

# Simulation software for biological processes in waste management (SimuCF)

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## **Abstract**

A literature review has shown that there is no software or model for simulation available for the aerobic and anaerobic degradation process for organic mixtures. The new software, SimuCF, can simulate the complex processes of aerobic, anaerobic, and combined treatments of organics such as waste with biogenic shares. This simulation software can be used to help answer energy- and emission-related questions in waste management facilities. This software can also be used for training courses.

## **Background**

Biogenic waste can be treated aerobically in composting systems and anaerobically in digestion systems. A combination of both systems, anaerobic digestion followed by composting, is e.g. frequently implemented in Germany. The optimization of the mentioned biological processes allows for example the reduction in energy consumption and the improvement of biogas production within a combined system. To be able to achieve an efficient and effective system the use of computer software can be highly beneficial. A literature review has shown that there is no software or model for simulation available for both, the aerobic and anaerobic degradation process for organic mixtures. Based on basic knowledge and findings in the literature, a new model, SimuCF, was developed. As software for programming LabVIEW™ was selected. The model structure is described. The developed software will allow future improvements like extended process integrations.



## ***Results***

The software SimuCF can simulate the degradation processes for biogenic substances on the computer to such an extent that statements regarding process sequences or process improvements can be made. This also includes the qualitative and quantitative description of the emissions during different degradation phases. The first validations by comparing simulated and empirically obtained values provided promising results for composting as well as for anaerobic digestion.

## ***Conclusions***

The software, SimuCF, can simulate the complex processes of aerobic, anaerobic, and combined treatments of organics such as waste with biogenic shares. This simulation software can also be used to help answer energy- and emission-related questions in waste management facilities. External environmental data and process inputs can simply be changed. Process optimizations reduced energy consumption and improved biogas generation and all other emissions. This software can also be used for training courses. Special adjustments are possible.

## ***Keywords***

simulation, model, software, App, biowaste, anaerobic, aerobic, composting, digestion, fermentation, degradation process, organics, waste, biogas, emission, energy, global warming

## 1. Introduction

Biological processes play a significant role in biogas and composting facilities and are important elements of waste management systems in many regions. In biogas facilities, the anaerobic biological processes are dominant, in composting facilities the aerobic. Biowaste can be used as an input feedstock for both process types. In the European Union (EU) separate biowaste collection became increasingly important with the transition towards bio-economy. With this, more efficient use of material and energetic utilization is the aim (European Commission, 2015) [1]. The combination of anaerobic and aerobic processes can enhance efficiency – both, energy-rich biogas and humus-rich compost can be produced. Combinations of both processes are increasingly being applied in biowaste treatment. For instance the German federal statistical office (Statistisches Bundesamt, 2018) [2] has counted a total of 849 solely-working composting plants in 2016 and 295 biological gas facilities and facilities combined aerobic and anaerobic processes. Combination plants were legislatively pushed by subsidies with the intention of increasing the output of renewable energy (Renewable Energy Law: EEG, 2017) [3]. Combined aerobic and anaerobic processes also occur in other areas of waste management, e.g., in plants for mechanical-biological waste pretreatment in landfills.

This work aims to present a tool (SimuCF) which can simulate the microbiological and biochemical processes of aerobic and anaerobic degradation processes. The background of the model development in more detail is described in Deipser (2014) [4]. All examples are from the area of waste management. The first example provides a comparison of simulated and laboratory results for a composting process. In the second and third examples, data for biogas production from literature and results from practice are shown in comparison. Examples of SimuCF applications includes the qualitative and quantitative description of the emissions during the different degradation phases in individual anaerobic digestion and composting processes and also in the combination process. A further application could be the use in education and training.

### 1.1 Overview of models and simulations

A comprehensive survey about models and simulations in the field of waste management was documented in (Deipser, 2014) [4]. In the following section, an overview is given.

### 1.1.1 Simulation models of aerobic biological waste management

The focus of present publications on simulation and modeling in the management of biological waste relies on composting (e.g. Haug, 1980 [5], Bach et al., 1987 [6], Nakasaki et al., 1990 [7], Kaiser and Soyez, 1990 [8], Soyez et al., 1995 [9], Hamelers, 2004 [10], Lin, 2006 [11], Woodford, 2009 [12]). Detailed reviews of simulations and modeling of aerobic biodegradation processes with associated physical and chemical environments and the problems and limitations are described in Fletcher et al. (2000) [13], Scholwin (2005) [14] and Mason (2006) [15]. An overview of process modelling relevant to the overall process and essential sub-processes of composting are presented and discussed in detail in Scholwin (2005) [14]. Simpler models calculate the biodegradation of the substrate based on empirical formulas derived from laboratory or environmental data. Examples of determining the reaction kinetics of oxygen consumption, carbon dioxide production or carbon emissions during composting under laboratory conditions are given by Seng and Kaneko (2011) [16], Papracanin and Petric (2017) [17], Tripathi and Srivastava (2012) [18], Stark (1995) [19] and Krogmann (1994) [20].

#### *Complex composting process*

For the complex composting process, no work is known in which a completely deterministic model was developed. Due to the heterogeneity of organic wastes and the complex physical, biological and biochemical processes, creating such a model does not appear realistic, so that simplified assumptions must be made to varying degrees. The complexity of the models can be very different. The most complex deterministic models for the biodegradation process include the entire process from cell growth to cell death (e.g., the models of Haug, 1993 [21] and Kaiser, 1999 [22]).

#### *Flow simulation models of ventilation*

Due to the heterogeneous porous storage structure of organic waste in the aerobic biological treatment, the mathematical description of the air flow through the waste matrix is hardly possible. In the field of biological waste treatment, only highly simplified models are used for airflow in forced-ventilation systems (Scholwin, 2005) [14]. Many authors tend to detect the airflow only indirectly, namely by mass balancing of the gas flow (Haug, 1993 [21], Kaiser, 1999 [22], Mohee et al., 1998 [23]).

### *Thermodynamical simulation models*

Not specific to waste treatments are the heat transfer and drying processes which must be considered respectively. Since the temperature has a decisive influence on the degradation activity of microorganisms, the computation of thermodynamics is a major component in many models (e.g., Keener et al., 2002 [24], Lomax et al., 1984 [25], Hsieh et al., 1997 [26]). The calculation includes information about the amount of heat supplied to the system with the supply air, the amount of heat removed by the exhaust air, the amount of heat released by biodegradation and the amount of heat lost to the system by heat conduction (Mohee et al., 1998 [23], Kaiser, 1999 [22]). The heat release can be calculated from the stoichiometric calculation of the degradation process, or it can be derived empirically from measurements (Scholwin, 2005) [14].

### *Simulation models of the water balance*

The water balance was used to model the biodegradation process by various authors (Nakasaki et al., 1987 [27], Haug, 1993 [21], Stombaugh and Nokes, 1996 [28], Hsieh et al., 1997 [26], Das and Keener, 1997 [29], Mohee et al., 1998 [23], Kaiser, 1999 [22]). The water content in the material, the water content in the supply and the exhaust air, as well as the specific water release during biodegradation for system sections or for the entire system, were taken into account.

## **1.1.2 Simulation models of anaerobic biological waste management**

There is a broad variety of mathematical models for the description of anaerobic digestion (continuous and discontinuous wet and dry fermentation), considering biological and physicochemical processes. An overview is given by, e.g. Echiegu (2015) [30], Demirel and Yenigun (2002) [31], Gall (1999) [32], Husain (1998) [33], Mata-Alvarez et al. (2000) [34] and Pavlostathis and Giraldogomez (1991) [35].

The aim of the model is mostly to calculate the biogas yield (e.g. Beba and Atalay, 1986 [36], Hashimoto, 1982 [37], Gunaseelan, 2004 [38], Hashimoto, 1984 [39], Chen 1983 [40], Mather, 1986 [41], Moller et al., 2004 [42]) and the description of other economic, technical and legal considerations (e.g., on material and energy balances) (e.g., Biogas 2000 [43], Langhans, 1997a [44], Langhans, 1997b [45], Mähnert, 2007 [46], Mertens et al., 1997 [47] and Mertens, 2001 [48] (as a concept for a combined composting and fermentation plant), KTBL, 2012, [49]). The models

are usually very specific to the kinetics of individual process variables (e.g., methane production, pH value, ammonium content, hydrogen sulfide emission, volatile carboxylic acid content) and often derive from wastewater management (sewage sludge digestion) and fermentation of manure in rural areas (wet fermentation).

The Working Group of the International Water Association (IWA) "Anaerobic Digestion Modeling" published a unified ADM1 model (IWA Anaerobic Digestion Model No. 1 (ADM1)), which includes a total of 19 process steps and 24 soluble components for wet fermentation (Batstone et al., 2002) [50]. Since then, the ADM1 model or parts thereof have been applied to complex processes on several occasions (e.g., Blumensaat and Keller, 2005 [51], Batstone and Keller, 2003 [52], de Gracia et al., 2006 [53], Jeong et al., 2005 [54], Nopens et al., 2009 [55]).

