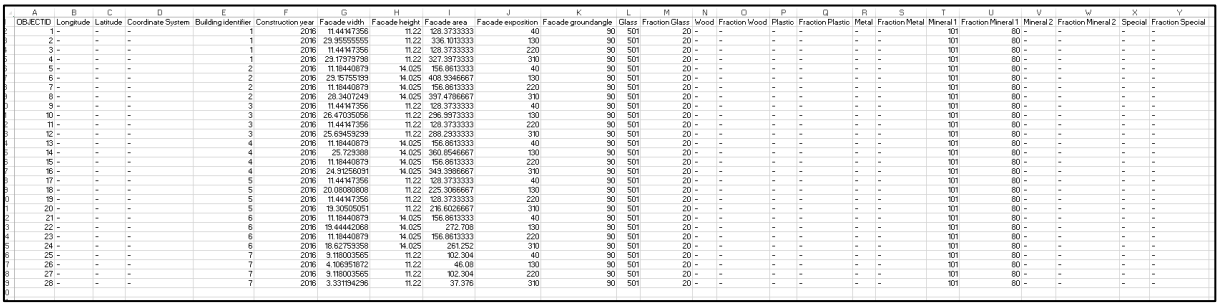
4.1.1 Input format

Geometries are imported by "*.csv"* files (Figure 37). The first row contains the column headings. Each subsequent line describes a single component. As a separator for the columns, a semicolon (;) is expected.

In total, 26 columns are defined. The first 11 columns describe the geometry and following 14 columns the materials. The last column is reserved for comments that are ignored during import.

Two columns each define one material, one of the columns specifying the material type by means of a 3- or a 4-digit code, the other the area proportion of the component that the material occupies. The list of all materials implemented in the COMLEAM database by default is given in the appendix in Table 13, page 46. If a user created new materials (as described in 3.6.2), the new created 4 digit code for the new materials must be picked out from the subtypes UI as shown in Figure 16.

If a material is not present on the component, the corresponding field pair is marked with a "-". The order of the columns is fixed. The required structure is described in detail in Table 12 in the appendix, page 45.



	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T	U	V	W	X	Y
1	OBJECTID	Longitude	Latitude	Coordinate System	Buildingidentifier	Construction year	Facade width	Facade height	Facade area	Facade exposition	Facade groundangle	Glass	Fraction Glass	Wood	Fraction Wood	Plastic	Fraction Plastic	Metal	Fraction Metal	Mineral 1	Fraction Mineral 1	Mineral 2	Fraction Mineral 2	Special	Fraction Special
2	1	-	-	-	1	2016	11.44147356	11.22	128.3733333	40	90	501	20	-	-	-	-	-	-	101	80	-	-	-	-
3	2	-	-	-	1	2016	29.95555555	11.22	336.1013333	130	90	501	20	-	-	-	-	-	-	101	80	-	-	-	-
4	3	-	-	-	1	2016	11.44147356	11.22	128.3733333	220	90	501	20	-	-	-	-	-	-	101	80	-	-	-	-
5	4	-	-	-	1	2016	29.17979798	11.22	327.3973333	310	90	501	20	-	-	-	-	-	-	101	80	-	-	-	-
6	5	-	-	-	2	2016	11.18440879	14.025	156.8613333	40	90	501	20	-	-	-	-	-	-	101	80	-	-	-	-
7	6	-	-	-	2	2016	29.15755199	14.025	408.9346667	130	90	501	20	-	-	-	-	-	-	101	80	-	-	-	-
8	7	-	-	-	2	2016	11.18440879	14.025	156.8613333	220	90	501	20	-	-	-	-	-	-	101	80	-	-	-	-
9	8	-	-	-	2	2016	28.3407249	14.025	397.4786667	310	90	501	20	-	-	-	-	-	-	101	80	-	-	-	-
10	9	-	-	-	3	2016	11.44147356	11.22	128.3733333	40	90	501	20	-	-	-	-	-	-	101	80	-	-	-	-
11	10	-	-	-	3	2016	26.47035056	11.22	296.9573333	130	90	501	20	-	-	-	-	-	-	101	80	-	-	-	-
12	11	-	-	-	3	2016	11.44147356	11.22	128.3733333	220	90	501	20	-	-	-	-	-	-	101	80	-	-	-	-
13	12	-	-	-	3	2016	25.69453239	11.22	288.2833333	310	90	501	20	-	-	-	-	-	-	101	80	-	-	-	-
14	13	-	-	-	4	2016	11.18440879	14.025	156.8613333	40	90	501	20	-	-	-	-	-	-	101	80	-	-	-	-
15	14	-	-	-	4	2016	25.723388	14.025	360.8546667	130	90	501	20	-	-	-	-	-	-	101	80	-	-	-	-
16	15	-	-	-	4	2016	11.18440879	14.025	156.8613333	220	90	501	20	-	-	-	-	-	-	101	80	-	-	-	-
17	16	-	-	-	4	2016	24.91256091	14.025	349.3586667	310	90	501	20	-	-	-	-	-	-	101	80	-	-	-	-
18	17	-	-	-	5	2016	11.44147356	11.22	128.3733333	40	90	501	20	-	-	-	-	-	-	101	80	-	-	-	-
19	18	-	-	-	5	2016	20.08888808	11.22	225.3066667	130	90	501	20	-	-	-	-	-	-	101	80	-	-	-	-
20	19	-	-	-	5	2016	11.44147356	11.22	128.3733333	220	90	501	20	-	-	-	-	-	-	101	80	-	-	-	-
21	20	-	-	-	5	2016	19.30505051	11.22	216.6026667	310	90	501	20	-	-	-	-	-	-	101	80	-	-	-	-
22	21	-	-	-	6	2016	11.18440879	14.025	156.8613333	40	90	501	20	-	-	-	-	-	-	101	80	-	-	-	-
23	22	-	-	-	6	2016	15.44442068	14.025	272.708	130	90	501	20	-	-	-	-	-	-	101	80	-	-	-	-
24	23	-	-	-	6	2016	11.18440879	14.025	156.8613333	220	90	501	20	-	-	-	-	-	-	101	80	-	-	-	-
25	24	-	-	-	6	2016	18.62753958	14.025	261.252	310	90	501	20	-	-	-	-	-	-	101	80	-	-	-	-
26	25	-	-	-	7	2016	5.11803565	11.22	102.304	40	90	501	20	-	-	-	-	-	-	101	80	-	-	-	-
27	26	-	-	-	7	2016	4.106951872	11.22	46.08	130	90	501	20	-	-	-	-	-	-	101	80	-	-	-	-
28	27	-	-	-	7	2016	5.118003565	11.22	102.304	220	90	501	20	-	-	-	-	-	-	101	80	-	-	-	-
29	28	-	-	-	7	2016	3.33194296	11.22	37.376	310	90	501	20	-	-	-	-	-	-	101	80	-	-	-	-
30																									

