Operating instruction

for the simulation program SimuCF

Program for process simulation of biological degradation processes

in the field of waste management

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1 Characterization of the simulation model

The simulation program SimuCF simulates the complex connections between most important biological degradation processes in the field of waste management under aerobic and anaerobic conditions, meaning rotting and gasification of biogenic waste and combined disposal operations. Here, mainly mathematical basic equations, physical laws and stoichiometric calculations were used. It is, therefore, assigned to the deterministic models.

After setting the initial conditions, iterative values are displayed in constant recalculation considering the dependencies. The preset parameters can be altered within the running simulation.

The program's main characterictics are:

- No strict separation between anaerobic and aerobic systems
- Many options for operation
- Thermodynamic effects included
- Thermophilic conditions and passive ventilation included
- Correction factors are integrated as changeable assumptions
- Spontaneously occuring temporary temperature rises are predictable
- Time-discrete process output, not only cumulative results
- Many influences included in degradation kinetics
- Water situation is fully adjustable

2 Installation

At first, the folder "SimuCF.zip" has to be extracted and opened. The files displayed in Figure 2-1 are located in the folder. For installation, the "setup.exe" must be executed. To open the program, the folder "programs" needs to be opened in Windows.

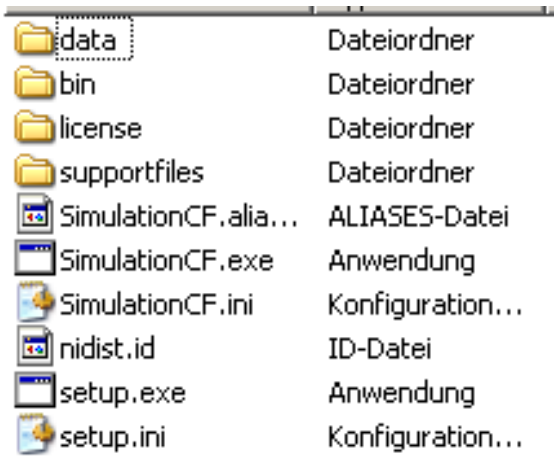


Figure 2-1: Files for installation

3 Functionality of the program

After the installation, the simulation tool can be used. When opening the program, an exemplary simulation is running.

Unique simulations can then be launched under variation of a great number of parameters, which will be described in the following chapter. The input of the parameters takes place directly on the program interface.
At first, some general information are provided:

- The input surfaces highlighted in pink include the starting values of the simulation.
- White areas and green switches include further input options.
- On brown-grey areas, the results of the simulation or the starting values are displayed.
- The simulation starts by pressing the button (Ctrl+R).
- The simulation runs when is displayed.
- Simulations can be stopped by pressing the STOP button (Ctrl+P).
- A reset of the simulation to the initial state is possible by using „Reinitialize All to Default“; this option can be found when pressing Operate on top of the program interface.
- The input of materials is only adopted if the simulation runs (see above).
- The saving of a whole simulation is achievable by pressing Operate > Data Logging > Log in the headline; for this purpose, you have to prepare a file.
- Saved simulations can be loaded by using Operate > Data Logging > Retrieve in the headline.
- For batch simulations, the simulation time is extended, therefore, it is needed to wait until the simulation stops by itself.
- The process is only feasible if diagrams and numbers are constant and no warning lights appear in the middle of the program interface.
- Thus, it is a requirement to reach a steady state without warning lights.
- Inputs and outputs happen simultaneously in batch processes.

3.1 Examples of application with the program

Individual examples for anaerobic digestion and composting are included which are anaerobic digestion of leaves and composting of food waste respectively. Settings meant for the examples will be included as shown in Figure 3-1. For ease of identification in the following manual, the interface of SimuCF is well defined into 21 zones labelled in alphabetically order, shown in Figure 3-2. All the zones are named individually as shown in Figure 3-3. Clear numeration has been created for fields found in SimuCF interface shown in Figure 3-4. A graph shown in Figure 3-5 is the result aimed to be generated with SimuCF.

Anaerobic Digestion of Leaves:

…… content ……

Composting of Food Waste:

…… content ……

Figure 3-1: Step-by-step guidance for setting up simulation interface according to examples given

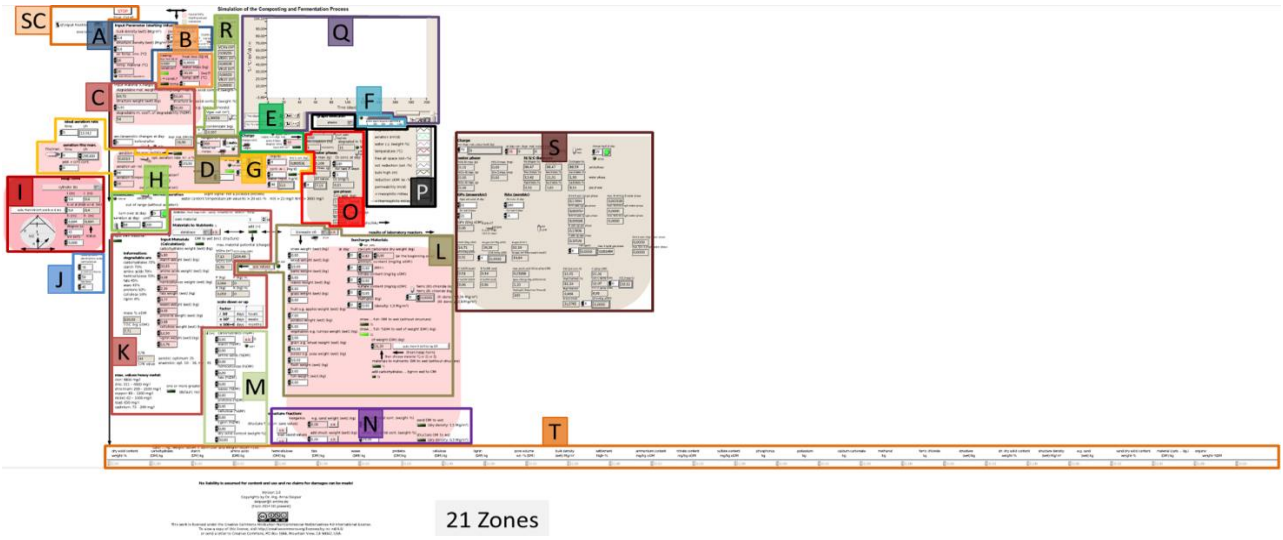


Figure 3-2: Well defined zones (total 21 zones)

A	Basic starting values	K	Material by components
B	Reactor casing	L	Biowaste-mixture by preset shares
C	Material characteristic	M	Additional components
D	Duration of treatment	N	Additional structure fraction
E	Charge (batch/continuous)	O	Additional fluid output characteristics
F	Inoculum and lag-phase	P	Graph selection and legend
G	Aerobic parameters	Q	Graph illustration
H	Anaerobic parameters	R	Gas output
I	Reactor form	S	Laboratory reactors results
J	Components degradability	T	Input overall sum
SC	ShortCut		