The models for the anaerobic utilization of liquid and solid substrates contain different emphases and differentiation. The bacterial growth and the substrate consumption are partly considered separately concerning substrate components such as volatile fatty acids (Vavilin and Lokshina, 1996) [57] or product components such as pyruvate formation by *Escherichia coli* (Zelic et al., 2004) [58]. The controlled supply of microorganisms with nutrients could not be modeled so far (Amon et al., 2003) [59].

A substrate and product inhibition by, e.g., acetate and propionate in anaerobic digestion in batch experiments were considered by a model with undissociated acid inhibition (Mosche and Jordening, 1999) [60].

For the growth of microorganisms in the methane fermentation, the use of the Monod equation is possible because all stages of degradation can be attributed to enzymatic reactions. Models from anaerobic wastewater management have also shown that the degradation kinetics of methanogenesis can be described very well with the Monod equation (Kroiss, 1986 [61], Linke and Kalisch, 1983 [62]). However, also first-order reactions for equilibrium states and the equations according to Haldane, Michaelis-Menten, Contois, and Arrhenius are used.

Also the fermentation of renewable raw materials became increasingly important. Literature data on biogas and methane yields from liquid manure and renewable raw materials show wide fluctuation ranges and are often not comparable with each other due to different reference quantities, normalizations, processes or process temperatures (Wilfert and Schattauer, 2003 [63], FNR, 2009 [3]). Mähnert (2007) [64] developed a model for the production of biogas from

renewable raw materials and liquid manure at any mixture and fermenter load in the mesophilic and thermophilic range, which still needs to be checked for reproducibility. In addition, substrate and process-specific parameters such as the maximum biogas yield, feed concentrations, density of the biogas and the reaction rate constants for other substrates and temperatures are to be determined additionally in the laboratory.

Due to the variety of substrates and the complex relationships of the anaerobic degradation processes, especially the supply of microorganisms with nutrients in solids, however, models cannot yet replace the laboratory experiments. The existing dynamic models for describing material turnover can only be used to a limited extent for solving real problems such as the planning and dimensioning of biogas plants (Radke, 2000 [65], Amon et al., 2003 [59]).

### **1.1.3 Simulation models for landfills**

There are also numerous publications regarding landfills in which gas, water and mass transport processes in various types have been investigated mathematically and empirically (e.g., Pommier et al., 2008 [66], Haarstrick et al. 2001 [67], Haarstrick et al., 2004 [68], El Fadel et al., 1996 [69], Findikakis et al., 1988 [70], Findikakis and Leckie, 1979 [71]). For the mathematical modeling, there are many proven software programs (e.g., Help, Rohaldep, Bowahald, Hydrus, Stanmod, SiWaPro DSS, Smart), which mainly serve the leachate forecast. The focus relies on spatially and discrete-time calculations of possible emissions. The accuracy and complexity of the models are different.

### **1.1.4 Summary of the state of the art**

In summary, there appears to be a lack of research regarding the thermophilic phase in composting models as well as concepts of passive ventilation. Temperature correction factors are included in almost all models. Correction factors for humidity, oxygen availability and free pore volume can be found in some models. Empirical correction factors exist for the humidity and the carbon/nitrogen (C/N) ratio. Theoretical correction factors are used for temperature and oxygen availability.

The mathematical models of the composting process are essentially based on heat and mass balances with respect to time in selected cases. A deterministic approach is always present; stochastic influences are less often incorporated. The energy from biodegradation processes was

modeled in all publications by a first-order reaction, Monod (Haldane inhibition), Michaelis-Menten, Contois, Arrhenius, or empirically obtained heat transfer factors. No model can predict the maximum or average temperature or spontaneously occurring short-term temperature increases with precise time and temperature accuracy.

The comparison of mathematical models of the composting process shows that further data on the specific degradability of substrates would be desirable. Associated with this, data on the development of temperature and moisture during the degradation of different substrates in combination with the different adhesive properties of water would also be helpful.

The models for the anaerobic utilization of liquid and solid substrates are mainly focused on the possible formation of methane or undesirable emission potentials (e.g., smell and hydrogen sulfide). But the utilization of organic wastes and the possibility of an anaerobic pretreatment of different material flows, also for those the composting are unsuitable, should process-technically be considered and be able to be simulated.

## **1.2 Conclusions for the development of SimuCF**

The simulation model, SimuCF, shall reduce the restrictions of existing simulations and models and represent the connections in an easy-to-use software. Furthermore, it should be able to serve as an alternative to time and resource-expensive laboratory experiments which are the main reason for the development of SimuCF. Moreover, a strict separation between aerobic and anaerobic biodegradation processes can rarely be observed. Hence, it seems plausible to also consider the possible processes simultaneously in the simulation and thus make it possible to simulate a large number of variants.

## **2. Methods**

For the production of a simulation software first basic conditions must be considered. They are described in the following.

### **2.1 Creating of the SimuCF model**

For the simulation of aerobic and anaerobic biological degradation processes mathematical and physical correlations and reaction equations from the basic fields of chemistry, biochemistry, microbiology, and physics were almost exclusively used. Only a few empirically obtained

mathematical equations were applied for the description of correlations equating to 42 equations in total. These do not include the stoichiometric reaction equations which were however used additionally as a basis of the program. Altogether, the reactions and equations are documented in detail in Deipser (2014) [4].

The simulation program was written with LabVIEW™ from National Instruments (company: www.ni.com). The programming environment of LabVIEW™ is, above all, employed in the instrumentation, control, and automation technology. It contains graphic programming elements which are composed of virtual instruments (VIs). The VIs consists of a front panel and a block diagram. The front panel functions as user interface where input and output values can be entered. The block diagram contains the graphical program code and processes the input values from the front panel. The verification of the program was finished during programming. The simulation results were compared thereby on correctness with observed values and balances were accomplished. The program code is compiled with the intention to be comparable with other high-level programming languages (e.g. Fortran, PHP, C).

## 2.2 Validation of the SimuCF model

For validation purposes, simulated and empirically obtained values were compared. The considered sectors were composting as well as biogas generation and digestion. Three sample applications are in this publication. The empirically obtained values were taken from a scientific laboratory experiment in technical scale conditions. A further dataset was collected from the scientific literature and represents values obtained under practice conditions.

The following validations were carried out:

- *Validation for an aerobic composting process:* Exemplarily, the composting validation is shown based on a laboratory experiment. It was implemented by comparing simulated values with experimentally gained data. The laboratory experiment was carried out in a system with 100 L reactors, documented by Körner (2008) [72]. In the experiment, a model waste was used which characterized a biowaste, mainly composed of easily degradable kitchen waste compounds. The results are shown in chapter 3.1.
- *Principal validation for anaerobic fermentation processes:* In this case, in chapter 3.2, the simulated values were compared with the common trends from anaerobic digestion and

the observed development tendencies of the gases by large quantities of organic wastes known from literature.

- *Specific validation of biogas generation:* For the validation of SimuCF with regard to the biogas quantities, large-scale produced biogas quantities from real biowaste fermentation plants, which work according to the wet process, were used and compared with the simulation on the basis of their process descriptions in the literature. Of the three plants “Nottensdorf” (Poetsch, 2005) [73], “Kehlheim” (Hoppenheidt et al., 1998) [74] and “Karlsruhe” (Gallert et al., 2002) [75], the key biogas indices were available for comparison and validation. The results are shown in chapter 3.3.

### 2.3 The simulation model with in- and output parameters

The structure of SimuCF is in more detail described in the following. The chapters are front page, value input, simulation model, value output and characteristics.

#### 2.3.1 Front page of SimuCF

The simulation software allows the user to input data and to view outputs via the front page (Figure 1).

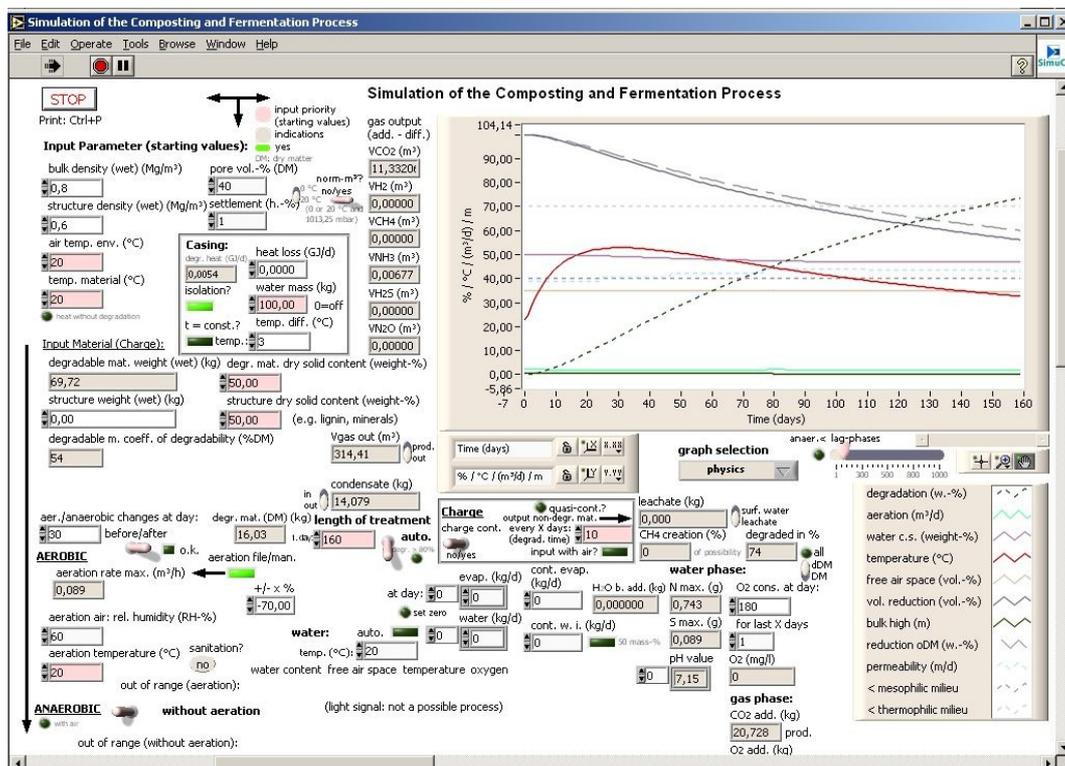


Figure 1: Part of the front view panel of the SimuCF software with input and output boxes