Figure 37: Exemplary excerpt of a geometry file

4.2 Module Weather data

Weather data are required in hourly resolution. This time resolution is necessary for the calculation of the WDR. The data records contain a station identifier, a time stamp, the hourly mean wind direction and wind strength as well as the hourly rainfall.

4.2.1 Input format

Weather data can be imported by ".csv" files (Table 4). The first row are the headings. Weather data are processed using defined algorithms to calculate missing values. Flow diagrams of the algorithms can be found in the appendix.

Table 4: Weather file structure. Column numbers, their names and the corresponding unit or format are shown

Column	Identifier	Unit / Format
1	Station name	-
2	Time stamp	YYYYMMDDhh
3	Hourly precipitation, sum	[mm] / [L/m^2]
4	Mean hourly wind speed	[m/s]
5	Mean hourly wind direction	[°]

4.3 Module Emission data

Emission data can be implemented in multiple ways.

4.3.1 Measured data

Measured data describing the substance emission [mg/m^2] as a function of the accumulated amount of water [L/m^2] can be used to directly parametrize emission functions. Data are expected in ".csv" format. The first line is ignored and reserved for column headings or comments (Table 5). For parametrization, the logarithmic function is recommended and

therefore is set as default when parametrize emission function via COMLEAM user interface. Also other emission functions as Michaelis-Menten, diffusion, and limited growth can be parametrized. The functions' description is described in chapter 5.6.

Table 5: Structure of a file containing measured emission data.

Column	Identifier	Unit
1	Cumulative runoff	[L/m^2]
2	Cumulative emission	[mg/m^2]

4.3.2 Direct parametrization

All implemented emission functions (logarithmic, Michaelis-Menten, diffusion, limited growth, linear) can be directly parametrized. To use these functions, the required parameters need to be derived by regression from the measured data (field / laboratory). The user must carry out this step in advance. A detailed description of the various functions and their expected parameters are described in chapter 5.6, page 38.

4.4 Building materials

A material describes a specific construction product. Therein, one or more substances are defined with their initial contents. In addition, a specific material type is defined for each material (e.g. mineral, wood, and plastic).

The initial substance content c_0 is expected for every emission function as stated in chapter 3.5.1. This opens the possibility to create several building materials with specific values for the initial substance content c_0 of a substance. COMLEAM is using c_0 in the emission function and the building material to scale the calculated emissions accordingly.

4.4.1 Material types and subtypes

The following five material types are predefined, each containing several material subtypes (e.g. concrete):

- Mineral, Glass, Wood, Metal, and Special (Various)

Runoff coefficients have been predefined for each material subtype and can be altered by the user if wanted. The runoff coefficient (proportion of runoff water) considers water losses as its whole due to water uptake by the material, by evaporation and splashing. More information to the coefficients see Table 13 in the appendix, page 46.

5 Mathematical Model

The mathematical part of COMLEAM consists of a system of coupled ordinary differential equations. For an interface compartment at the lower end of a façade, the water and material quantity is dynamically balanced. This section is intended to make the mathematical model concept reasonable by explaining the assumptions and boundary conditions.