Figure 3-3: Naming for individual zones

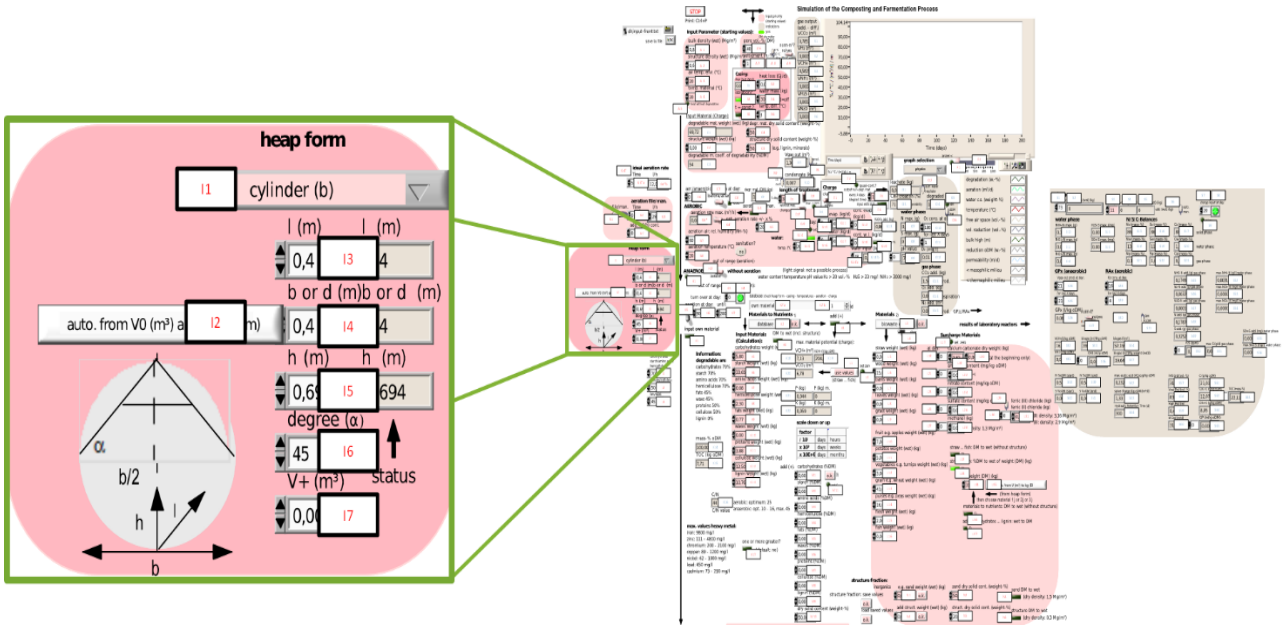


Figure 3-4: Numeration for each field in SimuCF

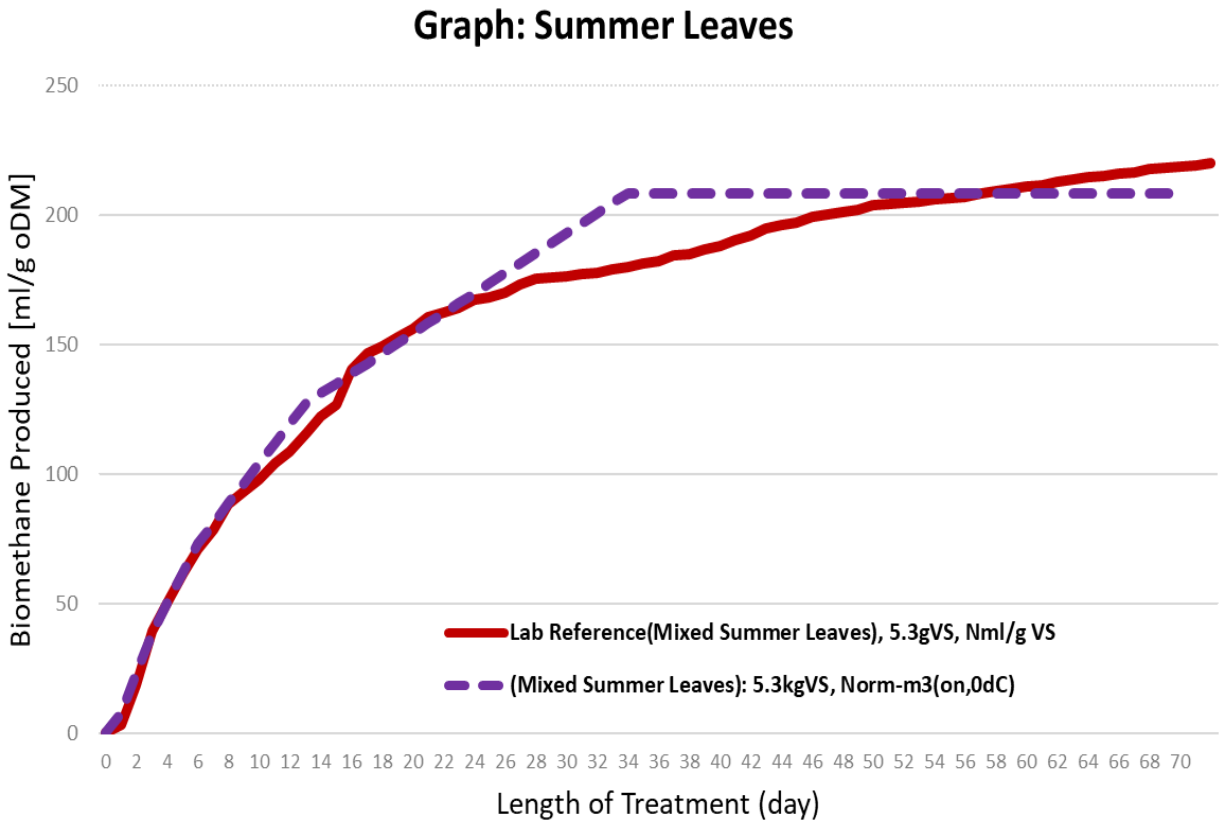


Figure 3-5: Graphs of comparison between laboratory experiment and SimuCF simulation

4 Input

To run the simulation, the following information about the input substrate should first be determined and analysed.

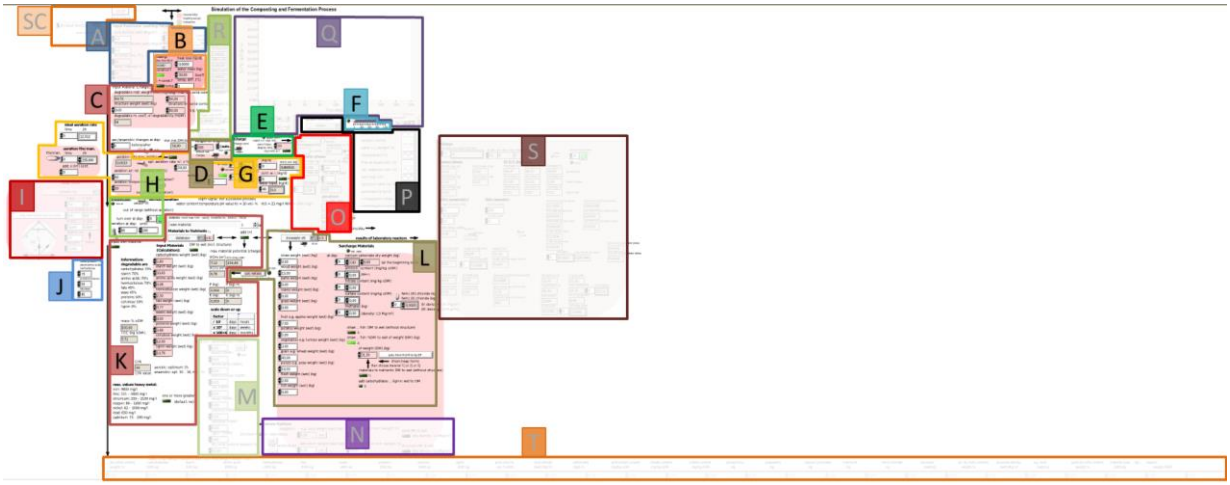
1. Physico-chemical analysis
    - Structure dry solid content *(also known as total solid content (TS))*
    - Degradable matter dry solid content *(also known as volatile solid content (VS) and organic dry matter (oDM))*
    - Structure weight *(also known as inorganic content and ash content)*
2. Bio-chemical analysis
    - Carbohydrates
    - Starch
    - Amino acids
    - Hemicellulose
    - Fats
    - Waxes
    - Proteins
    - Cellulose
    - Lignin
3. Type of materials
    - Straw
    - Wood
    - Barks
    - Leaves
    - Grass
    - Fruit (e.g. apples)
    - Potatoes
    - Vegetables (e.g. turnips)
    - Grain (e.g. wheat)
    - Pulsess (e.g. peas)
    - flesh
    - fish
4. Heavy metals concentration
    - Iron
    - Zinc
    - Chromium
    - Copper
    - Nickel

- Lead
- Cadmium

These initial values are then converted to match the units mentioned in the SimuCF interface before being entered into the respective fields. For a simulation to run more precisely, input information for category 2 (Bio-chemical analysis) is preferred over category 3 (Type of materials).

Anaerobic Digestion of Leaves:

- Zones important for input information in order to simulate anaerobic digestion process are zones B, C, D, E, F, G, H, J, K and L.



- Information about input substrate that are obtained from laboratory analysis are as follow:

Physico-chemical analysis		
Water content	%FM	50.12
Total solid content (TS)	%FM	49.88
Volatile solid content (VS)	%TS	92.36
Ash content/Inorganic content	%TS	7.64
Bio-chemical analysis		
Carbohydrates (wet)	kg	1.7054455
Starch (wet)	kg	0.00
Amino acids (wet)	kg	0.00
Hemicellulose (wet)	kg	0.8789604
Fats (wet)	kg	0.0393564
Waxes (wet)	kg	0.00
Proteins (wet)	kg	0.4722772
Cellulose (wet)	kg	0.8264851
Lignin (wet)	kg	1.3774752
Heavy metals concentration		
Fe	mg/L	0.3206
Zn	mg/L	0.1299
Pb	mg/L	0.0030
Cd	mg/L	0.0006
Cr	mg/L	0.0091
Cu	mg/L	0.0234
Ni	mg/L	0.0032

- Open the SimuCF software.

- Simulations can be stopped by pressing the STOP button (Ctrl+P) or ● button that is located on the upper left conner of the interface.

Composting of Food Waste:

- Zones important for input information in order to simulate composting process are zones A, C, D, E, F, G, H, I, J, and K.

4.1 Material

The input field for dry matter of the material is located in the upper part on the left side of the input surface, shown in Figure 4-1. If there is nothing given, this value is 50 weight-% or can be chosen. There are two terms to define: “degr. mat. dry solid content [C4]” is the degradable fraction, “structure dry solid content [C5]” is the non-degradable structure material.

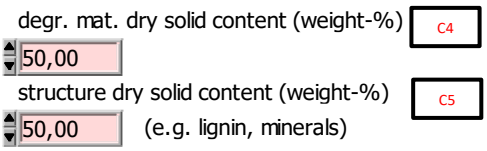


Figure 4-1: Adjustment of the dry content (Zone C)

Anaerobic Digestion of Leaves:

- The data obtained from physico-chemical analysis is required to fill up fields C4 and C5.

Physico-chemical analysis		
Water content	%FM	50.12
Total solid content (TS)	%FM	49.88
Volatile solid content (VS)	%TS	92.36
Ash content/Inorganic content	%TS	7.64

- C4 is defined as the VS content in fresh matter (FM).

$$Volatile\ solid\ content \times Total\ solid\ content \times 100\%$$
$$= 0.9236 \times 0.4988 \times 100\% = \mathbf{46.07}\%$$

- C5 is defined as TS in fresh matter (FM). Therefore **49.88%** should be filled in the field C5.