Table 1 and 2 summarizes (chapter 2.3.2 and 2.3.4) the model input parameters and the output options. In SimuCF, the input fields and the output diagrams are displayed over one front view page. The initial and the resulting parameter are connected in manifold calculations. The user can choose between many operation modes by setting their own values, e.g., for treatment times and conditions, material types and properties or users can choose pre-settings from the software. The simulation model operates in the background and follows an iterative approach (Deipser, 2014)[4].

### 2.3.2 Value input

An overview on the manifold input options is presented in Table 1, subdivided into basic parameters describing the input substrate, additional information for an advanced description of the input material and information to the treatment facility and the process operation there.

<b>VALUE INPUT INTO SIMUCF</b>
<b>basic material information</b>
<i>as dry or wet weight (in kg or weight-%)</i>
<b>pure materials</b> straw, wood, leaf, grass, fruits, potatoes, vegetables, grain, legume, meat, fish
<b>mixed materials</b> sewage sludge, green waste, mixed household waste, biogenic household waste (biowaste), wastepaper
<b>→ conversion into chemical composition data</b>
<i>automatic by use of entered data or direct input (in kg wet weight)</i>
carbohydrates (all types), starch, amino acids, hemicelluloses, fats, waxes, proteins, cellulose, lignin
<b>surcharge material information</b>
<i>as initial and time-exact defaults</i>
<b>physical material properties</b>
bulk density (of materials and structure material) – <i>in Mg wet weight / m<sup>3</sup></i>
pore volume – <i>vol.- % dry weight</i>
initial material temperature (in the range between 10 and 80 °C) – <i>in °C</i>
Settlement – <i>height-% over all</i>
<b>additional chemical properties</b>
<i>in mg/kg organic dry material</i>
ammonium, nitrate, sulphate content (time-exact defaults)
<b>surcharge materials</b>
structure material and sand (initial as kg wet weight) lime (kg dry weight), methanol (kg), ferric-(II or III)-chloride (kg) (time-exact defaults)
<b>facility and process information</b>

<b>bulk or reactor form</b>
<i>dimensions: height, width, length or diameter – in m; if necessary angles</i>
triangle or trapezoid front shape, cylinder, drum, sphere, box
<b>bulk or reactor tempering</b>
isolation, keeping at a given temperature, adjusting with reactor heating or higher
<b>process modes</b>
<i>as initial and time-exacts defaults</i>
batch, loads (interval), quasi-continuous
anaerobic, aerobic without and with ventilation: constant, optimal or direct defaults (in m <sup>3</sup> /h) ventilation temperature and humidity (in °C and RH-%)
water situation (water additions with water temperature (in °C) and evaporation (kg)) process-lengthens (automatic or default)

Table 1: Summary of the possible input data for the simulation model SimuCF with selection options

Important basic information regarding the material such as composition and proportions and supplementary information on the condition of the plant and the surrounding conditions influence the simulation result. The composition of the substrate exerts the greatest influence. The input of basic material values can take place as weight or optionally in percent on wet or on a dry weight basis. In SimuCF, some exemplary pure materials were given as selection. The provided selection was based on model wastes investigated by Körner et al. (1999) [76]. Körner et al. (1999) [76] also gave the chemical composition of these materials. Furthermore, the typical waste groups were included as mixed materials whereby example compositions were taken from Krogmann (1994) [20]. Data obtained from the literature were included and used for the simulations. Besides using values for the chemical composition from a database, the user can also choose to make a direct input of chemical composition data. Surcharge material information can be added to improve simulation outputs. This includes information on physical material properties as well as more specific chemical parameters. The properties and content data can be entered as initial values or, if needed, also as time-exact defaults (water in- and output, active or passive aeration, loads, surcharges) during the process.

Besides material data, information to the facility and process type can also be entered into SimuCF (Table 1). The bulk or reactor form of the material can be chosen for treatment. The

form can be described in more detail by the provision of the dimensions. Furthermore, it is possible to enter information regarding temperature conditions.

### 2.3.3 The simulation model

The model simulates the basic aerobic and anaerobic microbiological degradation processes using suitable substantial physical, chemical and biochemical equations and reactions. The calculations begin with the division of the dry material weight into “degradable” and “not (or hardly) degradable” portions. The “degradable portions” are assigned to three main compound groups of macromolecules: carbohydrates, proteins, and fats. The “not degradable portions” are subdivided into organic (e.g., lignin) and inorganic material (e.g., sand). Subsequently, further categorization is given such as that shown in the following model molecules: carbohydrates ( $C_6H_{12}O_6$ : easy degradable), proteins ( $C_{70}H_{110}O_{20}N_{20}S$ : moderately degradable) and fats ( $C_2H_5-COOH$ : difficult degradable) (e.g., Ottow, 1997 [77], Bekker, 2007 [78]). The share of degradable carbohydrates, proteins, and fats can be varied in the program. In addition, the different degradability extents of the organics under aerobic and anaerobic process conditions can be considered in the simulation program as a delay in growth of individual microorganism groups (acetic acid, hydrogen, carbon dioxide and methane creating microorganisms).

#### *Equations and calculations*

The modeling of the degradation rate and growth delay follows the approach of Monod (1949) [79] for both aerobic and anaerobic degradation models. The Monod kinetics is a rate model describing the dependence of the specific growth rate on the limiting substrate concentration. It results from the consideration of microbial growth since all enzyme reactions taking place in the cell.

In principle, the growth rate of continuously cultivated crops can also be transferred to degradation processes in microbiological waste treatment, such as composting and digestion or fermentation, because substrates are constantly being replicated or made available due to diffusion, transport, and dissolution processes such as hydrolysis (Kroiss, 1986 [61], Linke and Kalisch, 1983 [62]).

$$\mu = \mu_{max} \cdot \frac{c_S}{K_S + c_S}$$

- $\mu$ : Growth rate (1/Zeit)
- $\mu_{max}$ : Maximum growth rate (1/Zeit)
- $K_S$ : Substrate concentration, in which the growth rate is half of the maximum value (mass/volume)
- $c_S$ : Substrate concentration (mass/volume)

In this equation the growth rate of an idealized bacterial culture is shown. If the substrate concentration ( $c_S$ ) is significantly higher than the substrate concentration, at which the growth rate has reached half of its maximum value ( $K_S$ ), then it is a zero-order reaction. So the growth rate ( $\mu$ ) of the microorganisms is independent of the substrate concentration and almost maximum. If the substrate concentration ( $c_S$ ) is significantly lower than  $K_S$ , a first-order reaction is applied, i.e., an exponential growth rate, which means that the growth rate of the microorganisms ( $\mu$ ) is dependent on the substrate concentration ( $c_S$ ) (Lexikon der Chemie, 2000) [80]. It does not cover the specific sequence of microorganism species (e.g., succession in composting) or the different microorganism species in the different stages of digestion or fermentation.

Theoretical degradation rates for the three compound groups (carbohydrates, proteins, fats) and the delays are counted. The resulting curve computed in addition from each point of the curves. The calculated principal degradation rates are adjusted to more reality-close outcomes by consideration of different substrate-specific aspects. The delays are implemented in SimuCF for automatic use if the environmental conditions for the chosen process are incorrect and by the possibility to use the setting "lag-phases" and by the consideration of the total quantity of the material ("quantity delay"). The "quantity delay" considers the different availability of nutrients due to influence on transportation. The equations and calculations are descriptive in Deipser (2014) [4].