5.1 Mathematical Concept

The mathematical model of COMLEAM is based on a (vertical) component exposed to rain or WDR (chapter 5.4). The water on the material surface dissolves a substance out of the material. The runoff water and the mass of the released substance are taken into account as inflows into an interface compartment (IC). The runoff from the IC is discharged to surface waters (e.g. into receiving water).

The following parts of the mathematical model are needed for the calculation core of COMLEAM:

- Geometry of the component (width, height, exposition, angle to ground)
- Weather data (precipitation, wind heading, wind speed)
- Calculation of wind driven rain (exposition, building height, location to other buildings, location in the environment)
- Emission (diffusion, dispersion, adsorption, dissolution)
- Pathways to the interface compartments
- Runoff to surface water (dilution)

Additionally, the calculated data can be used for soil transport models (e.g. PELMO, PEARL) or in sewer network models (hydraulic, hydrological models like SWMM, MikeUrban).

5.2 Building Components

The component has a defined geometry by its width, height and surface area of the material. Only the fraction with the given material is considered for the emissions from a component. For example: If windows accounts for 40 % of a façade and 60 % are covered by the material, only 60 % of the component's area are considered for substance emissions (Figure 29). However, the runoff water is calculated for the entire facade area. This means, regarding the example above, that 40% of the façade's runoff is free of substance and leads to dilution.

Depending on the inclined position of the component, it is covered by rain (horizontal component) or wind driven rain (vertical component). Other forms of precipitation (e.g., snow) are neglected.

5.3 Weather Data

The weather affect the runoff directly on horizontal and vertical components. Weather data are essential for the mass flow, i.e. precipitation, wind direction and wind speed in hourly resolution. Weather data with daily resolution cannot be used for statistical reasons. The precipitation values are not normally distributed, the wind speed is distributed log-normal, and the distribution of the wind direction depends on whether it is raining or not (Figure 38, Figure 39, Figure 40, Figure 41).

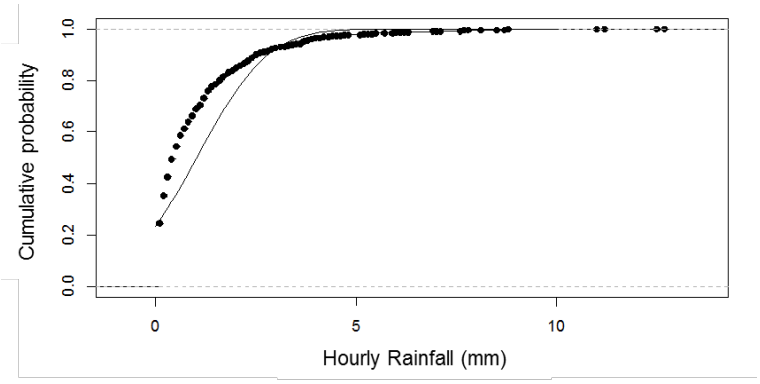


Figure 38: Probability function (cumulative) of the precipitation amount (dots) and the normal distribution (solid line)

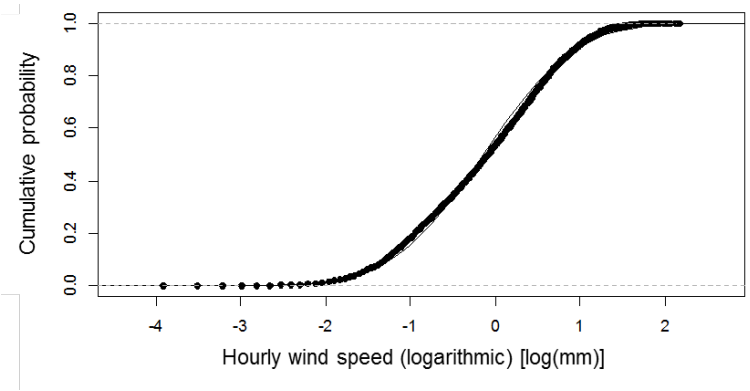


Figure 39: Probability function (cumulaitve) for the hourly wind speed (logarithmic, dots) and the lognormal distribution (solid line). Only hours with wind speed > 0 are considered

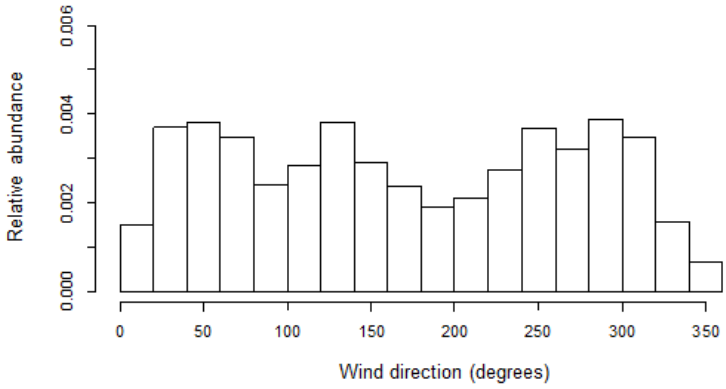


Figure 40: Frequency distribution for all wind directions shows an equal distribution