The degradabilities of the single substances [J1-J3] are based on assumptions and can be changed within the program on the left side of the input surface, if needed (Figure 4-2).

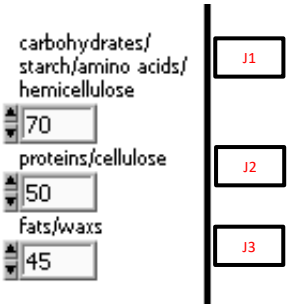


Figure 4-2: Degradabilities of substances by percentage (zone J)

Anaerobic Digestion of Leaves:

- The degradabilities could be changed when see fitting. In this example, J1 is set as 90%, J2 as 80%, and J3 is set as 45% (default).

With Figure 4-4, the 8 different input methods will be shown and described:

1. Enter material input with substrates (e.g. straw, wood, crust, sheets, fruits, meat etc.).

For this purpose, the values can be directly entered into the boxes marked in red color [L5-L16], which has to be confirmed and converted into constituents by pressing “use values [L1]” in the blue box. The constituents would only show after the simulation is pressed “to run”. “Set zero” [M11] could be clicked until a green light in turned on, in order to delete earlier inputs and define new waste categories, waste models or to carry out a direct input.

2. Enter material input with different waste categories incorporated in the program.

Use the grey drop-down button in the yellow box [K2] (Figure 4-4) and confirm with “o.k.” button next to it for option selected. The constituents will only appear after the simulation is pressed “to run”. The waste categories contain pre-defined biochemical compositions and values according to literature. Examples of waste categories available are:

- Sewage sludge
- Green garbages
- Household wastes
- Org. household wastes
- Organic wastes
- Newspaper
- Paper fibers
- Database (Hint: [K1, K2*a and K2*b] become visible after “database” is selected, shown in Figure 4-3)

- All zero (Hint: this option is selected if earlier inputs under [K5-K13] are preferred to be deleted, to define new waste categories or waste models or to carry out a direct input.)

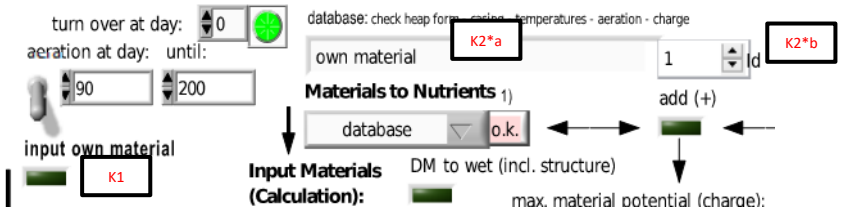
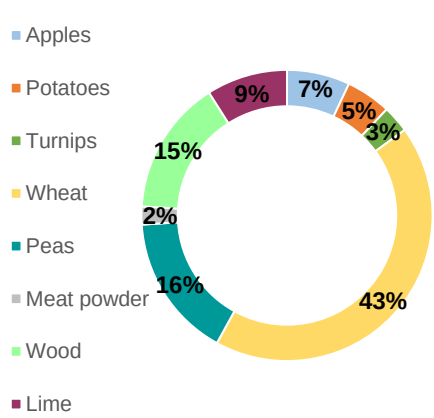
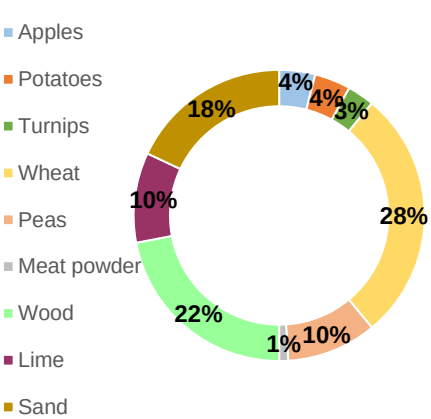


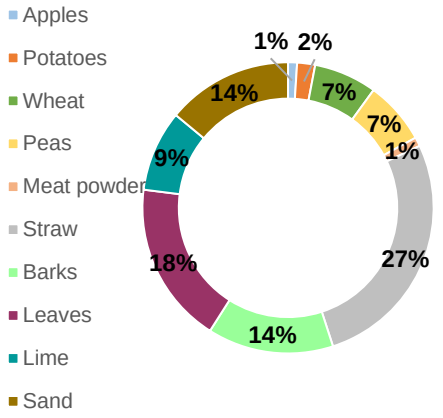
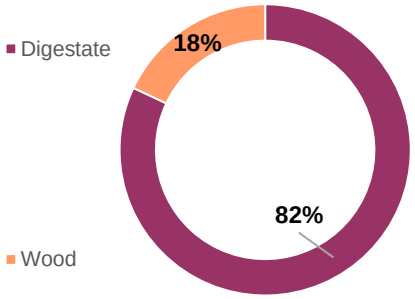
Figure 4-3: Hidden functions of "database" (Zone K)

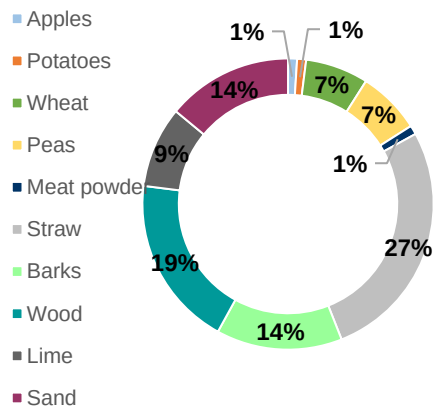
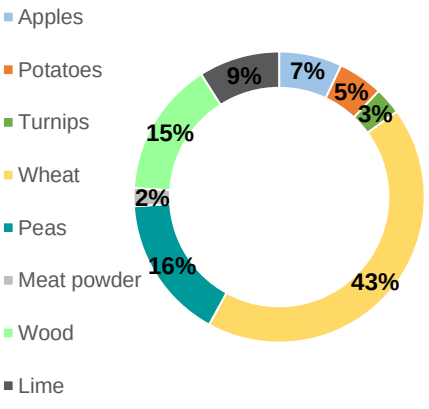
3. Enter material input with six waste models incorporated in the program.

Six waste models (biowaste e1 to e6) are chooseable, details about each waste model are shown in Table 1 that could be again access through “show” lever [L4] in the SimuCF interface. These waste models can be selected with the help of the grey dropdown button [L3] in the orange box (Figure 4-4) and confirmed with “o.k.” button next to it. The materials are automatically converted into their constituents (carbohydrates, starch, fats etc.) ([K5-K13], green box in Figure 4-4) after the simulation is pressed “to run”.

Table 1: Details about biowaste experiments e1-e6

[L3]	biowaste e1	biowaste e2
Status	Model waste	Model waste
Description	Easily degradable kitchen waste compounds	Easily degradable kitchen waste compounds, high concentration of inorganic substances (e.g. sand and soil)
Season (during which the waste is obtained)	Winter	Winter
Waste compositions		
Aeration rate	moderate	-
Water content (%)	49-50	54
pH value	6.1-6.5	6.3
Bulk density (Mg/m³)	0.8	0.7
N-content (%)	1.8-1.9	1.4
Organic content (%)	82-85	76
C/N ratio	20-25	24
Dry mass (kg)	31.30	60.55

[L3]	biowaste e3	biowaste e4
Status	Model waste	Real waste
Description	Rich in green waste compounds, containing some fractions of kitchen waste	Waste is first anaerobically degraded before composting process
Season (during which the waste is obtained)	Autumn	-
Waste compositions		
Aeration rate	-	-
Water content (%)	53	60
pH value	6.0	8.0
Bulk density (Mg/m³)	0.2	0.5
N-content (%)	1.5	1.2
Organic content (%)	66	39
C/N ratio	21	8
Dry mass (kg)	17.95	35.00

[L3]	biowaste e5	biowaste e6
Status	Model waste	Model waste
Description	Rich in green waste compounds, containing some fractions of kitchen waste	Easily degradable kitchen waste compounds
Season (during which the waste is obtained)	Sping, Summer	Winter
Waste compositions		
Aeration rate	-	Intense
Water content (%)	43	49-50
pH value	10.8	6.1-6.5
Bulk density (Mg/m³)	0.2	0.8
N-content (%)	0.6	1.8-1.9
Organic content (%)	64	82-85
C/N ratio	12	20-25
Dry mass (kg)	25.00	31.30

4. Enter material input directly with values.

Fill in values for the following directly ([K5-K13], green box in Figure 4-4):

- Carbohydrates
- Starch
- Amino acids
- Hemicellulose
- Fats
- Waxes
- Proteins
- Cellulose
- Lignin

These values will be read in for simulation after the simulation is pressed  "to run".

SimuCF works best between 1-1000 kg. However, input and output values can be scaled within each case (x0.1, x10, x1000 etc.).

5. Enter material input through conversion from dry to wet solid matter (kg).

This has to be done if material is given as dry matter. Use, therefore, the button in the purple box [K4] (Figure 4-4) (click it to light up in green). Changes would only appear after the simulation is pressed  "to run". The calculation is based on literature for some of the waste models, the waste categories and the single materials. Besides that, dry contents are changeable or choosable if nothing is given.