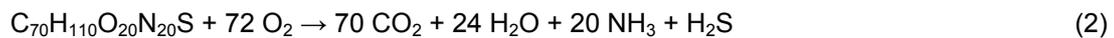
From specific importance is the consideration of the material degradation in dependence on the availability or absence of oxygen. For that reason, both types of degradation processes (for

aerobic and anaerobic environments) are included. In case of anaerobic milieus, the three major steps (acidogenesis, acetogenesis and methanogenesis) are considered separately. The main stoichiometric model reaction equations which are used in SimuCF and which are the basis of the calculations are listed below:

*Aerobic reaction equations*



glucose + oxygen → carbon dioxide + water



model protein + oxygen → carbon dioxide + water + ammonia + hydrogen sulphide



propionic acid + oxygen → carbon dioxide + water



acetic acid + oxygen → carbon dioxide + water



methanol + oxygen → carbon dioxide + water

*Acidogenesis – Acetogenesis*



glucose + water → acetic acid + carbon dioxide + hydrogen



model protein + water → acetic acid + carbon dioxide + hydrogen +  
ammonia + hydrogen sulphide



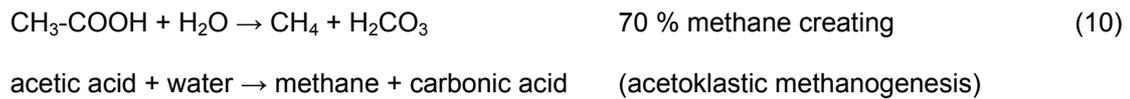
propionic acid + water → acetic acid + carbon dioxide + hydrogen

*Methanogenesis*



hydrogen + carbon dioxide → methane + water (hydrogenotrophic methanogenesis)

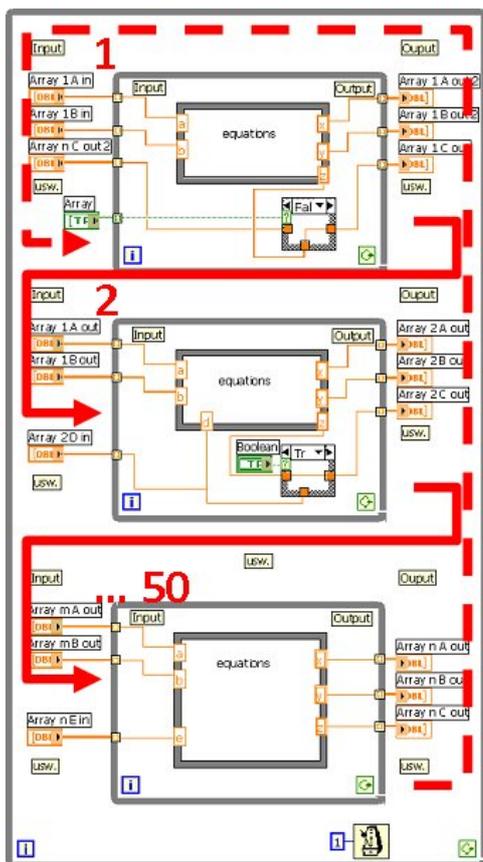




Using SimuCF, all material inputs and molecule amounts can be calculated. Based on the molecule data and the equations (1) to (11), all emissions of aerobic and anaerobic degradation processes can be computed. Only if all molecules for a reaction are present, a reaction takes place, and a calculation is carried out. In addition, SimuCF checks if the milieu conditions regarding water content, free airspace, temperature, pH as well as oxygen, hydrogen, hydrogen sulfide and ammonia concentration are in a feasible range for the aerobic and the three anaerobic processes. If not, the reaction cannot take place and is therefore not considered in the calculations.

In the simulation model, special attention is given to the water balance, thermodynamics, and ventilation conditions. The changes of the physical parameters such as temperature, humidity and the porous structure, which affect the milieu conditions and with it the biological dismantling processes, can be determined in this way with 53 equations for each time step (Deipser, 2014) [4].

The program essentially consists of iteration loops, in which reaction equations, physical functions, and other defaults are processed (Figure 2). The mutually affecting parameters again compute themselves for each time step. The computations are accomplished by feedbacks of initial values until a stable condition is reached (dynamic simulation).



### Explanations to the block diagram

The program consists of an infinite iteration loop. It contains further iteration loops, logical regulators and limits.

During the program run, the default values are used for the calculations. By converting all non-physical parameters into moles, the decomposition and inhibition functions can be used to form value arrays (two-dimensionally arranged similar data) for the given time. Dependent on this, the chemical and physical parameters such as temperature, water content and pH development also are summarized in arrays.

Further influences such as flow conditions, heat development and reaction limits are processed in subsequent iteration loops (approx. 50) with the corresponding functions and specifications.

The extensive logical rules, for example, to comply with the specified procedures and materials take place according to their tasks in or outside the iteration loops.

Figure 2: Schematic block diagram with iteration loops for reaction equations, physical functions and other defaults

### 2.3.4 Value output

The output of the result values of simulation is extensive and different. Table 2 summarizes the comprehensive output parameters, which can be obtained after SimuCF analysis. They can be chosen on the users demand.

VALUE OUTPUT FROM SIMUCF
<i>time-exact and maximum or added values</i>
<b>physical material parameter</b>
degradation rate (weight-%), ventilation (m <sup>3</sup> /d), water content (weight-%), temperature (°C), free pore volume (vol.-%), volume decrease (vol.-%), height decrease (m), reduction of the organic dry solid content (weight-%), water permeability (m/d)
<b>chemical material parameter</b>
<b>N/S/C balances</b>
nitrogen/ sulfur/carbon in the solid, water and gas phase (mass-%)
<b>Nitrogen</b>
ammonium-N (NH <sub>4</sub> <sup>+</sup> -N)(mg/L), nitrate-N (NO <sub>3</sub> <sup>-</sup> -N)(mg/L), nitrite-N (NO <sub>2</sub> <sup>-</sup> -N)(mg/L), ammonia-N (NH <sub>3</sub> -N)(g/d)

<b>sulfur/nitrogen</b>
dinitrogen oxide (N <sub>2</sub> O) (m <sup>3</sup> /d), produced dinitrogen (N <sub>2</sub> ) (m <sup>3</sup> /d), ammonia (NH <sub>3</sub> ) (m <sup>3</sup> /d), total nitrogen in water (N) (g/L), ammonium (NH <sub>4</sub> <sup>+</sup> ) (g/L), nitrate (NO <sub>3</sub> <sup>-</sup> ) (mg/L), nitrite (NO <sub>2</sub> <sup>-</sup> ) (mg/L), hydrogen sulfide (H <sub>2</sub> S) (m <sup>3</sup> /d), sulfur in the water (S) (mg/L), sulfate-S (SO <sub>4</sub> <sup>2-</sup> -S) (mg/L), pH correl.
<b>gaseous and liquid emission</b>
<b>gas/water</b>
methane (CH <sub>4</sub> ) (m <sup>3</sup> /d), hydrogen (H <sub>2</sub> ) (m <sup>3</sup> /d), carbon dioxide (CO <sub>2</sub> ) (m <sup>3</sup> /d), oxygen (O <sub>2</sub> ) (m <sup>3</sup> /d), pH value, acetic acid equivalent (ACeq) (g/L), C/N relationship, leachate (kg/d), surface water (kg/d), water in the material (kg/d)
<b>gas (vol.-%)</b>
oxygen (O <sub>2</sub> ), carbon dioxide (CO <sub>2</sub> ), nitrogen (N <sub>2</sub> ), methane (CH <sub>4</sub> ), hydrogen (H <sub>2</sub> ), dinitrogen oxide (N <sub>2</sub> O), ammonia (NH <sub>3</sub> ), hydrogen sulphide (H <sub>2</sub> S)
<b>water phase</b>
max. nitrogen (N) (g), max. sulfur (S) (g), oxygen consumption (mg/L) of the last x days starting from reference day y, pH values max. ammonium-N (NH <sub>4</sub> <sup>+</sup> -N) (g), max. nitrate-N (NO <sub>3</sub> <sup>-</sup> -N) (g), max. nitrite-N (NO <sub>2</sub> <sup>-</sup> -N) (g), max. hydrogen sulfide-S (H <sub>2</sub> S-S) (mg), max. sulfate-S (SO <sub>4</sub> <sup>2-</sup> -S) (mg)
<b>methane formation</b>
in percent related to the base substances acetic acid, hydrogen, and carbon dioxide: possible methane formation and calculated in m <sup>3</sup> and L/kg organic dry material
biogas (m <sup>3</sup> /Mg organic dry material, L/(m <sup>3</sup> ·d), m <sup>3</sup> /wet weight)
max. acetic acid concentration (ACeq g/kg dry organic material alternatively dry material)
<b>further output values</b>
leachate accumulation and surface water and/or expiration, water condensation, metabolic H <sub>2</sub> O
respired oxygen in mg O <sub>2</sub> /g organic dry material alternatively dry material
hygienization yes/no (at least 7 days 65 °C or 14 days 55 °C)
C/N-relationship - N/S/C-balance values in the solid, water and gaseous phase (mass-%)

Table 2: Summary of the output options of the simulation model SimuCF for aerobic and anaerobic degradation processes

Output values can be recalled as sum values or single values in tables or as diagrams. In this way, the physical and chemical material parameters, the parameters concerning gaseous and liquid emissions including the formation of methane as a product can be presented.