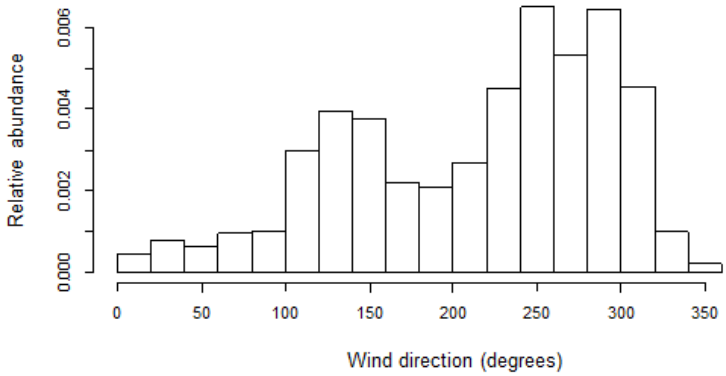


Figure 41: Frequency distribution for wind directions when rain occurs shows a cluster in the west direction

5.4 Wind Driven Rain Calculation

Wind driven rain (WDR) is the proportion of the rain that enters vertical surface. WDR is calculated from precipitation, wind speed and wind direction per the standard ISO-15927. The exposure of the component (angle of the component to the north), height of the building, position to other buildings and the location in the environment are considered (Figure 42).

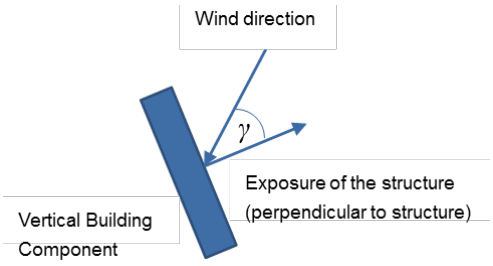


Figure 42: Angle γ in the formula for wind driven rain WDR

WDR r_{SR} is using the location factor α, current precipitation r, wind speed w and angle γ between component exposure and the current wind direction as:

$$r_{SR} = \alpha \cdot r^{0.88} \cdot w \cdot \cos(\gamma)$$

The local factor α considers:

- Terrain roughness C_R: whether and how much the wind speed is reduced by many and / or high buildings in wind direction
- Terrain topography C_T: whether and how much the component is being exposed to special weather due to ist location near a hill or lake
- Obstruction factor O: the obstruction of the component due to other buildings or obstacles
- Wall Factor W: the building's height.

Table 6: List of parameters for the calculation of wind driven rain

Parameter	Unit	Range	Comments
r	$\left[\frac{L}{m^2}\right]$	$0 \le r$	Precipitation amount
w	$\left[\frac{m}{s}\right]$	$0 \le w$	Wind speed
γ	[Grad]	$0 \le \gamma \le 360$	Angle between the component exposure and wind direction
α	[ ]	$0 < a_4 < 1$	Location factor $\alpha = C_r \cdot C_t \cdot O \cdot W$
C_r	[ ]	$0.1 \le C_r \le 1$	Terrain roughness coefficient
C_t	[ ]	$1 \le C_r \le 1.6$	Topography factor
O	[ ]	$0.2 \le C_r \le 1$	Obstruction factor
W	[ ]	$0.2 \le W \le 0.5$	Wall factor

5.5 Runoff Calculation

Since water (rain, WDR) r_{sr} on the component might be absorbed by the (porous) material, evaporate or splash, the amount of runoff from the component A_w becomes smaller. In principle, the runoff generated by WDR is calculated with respect to three assumptions:

1. The flow rate is the same as the amount of flow and evaporation is neglected.:

   $A_w = r_{sr}$

2. The losses results as a constant part of the rainfall quantity (proportional). The proportionality factor Ψ is the runoff coefficient:

$$A_w = \Psi \cdot r_{sr}$$

3. The evaporation results in a function of WDR (possibly non-linear). The function f_A is called the drain function:

$$A_w = f_A\left(r_{sr}\right)$$

The runoff function depends on the porosity and surface structure of the material. The difference between a linear or non-linear function and the resulting runoff proportional to the amount of WDR is small compared to the uncertainty resulting from the runoff coefficient which is known in most cases. This uncertainty is also small compared to the influence of the exposure of a component varying between 0 and 100% of the WDR amount.

In COMLEAM, the proportional dependency was implemented using a runoff coefficient. Hereby, it is also possible to neglect evaporation by setting the runoff coefficient ψ = 1.

5.6 Emission

The emission of substances from components occurs in the dissolved phase by runoff water. Based on experiences with field and lab studies it is assumed that a functional relationship between the runoff amount and the emission from a component exists. The function reflecting the specific leaching behavior is typically not known. Consequently, the mathematical function must be derived from experimental data with following conditions:

- The function increase monotonically
- Start at the origin (i.e. at the point (0;0))
- The slope of the function must constantly decrease (monotonically decreasing)
- The quantity released is smaller than the initial amount in the component
- The function must be fitted to the available data as best as possible (least squares)
- The function should be as universal as possible, i.e. various materials and substances should be described by the parameters without changing the shape of the function.