6. Enter material input by choosing material from a database.

Select "database" within the dropdown button [K2] in the yellow box (Figure 4-4) followed by the selection of a substrate (ID) [K2*b] that later shown on the appearing menu [K2*a] (Figure 4-3).

After selection is completely made, the selection is confirmed with "o.k." button next to [K2]. Values from the database would be read in after the simulation is pressed  "to run".

7. Enter material input by filling in own material.

As mentioned, [K1] would only appear after "database" at [K2] is selected and the simulation is pressed  "to run". After [K1] appeared, click on the area "input own material" [K1], until a green light is turned on. Own material is then defined in the lower area of the interface [T1-T28, Zone T]. Fields in zone T require information on dry matter (DM) instead of wet matter that are listed from [K5-K13].

8. Enter additional material input on top of existing quantities.

An addition on a percentage basis to already existing quantities is possible. Fill the white areas [M1-M10] with values and confirm with “o.k.” button (highlighted in the black box in Figure 4-4). “Set zero” [M11] could be clicked until a green light is turned on, in order to delete earlier inputs and define new waste categories, waste models or to carry out a direct input.

An addition of the values from the orange and red marked boxes to the input materials by using “add(+)” [K3] and “use values” [L1] respectively.

Actions would be read in after the simulation is pressed “to run”.

The field under “Input Material (Charge)” under Zone C, as shown in Figure 4-8, shows the wet content in kg.

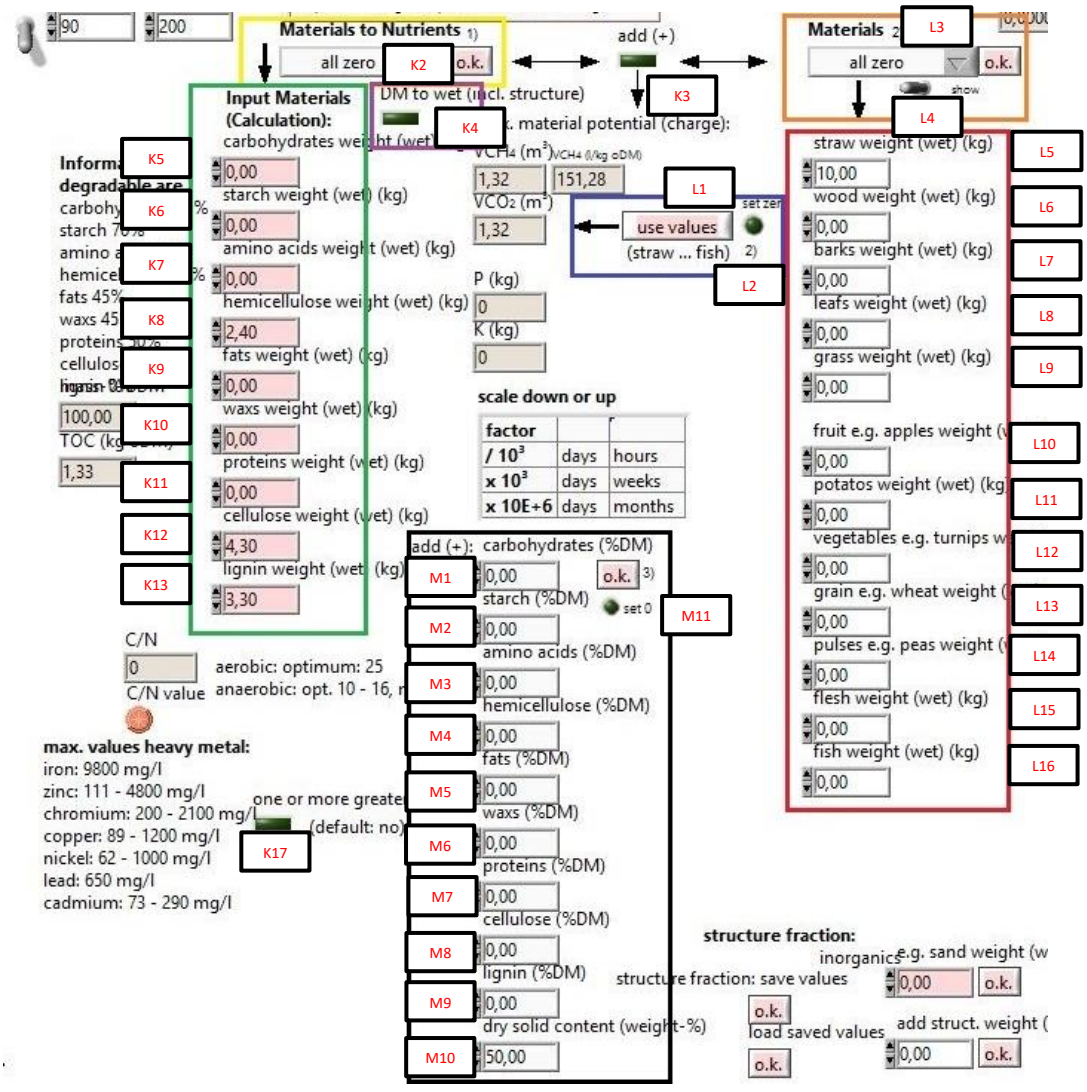


Figure 4-4: Overview of the material input

Anaerobic Digestion of Leaves:

- Information about input substrate that are obtained from laboratory analysis are as follow:

Bio-chemical analysis		
Carbohydrates (wet)	kg	1.7054455
Starch (wet)	kg	0.00
Amino acids (wet)	kg	0.00
Hemicellulose (wet)	kg	0.8789604
Fats (wet)	kg	0.0393564
Waxes (wet)	kg	0.00
Proteins (wet)	kg	0.4722772
Cellulose (wet)	kg	0.8264851
Lignin (wet)	kg	1.3774752
Heavy metals concentration		
Fe	mg/L	0.3206
Zn	mg/L	0.1299
Pb	mg/L	0.0030
Cd	mg/L	0.0006
Cr	mg/L	0.0091
Cu	mg/L	0.0234
Ni	mg/L	0.0032

- With these informations available, **method 4** could be used, by filling in values in fields K5-K13, green box in Figure 4-4.

- Since the heavy metals concentration mentioned in the table do not exceed the **max. values heavy metals** required by the SimuCF, therefore K17 does not need to be switched on.

4.2 Additional information

The bulk density [A1] and the density of the structure material [A2] are partly specified through the materials picked. The material temperature [A4] at the beginning has to be selected or adopted according to the process. The pore volume [A6] and the setting of the material [A7] are especially important for the aerobic degradation and can be estimated if necessary. It is, furthermore, possible to adapt the room temperature to the environment [A3]. This can lay between -40 and 80 °C. The information can be filled up in Zone A, as shown in Figure 4-5.

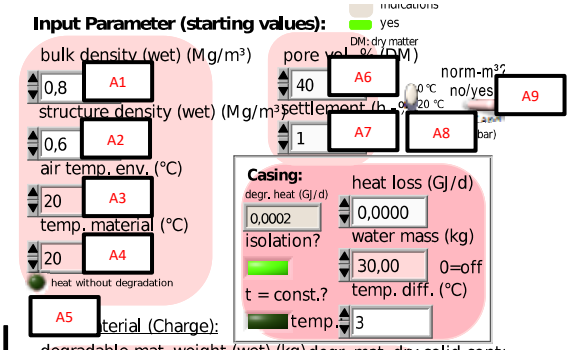


Figure 4-5: Input of additional information (important for aerobic degradation) (Zone A)

4.3 Further materials and/or contents

Calcium carbonate [L18], ammonium [L22], nitrate [L24], sulphate [L26], methanol [L28] and iron (II or III) chloride [L29, L31] can be added under “surcharge materials”. A defined day can be selected for this addition [L18, L21, L23, L25, L27, L30]. If there are absence of surcharge materials, ‘set zero’ [L17] could be switched on to erase the existing values that are already in the field. Mentioned fields for input of surcharge materials can be found in Zone L, these are shown in Figure 4-6.

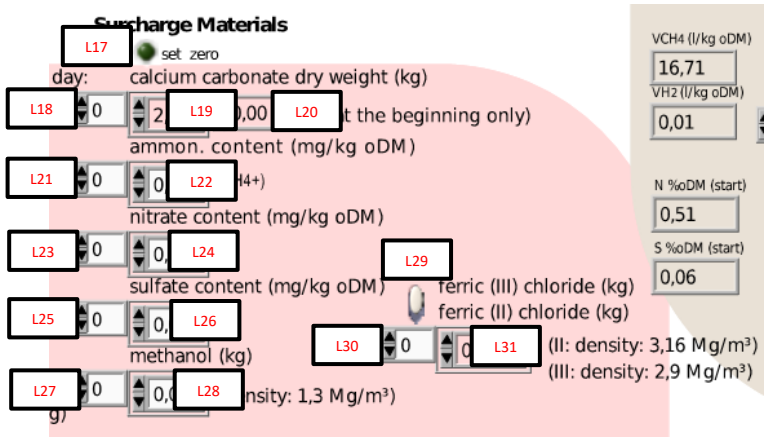


Figure 4-6: Input of surcharge materials (Zone L)

Inorganic materials like sand [N1-N3] and non-degradable material [N4-N6] can also be added additionally in Zone N on top of C2 from Zone C. These are shown in Figure 4-7 and in Figure 4-8. The values inserted at [N1 and N4] should then be confirmed with “o.k.” button next to it. Whereby the values will be read in for simulation after the simulation is pressed “to run”.