The simulation model indicates the complex relationships during the biological treatment of waste materials that contain carbohydrates, proteins and/or fats. The software SimuCF can, e.g., help to find process optimization approaches for both the aerobic treatment (composting) and the anaerobic biogas production (fermentation). Furthermore, conditions for changing milieu parameters, e.g., ventilated landfills or in combined treatments such as anaerobic fermentation followed by aerobic processes, can be simulated. Questions over the whereabouts of the nutrients

carbon, nitrogen and sulfur in the different treatment phases can be answered, also in comparison of different settings.

### 2.3.5 SimuCF characteristics

In summary, the simulation software can be characterized as follows:

- The software simulates aerobic and anaerobic microbiological, physical and chemical and/or biochemical processes in solids with a water content < 80 weight-% (dry fermentation). In addition, the simulation of wet fermentation is possible, if physical differences were not considered as crucial.
- The gas flow through a single-layer material is considered. The simulation of materials with different mixes, quantities, and forms is possible. The thermodynamics (heat conduction, thermal radiation, and convection) and the water balance are considered as well. The spatial distribution of the state parameters remains unconsidered (continuity of space).
- Five substance groups are considered: carbohydrates, proteins, fats, non-/hardly-degradable organic substances and inorganic substances (minerals). The basic constituents that are contained in a considered substrate must be assigned to these groups. The organic part of the material is further subdivided into carbohydrates (total of various types), starch, amino acids, hemicelluloses, fats, waxes, proteins, cellulose, and lignin, depending on the degradability.
- For carbohydrates, proteins, and fats different microbiological degradation curves are included in the model, following approximately Monod kinetics, whereas also degradation delays (lag-phases) can be selected. The amount of material is also considered as a time delay factor, to include solution, transport, and diffusion processes.
- Considering specified limit values, the program can automatically search the maximum degradation rate at a total given degradation time. Optionally the degradation time can be searched by the program with given minimum degradation rate.
- For selected organic fractions (e.g., straw, wood, bark, leaves, grass, apples, potatoes, turnips, wheat, peas, meat, and fish) the compositions are specified within the program, and only the quantities must be entered directly as a dry or as wet weight, or optionally as a percentage.

- Exemplary compositions are also specified for some mixed waste materials (e.g., sewage sludge, green waste, mixed household waste, biogenic household waste (biowaste), wastepaper (newspaper and paper fibers). If a material composition does not correspond to the given mixtures, nutrient concentrations can also be entered manually.
- The modes of operation comprise aerobic and anaerobic milieu conditions (also on an alternating basis) with the ability to select varying types of aeration. The following process feeding operations can be simulated: batches, loads with selectable time intervals or semi-continuous processes.

Based on the entry of approximately 30 initialization parameters, many process variations and influences can be simulated.

### 3. Results

A comparison of the simulation values with a variety of empirical values indicated that the results are comparable (Deipser, 2014 [4], Deipser and Körner, 2015 [81]). In the following section, three examples are shown.

#### 3.1 Exemplarily validation for an aerobic composting process

Experimental results gained in a laboratory composting experiment were compared with the corresponding simulation.

The laboratory test was conducted as follows by Körner (2008) [72]. The substrate in the laboratory experiment consisted of biowaste and rapidly degradable kitchen waste. Self-heating was supported by compensating the heat losses through the reactor wall to the environment by heating the reactors water jacket. During the process, the aeration rate has been manually regulated depending on the process progress. The aeration was carried out with fresh air at room temperature. The additions of water during composting were determined based on the water content of the substrates. For that purpose, samples were taken during turning of the substrate. Exhaust gas left the reactor and the cooled gas was analysed regarding its composition. A condensation water was generated, which was not led back to the reactor.

The input waste was well defined and composed of the following components (values in dry weight-%): apples (7 %), potatoes (5 %), turnips (3 %), wheat (43 %), peas (16 %), meat powder (2 %), wood (15 %) and lime (9 %). Wood was added to provide structure and lime to increase the pH value to a suitable range. The following parameters were determined from the initial mixture:

- > water content: 50 weight-%
- > pH value: 6.3
- > bulk density: 0.8 mg/m<sup>3</sup>
- > organic content: 84 weight-%
- > C/N: 23

The same contents and values were entered in SimuCF as basic and additional material information.

The simulation was carried out for the output parameters, which were also determined in the experiment. Water content and pH value were measured at the turning days, temperature of the material as well as oxygen and carbon dioxide content of the exhaust gas were continuously measured during composting.

The comparison of the laboratory results with the simulation results are shown in the following representations.

Figure 3 shows results for the changes in water, carbon dioxide and oxygen content, pH values and substrate temperature during composting from the laboratory experiment and from the simulation.

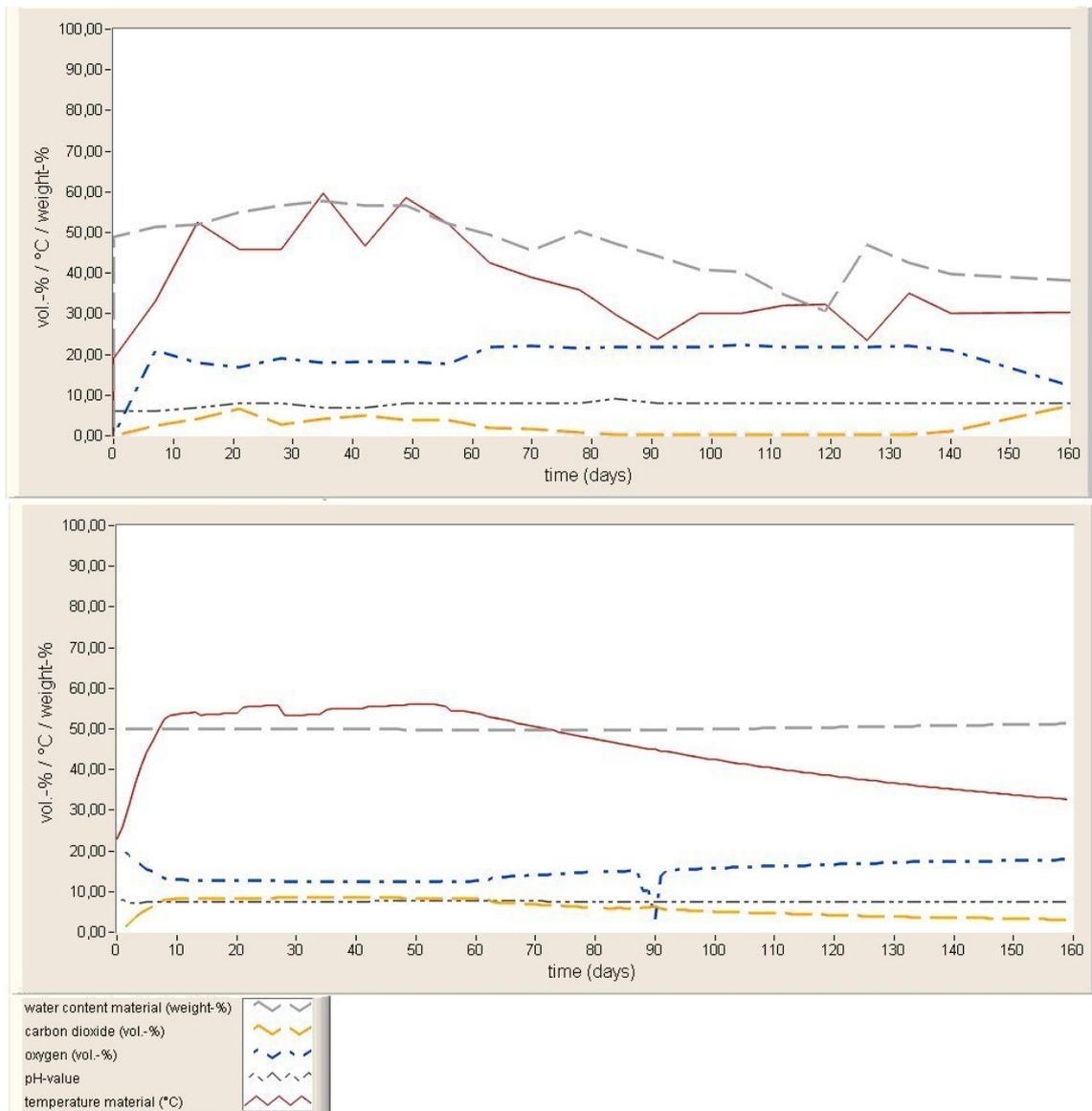


Figure 3: Changes of various process parameters during composting: Results from laboratory experiment (upper graph); and corresponding results from simulation (lower graph) (original graphics from the simulation program)

The results from the laboratory experiment and the simulation are comparable based on a similar trend. Differences could mainly be inferred based on the following reasons:

- In the laboratory experiments, inhomogeneities were formed during the process. In simulation, a homogeneous mixture is assumed.
- In the laboratory experiment, there were ventilation fluctuations, and the values were only intermittently measured. In the simulation, the few measured values were transferred and interpolated intermediate values.

- In the laboratory experiment, for many parameters (water content in the material, carbon dioxide and oxygen content, pH value, temperature in the material) measurement values were only produced once a week or every second week. For simulation, values must be given at the beginning and approximated if necessary, so that a process can be simulated and output values calculated.