COMLEAM provides six functions of type T as follows:

- Logarithmic
- Langmuir
- Michaelis-Menten
- limited growth
- Diffusion controlled.

Details to the emission functions and their relevance in modelling leaching are presented in Tietje *et al.* (2018)[1]. For all emissions $E(t)$:

$$E\left(t\right) = c_0 \cdot E_T\left(t\right)$$

with:

[1] Tietje, O., Burkhardt, M., Rohr, M., Borho, N., Schoknecht, U. (2018): Emissions- und Übertragungsfunktionen für die Modellierung der Auslaugung von Bauprodukten. Umweltbundesamt, Dessau-Rosslau.

$E(t)$ Amount of substance emission per square meter of façade area [mg/m²]
c_0 applied substance amount per square meter of façade area [mg/m²]
$E_T(t)$ emission function (dimensionless, $0 \le E_T(t) \le 1$) of type T,

For vertical component, the amount of runoff water $q_{c,cum}(t)$ is assumed as being dependent on the amount of WDR $r_{SR,cum}(t)$ and the runoff coefficient ψ (dimensionless, $0 < \psi \le 1$): $q_{c,cum}(t) = \psi \cdot r_{SR,cum}(t)$ [L/m²]. For horizontal component, no WDR is calculated. Instead, the amount of runoff water $q_{c,cum}(t)$ is calculated from the amount of precipitation $r_{cum}(t)$:

$$q_{c,cum}(t) = \psi \cdot r_{cum}(t).$$

5.6.1 Logarithmic Emission Function

The logarithmic emission function $E_{\log}$ is only adjusted by two parameters for the entire data range (Table 7):

$$E_{\log}(r) = a_{\log} \cdot \ln\left(1 + b_{\log} \cdot q_{c,cum}\right)$$

As an example: The initial substance amount in a façade coating is $c_0 = 1000 \frac{mg}{m^2}$. The parameters of the logarithmic emission function are $a_{\log} = 0.01$ and $b_{\log} = 0.172$. The runoff of $r_{\log} = 10 \frac{L}{m^2}$ is corresponding to the substance emitted from the façade $M = a_{\log} \cdot c_0 = 0.01 \cdot 1000 = 10 \frac{mg}{m^2}$.

Table 7: Parameters for the logarithmic emission function

Parameter	Unit	Range	Comment
$b_{\log}$	$\left[\frac{m^2}{L}\right]$	$0 < b_{\log}$	Comparison runoff $r_{\log} = \frac{1.72}{b_{\log}}$ in $\left[\frac{L}{m^2}\right]$
$a_{\log}$	$[\ ]$	$0 < a_{\log}$	Fraction of the amount of substance leached until the comparison runoff $r_{\log}$ is reached compared to the initial content c_0

5.6.2 Langmuir Desorption Function and Michaelis-Menten Kinetics

The Langmuir sorption-desorption function is used in mass transport modeling in soil to calculate the equilibrium between sorption and desorption of substances to the soil matrix when the number of sorption sites is limited. The Michaelis-Menten kinetics are used in pharmacokinetics to determine the release of an active substance in the body. These two functions are equivalent and differ only by using the inverse of a parameter. The approximation of the maximum emission quantity is calculated by the following expression:

$$E_{\text{Langmuir}}(t) = \frac{a_{\text{Langmuir}} \cdot q_{c,cum}(t)}{1 + a_{\text{Langmuir}} \cdot q_{c,cum}(t)}$$

Thus, the Langmuir desorption function only utilizes a single parameter, a_{Langmuir}, with the unit [L/m²] to describe the emission up to the maximum. The Langmuir desorption function corresponds to a Michaelis-Menten kinetics in which only the parameter a_{Langmuir} is replaced

$$K_{MM} = \frac{1}{a_{\text{Langmuir}}}$$

$$E_{MM}(t) = \frac{r(t)}{K_m + r(t)}$$

The time $t_{1/2}$ at which half of the emissions have elapsed is recognizable. For the "half emission time" $E_{MM}(t_{1/2}) = \frac{1}{2} = \frac{r(t_{1/2})}{K_m + r(t_{1/2})}$, the parameter K_m corresponds to the flow rate $r_{1/2}$ after which half of the emission has occurred $K_m = r_{1/2} = r(t_{1/2})$. In the T1/T2 scenario, there is just the assumption that $r_{1/2}$ marks the transition from fast emission to slow emission (Table 8).

Table 8: Parameters for the Langmuir emission function and the Michaelis-Menten kinetics

Parameter	Unit	Range	Comment
a	$\left[\frac{m^2}{L}\right]$	$a > 0$	$a = \frac{1}{K_m}$
K_m	$\left[\frac{L}{m^2}\right]$	$K_m > 0$	$K_m = r_{1/2} = r(t_{1/2})$ is the amount of runoff after which half of the emission has occurred.