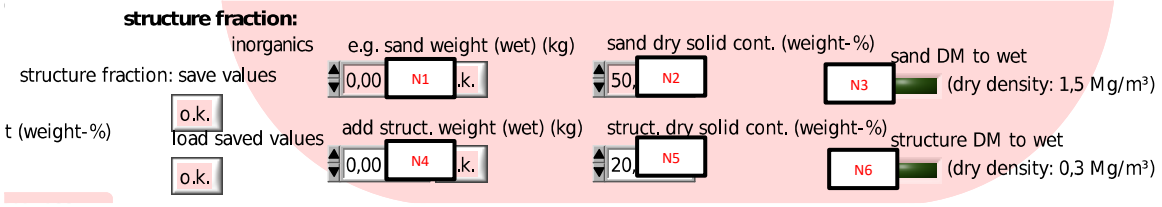


Figure 4-7: Input of inorganic materials (Zone N)

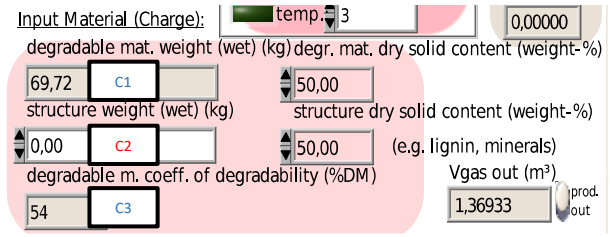


Figure 4-8: Input for inorganic content (Zone C)

Anaerobic Digestion of Leaves:

- The data obtained from physico-chemical analysis is required to fill up C2 in Zone C.

Physico-chemical analysis		
Water content	%FM	50.12
Total solid content (TS)	%FM	49.88
Volatile solid content (VS)	%TS	92.36
Ash content/Inorganic content	%TS	7.64

- C2 is defined for inorganic content or ash content. Since the volatile solid required for the experiment is 5.3kg, the volatile solid is calculated to be:

$$\frac{Mass\ of\ volatile\ solid\ content}{Volatile\ solid\ content\ (\%TS)} \times Inorganic\ content\ (\%TS) = Mass\ of\ inorganic\ content$$

$$\frac{5.3\ kg}{92.36\ \%TS} \times 7.64\ \%TS = \mathbf{0.4384}\ kg$$

4.4 Form of heap or reactor

Via a pull-down menu on the left side of the input surface in zone I as shown in Figure 4-9, the form of heap or reactor can be specified. A choice between triangular or trapezoid heaps and cylinder-shaped, drum-shaped, spherical or box-shaped reactors is possible [I1]. By specification of height [I5], width [I4] or diameter and length [I3], the volume of the material is calculated. A free volume can likewise be inserted in the field "V+ (m³)" [I7]. This is changing the reactor size but not the material quantity. The angle "α" [I6] must only be included for trapezoid heaps. In the dropdown menu, the used data for calculation are visible in the brackets behind the form of heap or reactor (e.g. "box (b,l)"). The calculated volume is shown in the illustrated graphic.

The material quantity in kg can directly be inserted centrally in the lower part of the input window or is calculated with help of the volume, [L34] shown in the red box in Figure 4-10.

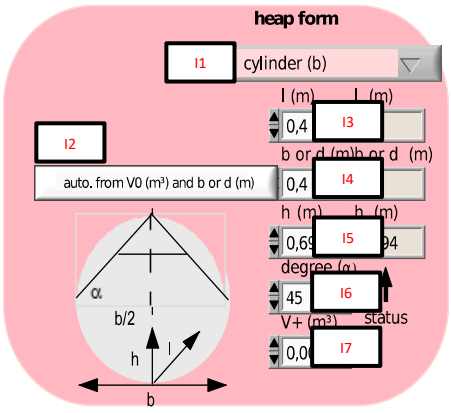


Figure 4-9: Input for form of heap or reactor (Zone I)

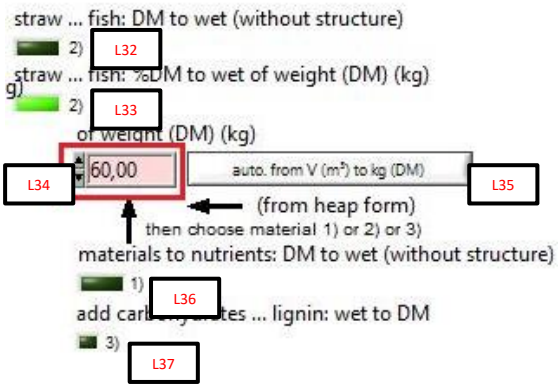


Figure 4-10: Input of material quantity (Zone L)

4.5 Isolation and waterjacket of the reactor

It is possible to choose within the program whether there is an insulation of the reactor/heap. Furthermore, expected heat losses and additional energy input by a water jacket can be entered. The water temperature inside the water jacket is assumed to be constant or is simulated as following the material temperature.

The setting of the named parameters can be conducted in the box outlined in Figure 4-11. By pressing the switch under “isolation?” [B3], the system can be identified as isolated when the green light is lit on. According to that, the value on top is defined [B1]; either it is named “degr. heat” (energy of degradation) or “heat loss”. Besides that, a further heat loss can be mentioned at [B2], which concerns the question of whether there is a heat loss in case of isolation. If the system is completely insulated, no water amount must be added.

The amount of water can be inserted in the pink field [B4]. A value of 0 means that no water jacket is present. If the indicated water mass is too low for the given temperature, an automatic increase takes place.

The energy needed is represented by the amount of water in the simulation.

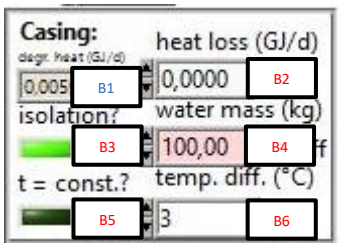


Figure 4-11: Input for isolation, temperature control and energy (Zone B)

Anaerobic Digestion of Leaves:

- The anaerobic digestion during the experiments is well isolated at the constant temperature of 38 ºC.

  B3 is switched **On**.

  B4 is set at **0** kg.

  B5 is switch **On**.

  B6 is set at **38** ºC.

4.6 Process selection and duration

The simulation of a semi-continuous process with selectable time intervals for the input can be performed with the help of the switch in the middle of the input window, at Zone E. Therefore, the switch in the green box in Figure 4-12 has to be shifted towards “yes”. The used amount of material is divided through the number of batches, which is why the same amount is considered like in a batch process. The number of charges can be inserted in the pink field [E3] in the blue box in Figure 4-12. The number corresponds to the difference between the single batches (in days). For a value of “1” in the field of [E3], the process is quasi-continuous. In this case, the button on top [E2], next to “quasi-cont.” can be pressed, which indicates that the startup phase is not included for the addition.

The points of time for the batches can also be defined separately for every time step, to this end, the settings from the red box in Figure 4-13 can be used. By converting the local shift to “man.” [S6], the days shown in the white field [S7] are defined as times of addition. For this purpose, the green button [S8] has to be activated for each day (lights up in green). Additionally, an automatic addition is definable, which can, subsequently, be edited (deletion, addition of days). The button “all no” [S9] deactivates all inputs.

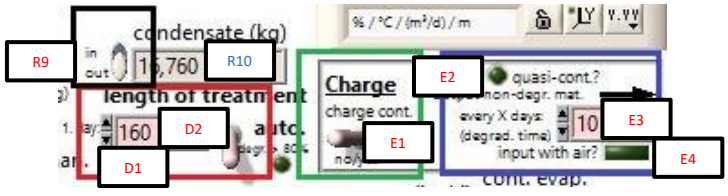


Figure 4-12: Inputs concerning process time, condensate and mode of operation (Zone D and E)

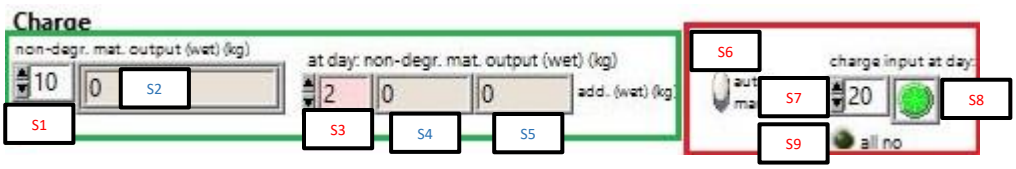


Figure 4-13: Further options for the times and amounts of inputs and outputs (Zone S)

The option to define the process time is likewise pointed out in Zone D, as shown in Figure 4-12 (marked in red). In the field of [D1], it is possible to define the process time by a fixed value. The switch in the red box must be flipped down for this purpose. A value (in days) can then be inserted in the pink field. For long processes, the simulation may take some time.

Furthermore, the program is able to find a value automatically by determination of the time at which 80 weight-% of the material is degraded. In doing so, the switch [D2] under Zone D has to be shifted upward (“auto.”). The start day should not be too wide away from the necessary day, to keep the simulation time short.

Anaerobic Digestion of Leaves:

- The length of the experiment was 70 days,
  D1 is set at **70** days.
- Since the experiment was batch process,
  E1 is then switch to **No**.