Regarding the investigated parameters, the comparison and the observed trends can be explained as follows:

The carbon dioxide and oxygen shares in the exhaust gas are generally comparable. If contemplated in detail, some differences can be found. The most obvious were:

- ❖ Decrease of O<sub>2</sub> content on day 90 in the simulation,
- ❖ Increase of CO<sub>2</sub> content from day 140 in the experiment.

The differences, in general, can be attributed to variations of the airflow through the material caused by changes in porosity during the process due to degradation, compacting and aeration irregularities. Aeration irregularities can be considered in the simulation through the exact day-by-day recording of the airflow in the experiment and data transfer into the program.

Further comparisons:

- In the experiment, the average water content in the material was 48 weight-% and 50 weight-% in the simulation. The water content did not decrease during the simulation and leachate did not accumulate in contrast to the experiment. This is probably due to the water-holding capacity not being exceeded in the simulated homogeneous mixture. In the laboratory experiment, dry and humid zones formed and leachate developed because of the inhomogeneous mixture. The aeration also exerted significant influence on the water content. A resulting material drying could be simulated by the enhancement of the uneven aeration flow, and with it, the experiment and simulation result further converged.
- The pH value was dominantly influenced by lime addition in the laboratory experiment. Lime addition was also considered in the simulation. Inhomogeneities due to an uneven lime distribution in the experiment were considered in the simulation by only including 90 % of the practical lime additions in the simulation. In both cases, laboratory experiment and simulation, slightly lower pH values developed initially because of the initial acidification by biological processes. The pH values were mainly between 7 and 8 during the process in both variants.

- The simulated substrate temperature gradient is similar in the laboratory experiment. At the beginning, it increases up to almost 60 °C and drops down to approximately 30 °C at the end.

Here, further approximations would also be possible, if the aeration entries would be adapted.

The results of Körner (2008) [72] are used again for the comparison of simulation results concerning nitrogen during composting since numerous laboratory tests (number: 53). Körner (2008) [72] found that much of the processes known from the global nitrogen cycle are also important for composting. The main transformation processes are the ammonification of organic nitrogen compounds, nitrification, denitrification and ammonium/ammonia immobilization. In the substrate, organic nitrogen always has the largest nitrogen content during composting. Ammonium/Ammonia nitrogen is continuously present, but the levels vary widely throughout the process. Nitrate-N and especially nitrite-N are rarer and only present in certain phases and usually only in low concentrations. Dinitrous oxide is rare and quantitatively not relevant but can be climate-effective as a trace substance. The main nitrogen emissions occur via the exhaust air in the form of ammonia and produced dinitrogen with phase-wise different intensity. In the substrate contained ammonium/ammonia can escape as ammonia via the exhaust air. The substance discharge occurs increasingly through active ventilation or natural convection. This results in a re-adjustment of the ammonium/ammonia balance in the substrate (Körner, 2008) [72].

The ammonification and the associated possible loss of ammonia via the exhaust air and the denitrification with entering dinitrogen emission are therefore the main processes of nitrogen loss during composting.

In the simulations with SimuCF, the same set of values as described in this chapter were used. In the simulation results, nitrate-N and especially nitrite-N also occur rarely, only in certain phases and in low concentrations (Deipser, 2014) [4]. The main nitrogen emissions occur via the exhaust air as ammonia and as dinitrogen with phase-wise different intensity.

For a more differentiated presentation, the nitrogen simulation results of the described laboratory experiment are described as follows.

The simulation of the laboratory test showed ammonia-N emissions totaling 8.4 g (corresponding to 14.5 liters of ammonia at 20 °C and 1013.25 mbar) and ammonium-N concentrations of up to 37.8 mg/L at a C/N ratio of 44. A total of 7.8 g of dinitrogen-N

(corresponding to 6.7 liters of dinitrogen at 20 °C and 1013.25 mbar) was formed at the beginning and from the 88<sup>th</sup> day. Also from the 88<sup>th</sup> day, Nitrate-N has been calculated up to 39.3 mg/L in the water phase from the simulation program. Nitrite-N and dinitrous oxide-N did not calculated. A total of 16.2 g of nitrogen was lost via the gas phase.

Figure 4 shows the concentration curves of the resulting nitrogen compounds in the simulation of the laboratory experiment.

Leaps in the curves, thus concentrations or quantities, arise in simulation and in the laboratory experiments. For this there are different causes like e.g. Inhomogeneity of the solid substrate or changes of the gaseous phase composition.

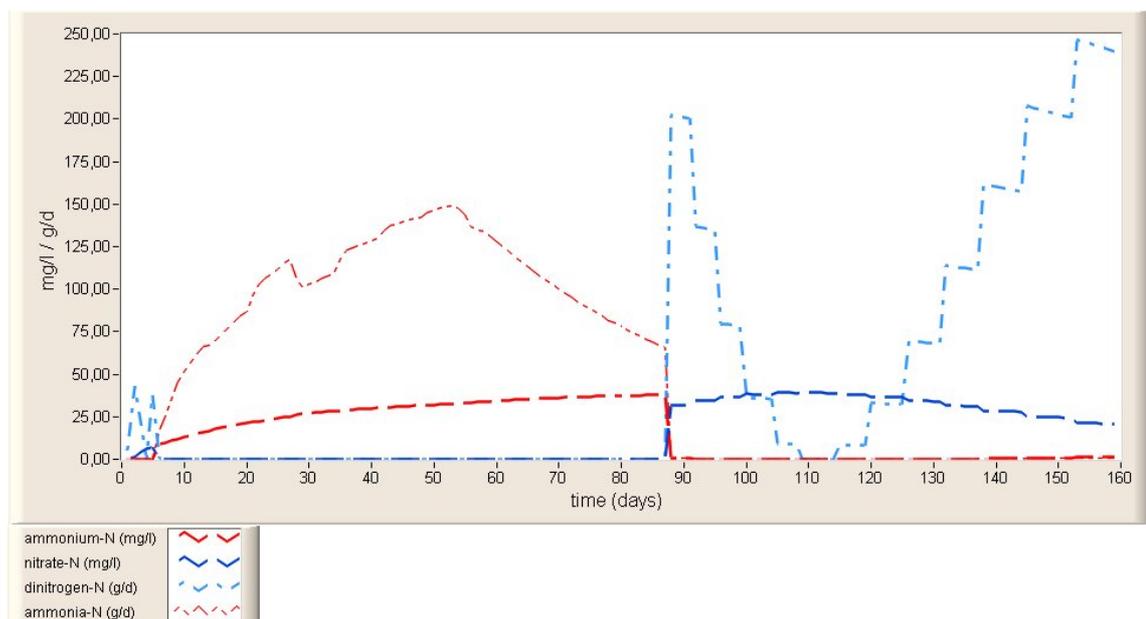


Figure 4: Ammonium-N, nitrate-N, nitrogen-N produced, and ammonia-N from laboratory testing results from simulation (original graphic from the simulation program)

The laboratory test showed a comparable result at a similar rate of degradation (77 % by weight material loss, in the simulation 81 % by weight of the degradable material). Dinitrogen and dinitrous oxide could not be detected. As estimated by Körner (2008) [72], total dinitrogen-N formation was in average 35.7 g (range: 11.9 - 59.5 g, maximum: 118.9 g) in the laboratory experiment. From the 126<sup>th</sup> day, low nitrate concentrations up to a maximum of 0.15 mg/L nitrate-N were measured, nitrite was not detected and ammonia-N can be calculated on the basis of measured values (Körner, 2008) [72] with 29.7 g emission be assumed in total via the gas phase (range: 29.7 - 267.6 g, maximum: 416 g).

Furthermore, ammonium-N concentrations in the water phase in comparable experiments are between 0.01 to 17 g/L (average: 2.1 g/L) and nitrate-N concentrations in further experiments in one fifth of the samples between 0.1 and 2700 mg/L (mean: 351 mg/L, median: 15 mg/L). Nitrite-N rarely appeared and if so, then no more than 0.2 % of the substrate solids. Due to literature reviews, the formation of dinitrous oxide is rarely detectable and quantitatively irrelevant (Körner, 2008) [72].

It should be underlined that the total emissions are dependent on the rate of degradation. At a degradation rate of 81 weight-% as in the simulation is therefore expected to higher loads than at a rate of degradation of 77 weight-% in the laboratory experiment. The nitrogen emissions are also dependent on the C/N ratio. A high C/N ratio means a lower nitrogen content and a relatively lower possible emission of nitrogen compounds (Körner, 2008) [72].

The comparison of the laboratory experiment concerning nitrogen with the simulation results of SimuCF are shown in Table 3.