5.6.3 Limited Growth

Another emission function is the limited growth function:

$$E_{LG}(t) = \left(1 - e^{-a \cdot r(t)}\right)$$

This approach assumes that the emission decreases continuously. The parameter a here signifies the decay rate of the emission. It can also be determined as $a = \frac{0.69}{r_{1/2}}$ from the runoff amount $r_{1/2}$, after which half of the emission has been carried out. The limited growth function as well uses only one parameter a in [m²/L] to describe the course of the emission to the maximum. See Table 9 for details on the parameter.

Table 9: Parameter for the limited growth emission function

Parameter	Unit	Range	Comment
a	$\left[\frac{m^2}{L}\right]$	$a > 0$	$a = \frac{0.69}{r_{1/2}}$ can be calculated from the amount of runoff after which half of the emission has occurred.

5.6.4 Diffusion Controlled Function

The following process-based function is reflected by a combination of diffusion and sorption:

$$\frac{\partial C}{\partial t} = \frac{D_{eff}}{K_{pw} + 1} \cdot \frac{\partial^2 C}{\partial x^2}$$

A sorption-desorption function can be derived between a zero-order sorption-desorption and first-order sorption-desorption. With the assumption that the mean rain intensity is constant, this approach can be applied as follows:

$$E_{\text{Diffusion}}(t) = a \cdot \sqrt{r(t)}$$

Therefore, only one parameter a in $\left[\frac{m}{\sqrt{L}}\right]$ is used in the diffusion approach to describe the course of the emission to the maximum. The parameter a (Table 10) is calculated as $a = \frac{1}{2 \cdot \sqrt{r_{1/2}}}$ using the runoff amount $r_{1/2}$ after which half of the emission has occurred.

Table 10: Parameter for the diffusion controlled emission function

Parameter	Unit	Range	Comment
a	$\left[\frac{m}{\sqrt{L}}\right]$	$a > 0$	$a = \frac{1}{2 \cdot \sqrt{r_{1/2}}}$ is calculated from the runoff amount $r_{1/2}$, after which half of the emission hasoccurred.

5.6.5 Linear emission function

If the emission is constant over time, the corresponding emission function as a cumulative function is linear with the emission rate a_{linear} in [mg/L]:

$$E_{\text{linear}}(t) = a_{\text{linear}} \cdot r(t)$$

Linear emission functions occur when the emissions are very small compared to the amount of the substance present on the component. For example, in the case of copper façades, a constant emission of copper into the runoff water is assumed. In this case, the applied quantity c_0 is not specified ($c_0 = 1$) and the linear emission function is given [mg/m^2] (Table 11).

Table 11: Parameter for the linear emission function

Parameter	Unit	Range	Comment
a_{linear}	$\left[\frac{mg}{L}\right]$	$a_{\text{linear}} > 0$	The parameter of the linear emission function is specified in $\left[\frac{mg}{L}\right]$.

5.6.6 Parameter Identification

The logarithmic emission function has two parameters with an illustrative interpretation, however, also must be calculated statistically.

The other emission functions have only one parameter which describes the course of the emission. This can easily be calculated from the flow rate after which half of the emission has occurred. Since the flow rate itself must be calculated statistically, it is recommended to adjust the parameters uniformly with the statistical software by non-linear regression ("nls": non-linear least squares) to the available data.

5.6.7 Example for Emission Functions with Reference Data

Various parameters of the emission functions were calculated using emission data of Terbutryn determined in a field study (Burkhardt et al., 2012).

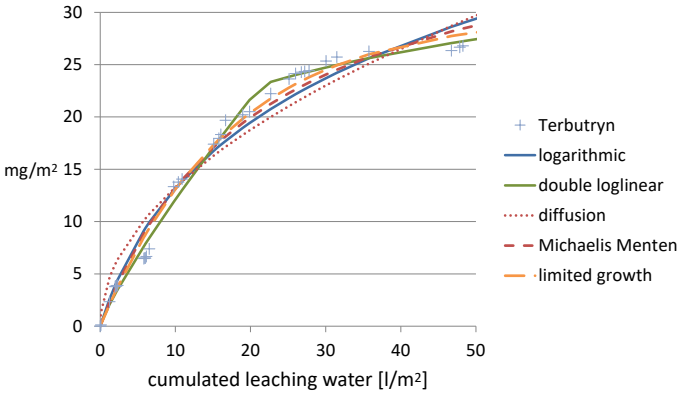


Figure 43: Fitting of various emission functions for Terbutryn emission recorded in the field.