4.7 Configuration of the ventilation

The most important choice exists in case of the fundamental process: Without aeration, primarily an anaerobic degradation takes place (for example: alcoholic fermentation) and, with aeration, an aerobic degradation is simulated (for example composting). For adjustment, the switch [H2] in Figure 4-14 in the red box can be switched to either left or right ‘without aeration’. When the switch is turned to the right, an anaerobic process takes place; if it is turned to the left, an aerobic process is simulated by the program.

If the switch in the red box [H2] is flipped to left, an aerobic process is simulated. There are several possibilities to define the input of air. At first, there is the green rectangular button [G4] on the top right in the right brown box in Figure 4-14, which can be switched on or off. If it is switched on, it lights up in green. Modification of data can be executed in the area of the left brown box [G1*, G1-G3] (Figure 4-14). There is the opportunity to switch the pink slider on “file” [G1], which makes it possible to perform a continuous increase of the presetted values for ventilation. If the slider is switched on “man.”, the ventilation for every single day (“Time” corresponds to the days) can be specified. If the [G4] is switched off (no light), a continuous ventilation in m^3/h can be defined. The input field below “aeration rate max.” [G6] in the right brown box changes to a pink input field. In this case, it is feasible to tilt the switch [G4*] next to the field to simulate an ideal ventilation. This can be seen in the green box [G4**a-b]. The values are calculated according to the stoichiometry of the biochemical reactions. Additionally, the precision of the ventilation can be adopted. Therefore, the input field below “+/- x %” [G5] in the right area of the brown box can be used.

If the switch [H2] is flipped to an anaerobic process (right), there is still the possibility to simulate an input of air into the system. This is achievable by pressing the small button [H1] to be lit up in green. This simulates an anaerobic process with air introduction. The introduction of air is defined in the same way as in the aerobic process. Such a simulation can usually be described as a “failure”, for example because of leakage incidence.

Alternatively, the abovementioned ventilation can be adjusted for a defined time period under the yellow box in Figure 4-14. For this case, [D2] must be shifted upward so that the duration from beginning to the end can be defined in days. The opportunity to simulate a turnover for single days (“turn over at day:”) of the material is also possible in fields [H3-4]. Then, the pore volume of the material surface with 10 cm depth is simulated as gas volume.

Intermediate processes dependant on the amount of air and can also be simulated. Furthermore, it is possible to perform a change between aerobic and anaerobic (milieu condition) as shown in the blue box in Figure 4-14. With the help of the “before/after” [C7], the already degraded or the residual substrate from the specified day is displayed [C9]. If an aerobic process is simulated and the button “o.k.” [C8] has been pressed, the simulation will change to anaerobic and vice versa. With this feature, optimizations and changes in the process can be simulated.

Moreover, it is also feasible to define the relative humidity of the input air [G7] and air temperature [G8] as shown in Figure 4-14.

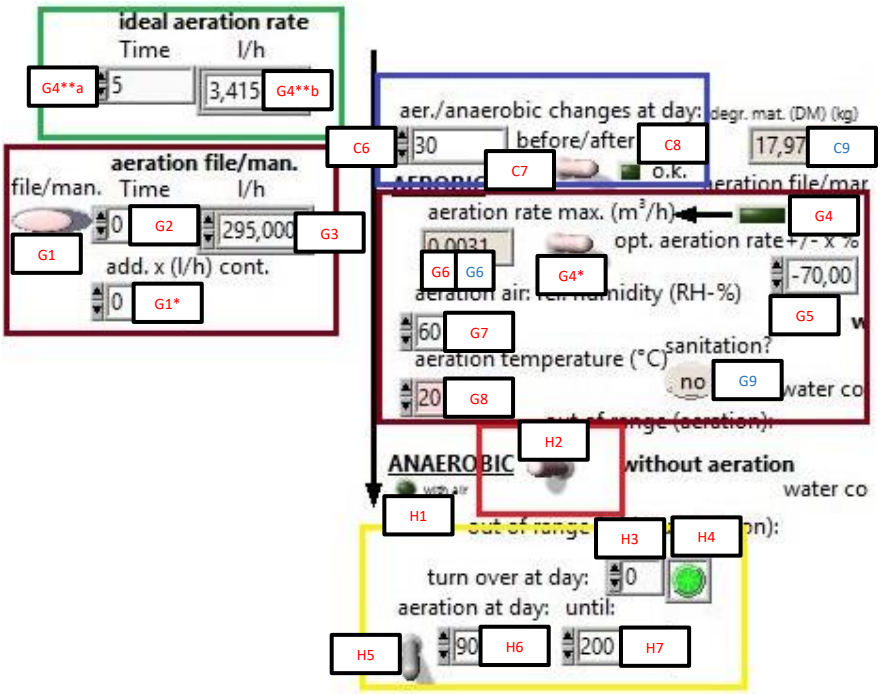
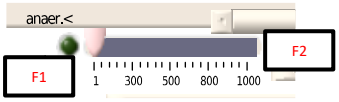


Figure 4-14: Inputs for process selection, aeration and turnover (Zone C, G and H)

Anaerobic Digestion of Leaves:

- Since fermentation happens in anaerobic condition (without air/oxygen), **H2** is switch to the **'right' (without aeration).**
- Since inoculum is added into the reactor at the beginning of the experiment,



F1 is switched **on (green light)**, whereas

F2 is dragged to the **most left** to indicate zero lag-phase.

4.8 Configuration of the water situation

The supply with water by precipitation or irrigation and evaporation can be simulated by SimuCF. Additionally, it is possible to calculate the missing amount of water for a water content of 50 weight-% and to keep this value on a constant level over the degradation time.

The adjustments for water supply and evaporation are demonstrated in Figure 4-15. In the red box, information about the evaporation can be entered at a specific time (indication of day and mass) [G10-12] or continuous (mass per day) [G13]. A combination is also possible. In the green box, the same configuration option for the water supply is given. Besides that, there is the possibility to simulate a recirculation of the evaporated water. Shift the switch [R9] in the black box in Figure 4-12 to "in". If there is no recirculation, then the switch is set to "out".

An automatic adjustment of the water content to 50 weight-% during the process is activatable by using the button [G15] next to "auto.". Furthermore, it is possible to define the temperature of the fed water by the button to the right of "temp. (°C)" [G16]. The control of the water content to 50 weight-% at the beginning of the process is feasible with the help of the button on the right side next to "cont. w. i." [G20].

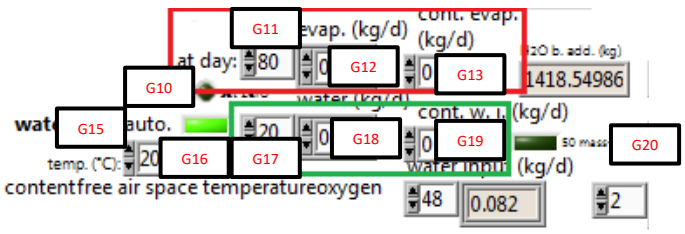


Figure 4-15: Configuration of the water situation (Zone G)

5 Output

After data processing, the presentation of the most important trends is displayed in a graphic form. Additionally, single values are shown. Connections between the data are clarified by the graphical representation and it allows a quick reading.

Enlargement and scaling of the axes are freely selectable in the green box as shown in Figure 5-1. Additionally, a visual adaption of the graphs can be performed by a right-hand click in the yellow box [P2] and right-hand click on the presentation surface [Q].

The time-discrete output occurs on a daily basis, but this can be changed to an output by month, hour or week. To estimate the amounts of gas and water, freights and the degradation and emission times for much smaller and bigger material quantities, the following Table 2 can be used:

Table 2: Conversion table for the assumed amounts of substrate and degradation times

Quantities multiplied by:	
10^{-3}	from days to hours
10^{3}	from days to weeks
10^{6}	from days to month

The calculated quantities must be multiplied with the given conversion factor from Table 2 to get an estimation of the changed quantities. The factors are valid for inputs and outputs and based on values from literature. The table can also be found in the interface under Zone K.

In addition to the graphical representation, the results of gas, water and solid material can be read as single values. All values can be exported.

5.1 Graphical output

There are six different options (physics, N/S/C balances, Nitrogen, S/N, gas/water, and gas (vol.%)) to illustrate the outcomes, which can be chosen through the red box [P1] in Figure 5-1 by the selection from a dropdown list. The legends are then displayed in the yellow box [P2].

5.1.1 Physical parameters

The physical parameters can be found at “physics”. This includes the degradation rate, ventilation volume, water content of the material, temperature inside the material, free pore volume, reduction of the material volume, height of the material, reduction of the organic dry matter and the water permeability of the material.

5.1.2 N/S/C balance

The diagram for nitrogen, sulphur and carbon balance includes the respective atoms in solid, water and gaseous phase in weight-%. The degradable solid material is considered here.

5.1.3 Nitrogen

The nitrogen diagram contains ammonium-N, nitrate-N and nitrite-N in the water phase and ammonia-N in the gaseous phase.

5.1.4 Sulphur/Nitrogen

In the diagram for the sulphur- and nitrogen compounds, the pH-values in the water phase, nitrous oxide (N_2O), produced nitrogen (N_2) and ammonia (NH_3) in the gaseous phase, total nitrogen (N), ammonium (NH_4^+), nitrate (NO_3^-), nitrite (NO_2^-) in the water phase, hydrogensulfide (H_2S) in the gas phase, sulphur (S) and sulphate-S (SO_4^{2-}-S) in the water phase are illustrated together.