	<b>Laboratory experiment</b>	<b>SimuCF</b>
Degradation rate	77 weight-%	81 weight-%
C/N ratio	20 – 25	44
Ammonia-N (total emissions)	29.7 - 267.6 g	8.4 g
Ammonium-N (total formation)	0.01 - 17 g/L	0.038 g/L
Dinitrogen-N (total formation)	11.9 - 59.5 g	7.8 g
Nitrate-N (total formation)	39.3 mg/L	0.1 - 2700 mg/L
Nitrite-N	not detected	0
Dinitrous oxide-N	not relevant	0

Table 3: Summary of the comparison of the laboratory experiment with the simulation results from the model SimuCF

### 3.2 General validation for anaerobic digestion processes

In this case, the simulated values were compared with reported common trends, presented in Figure 5. This refers specifically to the observed development tendencies of the gases by large quantities of organic wastes, which is manifold described in the literature (e.g. Farquhar and Rovers, 1973) [82]. The simulation of digestion presented in Figure 6 was carried out for mesophilic conditions and the most important anaerobic digestion parameters. In the simulation, for the substrate amount 1 Mg wet weight organic waste with 10 kg lime addition was used.

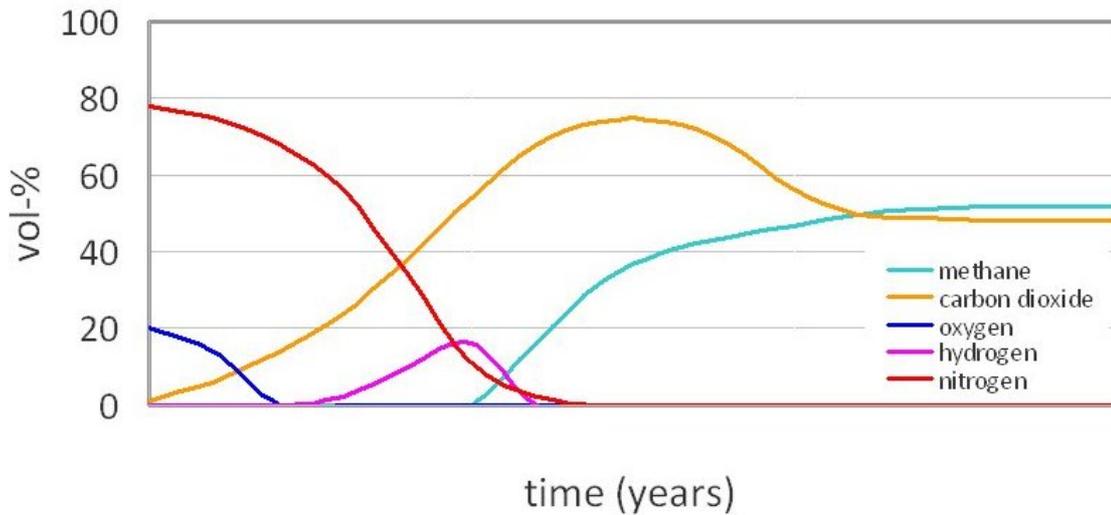


Figure 5: Trend for the development of the composition of emitted gas as an example for the anaerobic digestion processes in landfilling of organic wastes (Farquhar and Rover, 1973) [82]

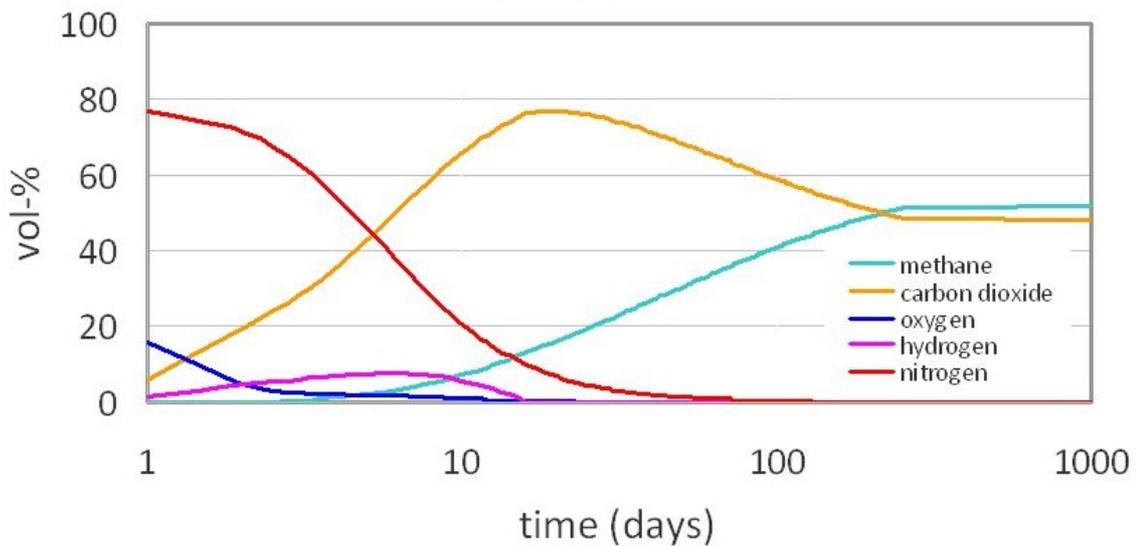


Figure 6: Simulation: Anaerobic gas composition development over 1000 days with logarithmic time representation

In both, the general trend visualisation (Figure 5) and the simulation (Figure 6), in the initial digestion phase the molecular air components of oxygen and nitrogen decrease. The available oxygen is consumed quickly while the unused nitrogen escapes slowly together with carbon dioxide, molecular hydrogen and later-on methane. The hydrogen is used for the creating of methane after an initial phase in which the methane-creating microorganisms increase and the milieu conditions change. In Figure 5 and 6, the carbon dioxide concentration rises at the

beginning strongly (to approx. 78 vol.-%) because of the initial acidification due to anaerobic bioactivity. In the simulation, the methane concentration constantly rises up to approx. 52 vol.-%. The carbon dioxide concentration decreases to approx. 48 vol.-%. Hydrogen increases at the beginning, in the simulation and also in the example of Farquhar and Rover, 1973 [82]. In Figure 5, a hydrogen generation is assumed to take place after the disappearance of oxygen. However, both gases might be able to occur at the same time due to inhomogeneities in the landfill body, like it is shown in Figure 6. Under increasing anaerobic conditions the hydrogen is converted quickly to methane in the simulation as well as the reality trend. Thus, the oxygen and hydrogen concentrations are reduced to zero within the first few days due to the quantity and existing oxygen at the beginning.

In Figures 5 and 6 the different displayed time periods vary. They depend on the quantity, the composition of the substrate and the milieu conditions. The anaerobic microbiological dismantling can extend from hours with the easily degradable substrate and optimal milieu conditions up to weeks, months and years with a substrate that is difficult to degrade and/or unfavourable milieu conditions are present. Therefore, the simulation results show a correlation of the gas concentration curves with consideration to the implemented conditions.

### **3.3 Specific validation with parameters of large-scale biogas plants**

A quantity conversion to higher or lower values makes the use of SimuCF possible within many ranges, thus from the laboratory test up to the large-scale plant.

The comparability is limited by different rates of degradation, different material compositions and reproducible material contents, also different measurement methods and reference values (e.g. dry weight (DM), organic dry weight (oDM), wet weight (WM)) and operations or system designs.

Nevertheless, three German quasi-continuous biowaste digestion plants (Nottensdorf: Poetsch, 2005 [73], Kehlheim: Hoppenheidt et al., 1998 [74], Karlsruhe: Gallert et al., 2002 [75]) were compared with simulations to show results with SimuCF.

The biogas plant in Nottensdorf (volume load: 2.5 kg oDM/m<sup>3</sup>d, thermophilic) was reported with 135 m<sup>3</sup>/Mg WM, 673 m<sup>3</sup>/Mg oDM and 1710 L/m<sup>3</sup>d biogas production, the biogas plant in Kehlheim (volume load: 5.2 kg oDM/m<sup>3</sup>d, mesophilic) with 68 m<sup>3</sup>/Mg WM, 380 m<sup>3</sup>/Mg oDM and

1800 L/m<sup>3</sup>d biogas production and the biogas plant in Karlsruhe (volume load: 3.5 kg oDM/m<sup>3</sup>d, mesophilic) was reported with 91 m<sup>3</sup>/Mg WM, 394 m<sup>3</sup>/Mg oDM and 1364 L/m<sup>3</sup>d biogas production.

The procedure for implementing the reported data into SimuCF and comparing the practice and the simulation results is described in the following for the Karlsruhe plant. In the Karlsruhe case municipal biowaste was used without co-substrates as input. The category “biowaste” is integrated in the SimuCF program as category and was selected as default. Co-substrates may be added but must be known as a fraction or composition. In the Karlsruhe case, this was not necessary. Further key information for the Karlsruhe plant with respect to parameters reported in Table 4 were taken from the description of Gallert et al. ( 2002) [75].

Parameter	Reported data for biogas plant Karlsruhe <sup>1</sup>	Chosen input data for SimuCF
Waste amount (charge)/day	20 Mg/d WM biowaste	20 kg/d WM biowaste
Hydraulic retention time	68 days (calculated)	70 days (rounded up)
Additives	not reported	1 kg lime at the beginning
Temperature	mesophil	45 °C
Volume load	3.5 kg oDM/m <sup>3</sup> d	3.7 kg oDM/m <sup>3</sup> d (calculated)
Operation mode	quasi-continuous	quasi-continuous
Degradation rate	86 weight-%	85 weight-%
Reactor volume	1350 m <sup>3</sup>	about 2000 m <sup>3</sup> for 70 x 20 kg

<sup>1</sup>(Gallert et al., 2002) [75].