5.7 Interface Compartment

For each component i $(1 \le i \le n)$, the mass balance of water and substance are calculated. The inflow from the component is compared with the outflow to the receiving compartment. The temporal change in the amount of water in the IC is temporal varying, which is increased by the

water outflow from the component and is reduced by e.g. the discharge into the sewer or surface water. The outflows into drains and/or a surface water represents a linear storage y_L:

$$\frac{dy_L}{dt} = (k_K + k_O) \cdot y_L$$

Herein, the runoff rate $k_K \left[h^{-1}\right]$ determines runoff into the sewer system and $k_O \left[h^{-1}\right]$ runoff into surface water. If water flow is not discharged into the drainage system or into a surface water ($k_K = k_O = 0$), the runoff $k_B \left[h^{-1}\right]$ is retained in an external file and can be used for an soil transport model. The water balances in the IC in liters per component is as follows:

$$\frac{dy_i}{dt} = A_{W,i} - (k_{K,i} + k_{O,i} + k_{B,i}) \cdot y_i$$

The substance leached from the component (mg or µg per component) is in the runoff water. The mass inflow *E* is calculated by the emission function. The ratio of the mass of the substance to the quantity of runoff water equals the concentration c_i in the interface compartment (in mg/L or µg /L per substance). The mass outflow m_{sk} of the substance from IC is obtained from the concentration multiplied by the water outflow $m_{sk,i} = c_i \cdot (k_{K,i} + k_{O,i} + k_{B,i}) \cdot y_i$.

In addition, the mass of the substance in the IC is reduced by degradation in the water with the decay rate k_a.

$$\frac{dz_i}{dt} = E_i - m_{ms,i} - k_a \cdot z_i = E_i - c_i \cdot (k_{K,i} + k_{O,i} + k_{B,i}) \cdot y_i - k_a \cdot z_i$$

5.8 Runoff to Surface water

It is assumed that the amount of water present in the IC flows directly into surface water typical for separated sewer systems.

The modeling of the effluent from the interface compartment is a linear storage, in which the flow rate is proportional to the amount of water present. The concentration of the substance in the IC is also the concentration in the current outflow.

The discharge into a surface water can be calculated for different surface waters. The Q_{347} value is assumed as the parameter for the size of the surface water. The Q_{347} value determines the minimal water flow of a surface water during 95% of the year (dry-weather runoff). It thus determines the amount of water in which the outflow from the component is diluted and at the same time the period after which the substance has flowed further in the surface water.

Figure 44: Example of a creek with a Q_{347} of 2.9 L/s.

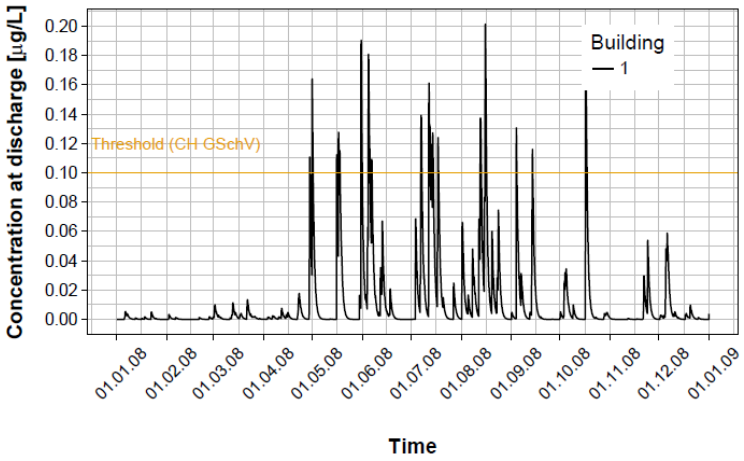


Figure 45: Substance concentration in a creek with Q_{347} = 2.9 L/s.

5.9 Runoff to Soil and Groundwater

COMLEAM provides an output interface (csv file) for water and substance flowing from a component which may enter the unsaturated soil and groundwater. These output data can be used as input data in a simulation program as the upper boundary condition of a soil model like PELMO or PEARL.

Appendix

Table 12: Geometry file structure

Column	Identifier	Data type	Range	Description
1	Component id	Integer	>0	Unique numerical identifier
2	X coordinate	Real number	>0	Geographical width of the component's center
3	Y coordinate	Real Number	>0	Geographical length of the component's center
4	Coordinate system	Alpha numerical	-	Coordinate system denomination (i.e. WCS, CH95)
5	Building id	Alpha numerical	-	Identifier grouping individual components to a building
6	Construction year	Integer	>1900	Construction year of the component / building. [YYYY]
7	Component length	Real Number	>0	[m]
8	Component height	Real Number	>0	[m]
9	Component area	Real Number	>0	[m^2]
10	Exposition	Real Number	0 … 360	Orientation of the surface normal in [°] from north, clockwise.
11	Angle to ground	Real Number	0 … 90	90° for façades, other angles are interpreted as horizontal surfaces
12	Glass	3-digit Integer	See Table 13	Material type Glass
13	Percentage glass	Real Number	0 … 100	Percentage of the component area covered with glass.
14	Wood	3-digit Integer	See Table 13	Material type wood
15	Percentage Wood	Real Number	0 … 100	Percentage of the component area covered with wood.
16	Plastic	3-digit Integer	See Table 13	Material type plastic
17	Percentage Plastic	Real Number	0 … 100	Percentage of the component area covered with plastic.
18	Metal	3-digit Integer	See Table 13	Material type metal
19	Percentage metal	Real Number	0 … 100	Percentage of the component area covered with metal.
20	Mineral 1	3-digit Integer	See Table 13	Material type mineral 1
21	Percentage mineral 1	Real Number	0 … 100	Percentage of the component area covered with a mineral material
22	Mineral 2	3-digit Integer	See Table 13	Material type mineral 2 (i.e. a concrete socket)
23	Percentage mineral 2	Real Number	0 … 100	Percentage of the component area covered with a mineral material.
24	Special materials	3-digit Integer	See Table 13	Photovoltaics, textile, greenery, …
25	Percentage special material	Real Number	0 … 100	Percentage of the component area covered with a special material
26	Comments	Free	-	