5.1.5 Gas/Water

The diagram for the gas production and the water situation shows the gas quantities of methane (CH_4), hydrogen (H_2), carbon dioxide (CO_2) and oxygen (O_2). Additionally, the pH value, the acetic acid equivalent (AC_{eq}) in the water phase, the C/N ratio in the solid phase, the accruing amount of leachate (declared as “leachate” in the program), the quantity of surface water (not infiltrated water) and the amount of water in the material are calculated.

5.1.6 Gas (vol. %)

In this case, the percentage gas composition is illustrated. The oxygen (O_2), carbon dioxide (CO_2), nitrogen (N_2), methane (CH_4), hydrogen (H_2), nitrous oxide (N_2O), ammonia (NH_3) and hydrogen sulphide (H_2S) are displayed in percent by volume.

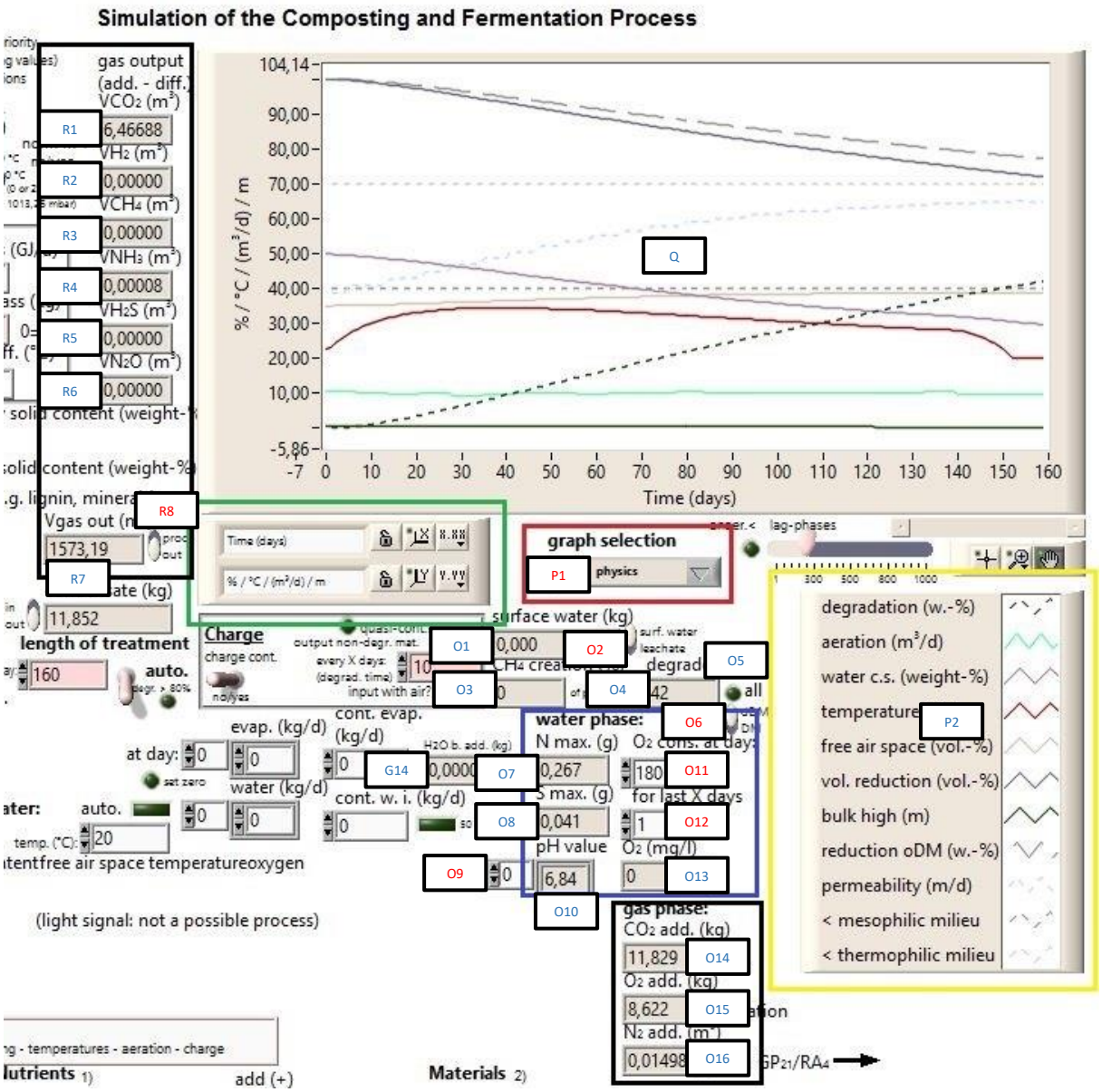


Figure 5-1: Graphical output and single values (Zone G, O, P, Q and R)

5.2 Output of single values

The single values, which are additionally readable, will be mentioned and described in the following part.

5.2.1 Water balance

The amount of leachate or surface water [O1] is shown underneath the red box in Figure 5-1. For this purpose, the virtual switch [O2] can be shifted between “surf. water” and “leachate”. On the left side next to the green box, the final amount of condensate [R10, shown in Figure 4-12] can be read.

A virtual switch can be shifted between “in” and “out” [R9] in that case. This defines whether the condensate is recycled or an output has taken place. In addition, the amount of water built via microbial degradation is defined as “H_2O b. add.” [G14] as shown in Figure 5-1.

5.2.2 Aqueous phase

The values for the water phase are shown in the blue boxes of Figure 5-1 and Figure 5-2. The pH value [O10] (adjustable with the arrow keys and readable for each day [O9]) and the maximum values of nitrogen [O7] and sulphur [O8] as well as the sum of consumed oxygen [O11] for a defined time period (from a defined day for the last x days) are outlined in the blue box shown in Figure 5-1. The maximum values for single compounds of nitrogen and sulphur [S10-14] are listed in Figure 5-2. The values refer to the gas phase and the water inside the material. If there is no leachate, an output does not happen.

5.2.3 Gas phase

The cumulative values for the oxygen consumption, formation of carbon dioxide and nitrogen production are shown in the program surface. This information [O14-16] is found in the lower black box shown in Figure 5-1.

Additionallly, the biogas formation with different references and the methane- and hydrogen production [S32-38] are also displayed, viewable in the bigger black box on the left side in Figure 5-2.

In the black box in Figure 5-2, down on the right, the total carbon emissions and the carbon emissions by carbon dioxide and methane formation (C, CO_2-C, CH4-C) [S63, S64 and S67] are listed. In the black box on top, the development of the hydrogen sulphide concentration in ppm [S52] is shown in addition to the graphical output. Thereby, a day [S51] can be chosen by using the arrow keys on the left.

Furthermore, the total gas emissions at the end of the process are shown for carbon dioxide [R1], hydrogen [R2], methane [R3], ammonia [R4], hydrogen sulphide [R5] and nitrous oxide [R6] in the black box as shown in Figure 5-1. In the same box, the cumulative total gas emission value or, alternatively, the produced amount of gas is displayed under ‘Vgas out (m^3)’ [R7]. The switch on the right side [R8] allows to change between “prod” and “out”. The cumulative total gas emission value contains emitted carbon dioxide and emitted molecular nitrogen and oxygen, molecular hydrogen, methane, ammonia, hydrogen sulphide and nitrous oxide. The produced amount of gas covers the produced carbon dioxide, produced molecular nitrogen, molecular hydrogen, methane, ammonia, hydrogen sulphide and nitrous oxide.

Since temperature, air pressure and water vapour pressure affect the gas volume, they are adjustable [A8-9] to standard conditions as shown in Figure 4-5. The values are then converted to 0 °C with air pressure of 1,013.25 mbar. The water vapour pressure is not considered. For a better comparability, the temperature is, likewise, changeable to 20 °C [A8] as well as the switch underneath “norm-l?” [A9]. This similar function could again be found in Zone S, [S27] as shown in Figure 5-2. If it is switched to the right (“yes”), the temperature is at 0 °C. Is it switched to the left (“no”), the temperature is at 20 °C.

5.2.4 Gas-formation potential and breathability

Under aerobic conditions, the oxygen consumption (RAx) and, under anaerobic conditions, the gas formation potential (GPx), are displayed in the red box in Figure 5-2. For an anaerobic process with aeration in a defined time period, the GPx and RAx is displayed [S26 and S30]. Time and measuring period can be chosen freely in both cases [S24-25, S28-29].

At a degradation of nearly 100 weight-% of the degradable dry matter, the potential is displayed. In other cases, the simulated process-specific gas formation or the oxygen consumption is shown.