Table 13: List of valid material subtypes

Code	Material	Runoff Coefficient	Remarks
1	Mineral		
101	Render matte	0.9	Purely mineral, possibly with finishing coat
102	Render shiny	0.9	Organic matrix, possibly with finishing coat
103	Ceramic brick	0.9	Coarse ceramic, natural finish
104	Ceramic (coated)	0.98	Fine ceramic
105	Fiber cement colored (boards)	0.98	Eternit boards
106	Exposed concrete dull	0.85	Naked concrete
107	Exposed concrete shiny (coated)	0.9	Coated
108	Exposed concrete (glazed)	0.85	Glazed (concrete structure shines through)
109	Stone	0.85	Granite, lime, sandstone etc.
199	Undetermined mineral	0.9	
2	Wood		
201	Natural raw surface	0.85	Uncoated wood
202	Natural (glazed)	0.85	
203	Natural (coated)	0.85	Coated
204	Composite laminated (boards)	0.85	Composite glued / laminated
299	Undetermined wood	0.85	
3	Metal		
301	Aluminium (polished)	0.98	Elements bolted together
302	Steel (galvanized)	0.98	Hot zinc dipped
303	Steel colored (coated)	0.98	Coated, matte or shiny
304	Stainless steel	0.98	
305	Copper	0.98	
399	Undetermined metal	0.98	Tin, bronze, brass
4	Plastics		
401	PVC	0.98	
402	HDPE	0.98	
499	Undetermined plastic	0.98	
5	Glass		
501	Glass	0.98	
599	Undetermined glass	0.98	
6	Special Forms		
601	Textile fabric	0.8	
602	Green facade	0.7	
603	Photovoltaics	0.98	Building-integrated
604	Bituminous sheeting	1.0	Roof sealing per DIN 1986-100-A1
605	Green roof	0.5	Assumption: Inclination <= 5°, per DIN 1986-100-A1
699	Undetermined special type	0.2	

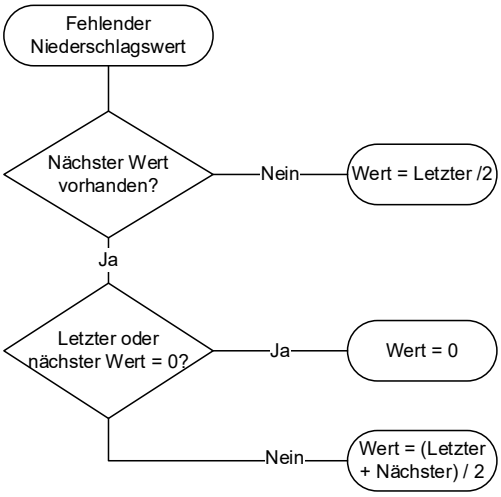


Figure 46: Algorithm for missing precipitation values

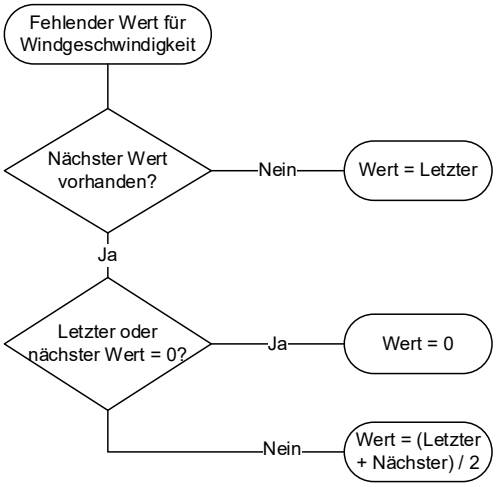


Figure 47: Algorithm for missing values for wind speed

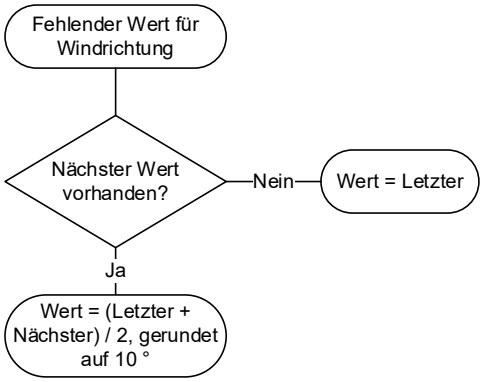


Figure 48: Algorithm for missing values for wind heading