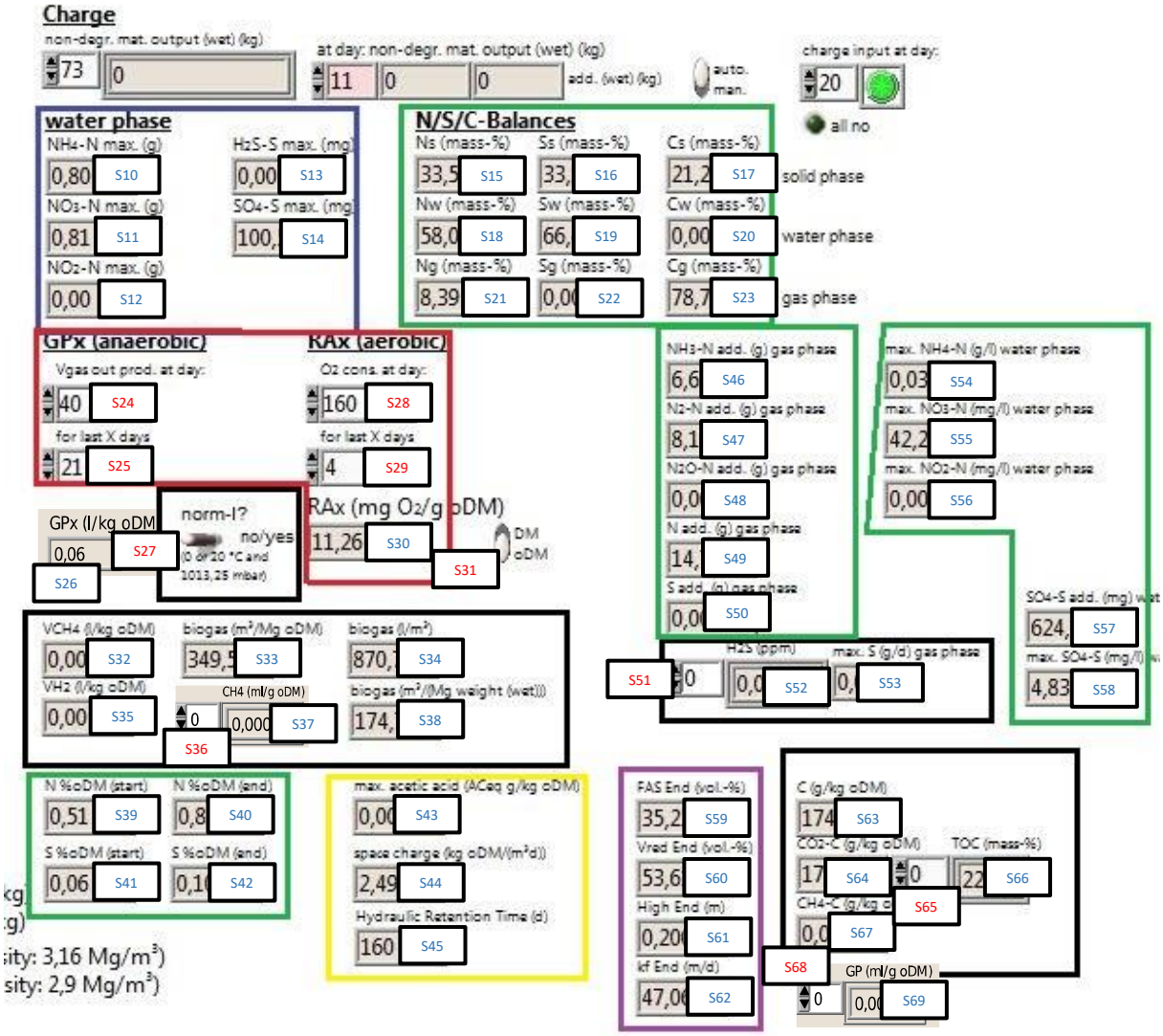


Figure 5-2: Output of single values (Zone S)

5.2.5 Output of the material values

For comparison with analytical data, the initial values of the organic percentage by mass of the dry matter [K14], the organic carbon (TOC) [K15] and the C/N ratio [K16] are given. These are illustrated in Figure 5-3.

To compare the results of the methane [K18] and carbon dioxide production [K20], the potentials [K19] (as maximal total values) are also described. They are calculated with the help of the input material and are displayed in cubic metre in standard state in the upper right box shown in Figure 5-3. The phosphorous (P) [K21-22] and potassium (K) content [K23-24] results from a correlation with the help of the nitrogen content and displayed below. From this follows that, if the input material contains no nitrogen, there are no values for P and K displayed. The same applies for the C/N ratio.

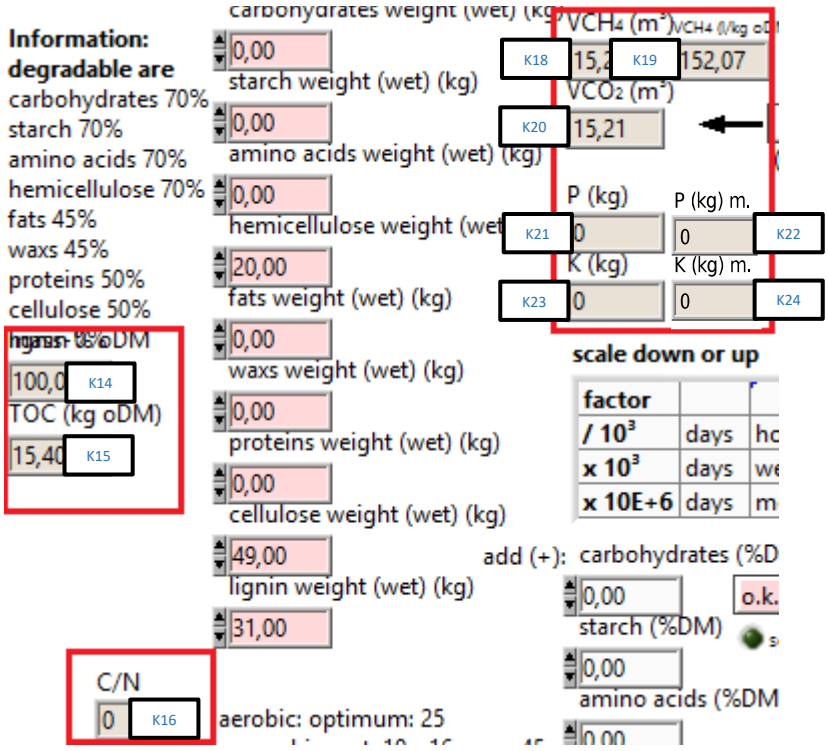


Figure 5-3: Output of material-dependent calculations (Zone K)

5.2.6 Degradation rate and methane formation

The degradation rate (or level of degradation) of the total material [O4] is given out by the simulation program and the aerobic and anaerobic process-specific achievable methane formation [O3]. Both are expressed as a percentage, shown in Figure 5-1. The green LED on the right side [O5] of the degradation rate lights up if any degradable material is degraded. The degradation rate can either be related to the degradable or the total material (switch below). Additionally, there is the possibility to adapt the degradation rate within the simulation program.

5.2.7 Nitrogen and sulphur values

The total nitrogen and sulphur contents are displayed for the beginning and the end [S39-42], shown in Figure 5-2 in the small green box down on the left. The values always refer to the dry matter at this point of time.

Likewise, the final values for the N/S/C balances of the degradable substrate in the solid, liquid, and gas phase [S15-23] are displayed in cumulative percent by mass in the upper area of Figure 5-2 in the green box.

Moreover, the nitrogen and sulphur emissions [S46-50] are displayed by the gas and water phase underneath the N/S/C balances in the green box. The gas phase contains the total emissions of

ammonia-N (NH_3-N), nitrous oxide-N (N_2O-N), di-nitrogen-N (N_2-N), nitrogen (N) and sulphur (S) as well as the hydrogen sulphide (H_2S) [S51-53], as daily emissions and the maximum sulphur emissions (max. S). The water phase is displayed in the green box next to it on the right and contains the maximum ammonia-N (max. NH_4^+-N), maximum nitrate-N (max. NO_3^--N), maximum nitrite-N (max. NO_2^--N) [S54-58], cumulative sulphate-S (SO_4^{2-}-S) [S57] and maximum sulphate-S (max. SO_4^{2-}-S) [S58] emissions.

5.2.8 Acetic acid, volumetric load and residence time

The maximum acetic acid concentrations [S43] during the simulated degradation and the volumetric load [S44] are similarly displayed in the program. They are shown in the yellow box of Figure 5-2. The residence time relates to the chosen or indicated degradation time [S45].

5.2.9 Further final values

The free pore volume (Vol.-%) [S59], volume reduction (Vol.-%) [S60], material height (m) [S61] and the calculated coefficient of permeability (m/d) [S62] are additionally indicated for the end of the process. The mentioned data are displayed in Figure 5-2 in the purple box down in the right corner.

If a sanitation [G9] has occurred or not is indicated in the area of process choice (see brown box on the right in Figure 4-14). There, a brown-grey output area in the middle underneath “sanitation?” displays “yes” or “no”. To fulfil the criteria of a hygenization, the process has to run 7 days at 65 °C or 14 days at 55 °C at the least.

6 Data Handling

6.1 Create logfile

This function is used when the simulation model created is preferred to be saved and for ease in opening the saved model in the future.

1. In order to create a logfile:

Operate > log at completion > run SimuCF > save the file at desired location

2. To open up a logfile:

Operate > Data logging > Log… > select a desired file > select "o.k." > back to SimuCF interface > Operate > Data logging > Retrieve… > Press a "tick" on the upper left of the SimuCF interface > all values from the logfile created previously would appear in the interface.

6.2 Data extraction

In order to extract the data:

Right-click on Zone Q > Export > select an option from the list

There are options such as:

- Export data to Clipboard
- Export data to Excel
- Export data to DIAdem
- Export Simplified Image

The data exported is dependant on the graph selection [P1] as shown in Figure 5-1.