Table 4: Summary of the input data for the biological gas facility and the simulation model SimuCF

The degradation rate of the organic substance in mesophilic operation was about 86 %. Since the reactor volume was 1350 m<sup>3</sup> and the processed wet amount of waste 20 Mg/d, the hydraulic retention time was about 68 days (Gallert et al., 2002) [75].

For the implementation in SimuCF, 20 kg of WM biowaste, a hydraulic retention time of 70 days and an addition of 1 kg of lime were taken daily for adjustment the pH value (Table 4). The simulation was carried out with a 1000 times smaller amount of substrate than in the biogas plant Karlsruhe to simplification for calculations.

The temperature was set at 45 °C, which corresponds to the upper mesophilic range. The space load calculated with these values in the quasi-continuous simulation was 3.7 kg oDM/m<sup>3</sup>d. The share of the degradable organic substances was about 85 % by weight.

So the inputs for the processing mode (quasi-continuous operation), the processed waste amount (20 Mg/d after conversion 20 kg/d), the volume loads (3.5 and 3.7 kg oDM/m<sup>3</sup>d), the

hydraulic retention times (68 and 70 days) and the degradation rates (86 and 85 weight-%) were comparable between the biogas plant Karlsruhe and the simulation with SimuCF.

Figure 7 shows the biogas indices of all three biowaste digestion plants in comparison with the simulation results (outputs).

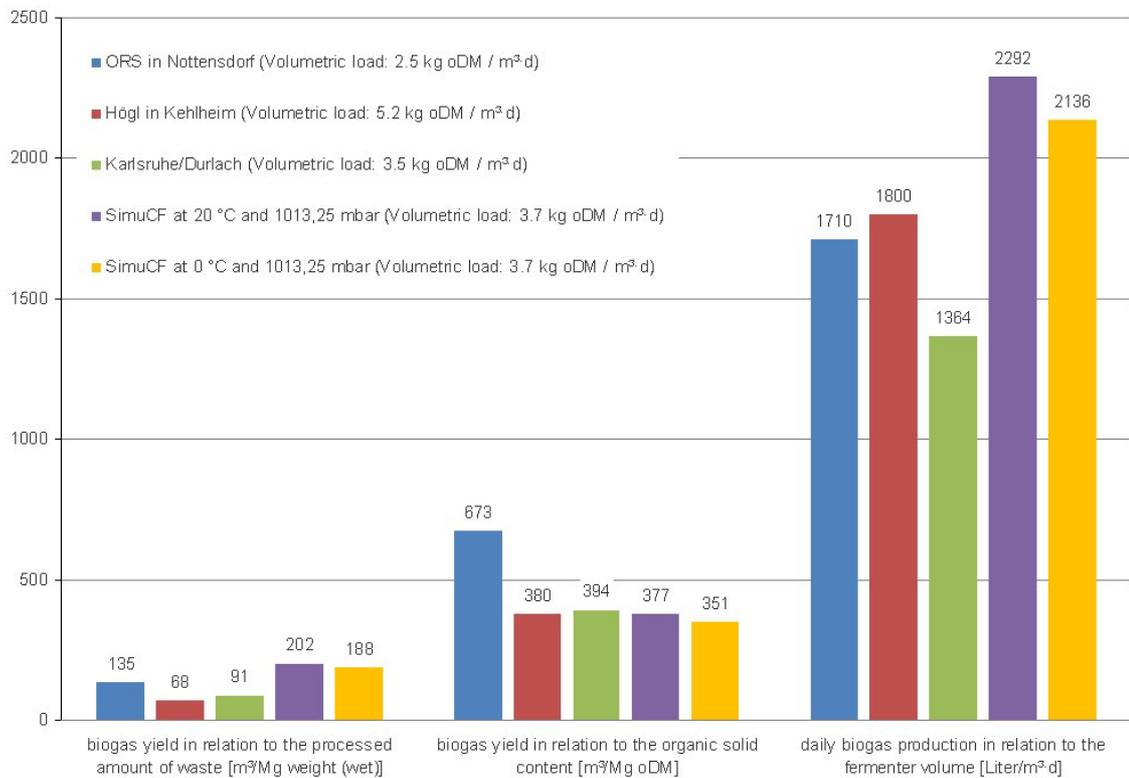


Figure 7: Digestion gas characteristics of three biogas digestion plants and digestion gas characteristics calculated with simulation by SimuCF

The biogas production in the simulation with SimuCF was 202 m<sup>3</sup>/Mg WM (based on the wet matter basis), 377 m<sup>3</sup>/Mg oDM (based on dry matter basis) and 2292 L/m<sup>3</sup>d (related to the reactor volume). These values refer to biogas conditions of 20 °C and 1013.25 mbar. The biogas conditions from the reported practice values were not given in the publications mentioned, but are assumed to be in this range.

The biogas production based on the dry organic matter basis of the biogas plant Karlsruhe and the simulated quasi-continuous operation was almost identical (Figure 7). The deviation is only about 4 %.

In Nottensdorf (Poetsch, 2005) [73] and Kehlheim (Hoppenheidt et al., 1998) [74] less information to the process were available. Therefore, the same starting conditions as in Table 4

were assumed. The biogas results, displayed in Figure 7, were provided by the mentioned authors.

The deviation of the biogas production on dry matter basis between practice and simulation for the Kehlheim plant is only 0.8 %. For the Nottensdorf plant it is high with 79 %. In Nottendorf, fatty co-substrates were co-fermented. In the simulation, only “biowaste” was assumed as input, which explains the large deviation.

Similar to the Karlsruhe case, the deviations are also large when the biogas production is related to the reactor volume (27 - 68 % lower values in practice compared to the simulation). This can be due to differing filling levels and resulting reactor outputs.

Even when referring to the amount of waste (on wet matter basis) processed, the deviations are high (50 – 300 % lower than in the simulation). Since it concerns material wet digestion plants, the water content will have been probably still higher. The water content in simulation amounted only to 40 weight-% for biowaste.

Differences in biogas production are generally to be explained primarily by different types of biowaste, co-substrates and degradability of the constituents (FNR, 2009) [83]. A higher water content of the material and additional free reactor volume may also result in lower values when related to wet weight or reactor volume. The values of the simulation are to be optimized if respective information are known. SimuCF has input areas for water contents, chemical composition of substrates and co-substrates as well as free reactor volume. The practice biogas productions related to the dry organic substance are best comparable with the simulation results because of their independence from the water content and reactor volume.

When referring to the wet substance and the reactor volume, the deviations of the measured values from the simulation results decrease when the values are referred to 0°C instead of 20°C. Then the gas volumes are about 15 % lower.

For further comparisons between practice and simulation, the gathering of the specific missing data regarding waste density, free pore volume, water content, free reactor space as well as on co-substrates from the facilities is a task.

### 3.4 Possibilities of the field use with the simulation program

Optimizations can contribute to more efficient working modes and uses of waste management facilities. Improvements are possible e.g. with regards to resources consumption, energy generation, and operational sequences to allow savings. Processing modes can be found, so that desired products such as methane in biogas can be increased and unwanted emissions reduced. In practice, optimizations are often complicated to investigate, especially if different changes of the routine working mode need to be tested. It is, therefore, useful to make predictions using the SimuCF program.

Plants with aerobic and/or anaerobic processes e.g. in composting, anaerobic digestion or fermentation, and landfilling can be tested and optimized with modifications in the following settings:

- changes of process and/or milieu conditions
- temperature
- water content
- pH value attitude (e.g. by simulated lime addition)
- changes in the material (substrate types, structural improvement)
- ventilation
- hydraulic retention time
- degradation
- emissions (e.g., methane, ammonia, nitrate, nitrite, hydrogen sulfide in gases, leachate)
- products (e.g. biogas and compost amounts and compositions)

## 4. Discussion

The simulation model SimuCF covers a large area of biodegradation-related topics regarding organic materials (Deipser, 2014), unequal in which physical state (liquid or solid) they are since a mixed reactor is simulated. Due to the lack of pores, liquids can only be simulated anaerobically. However, the necessary shortening of the degradation pathways with the use of model molecules and model degradation reaction equations could be enough to answer many questions in this area.

The mechanical, chemical and biological decomposition of macromolecules is only indirectly included in SimuCF. But these removal steps can essentially inhibit the overall reduction. A general reduction delay can be simulated in the program.

SimuCF considers the final reaction equations. Intermediates that are formed at the beginning of the degradation can therefore not be simulated in detail. The distribution and generation of emissions in the different phases (solid, liquid and gas phase) can therefore only be compared based on the final products.

Whether the assumptions and simplifications made suffice to show consequences sufficiently for the practice, applications will have to indicate.

## 5. Conclusions

The simulation model SimuCF (<https://www.simucf.de>) simulates aerobic and anaerobic degradation processes and microbiological, chemical and biochemical processes including physical effects. It can be applied in practice, for example for the emission optimization, also climatic effective emissions, or plant planning, and for training and education purposes. Due to many setting possibilities, almost all of the standard process operating models for the biological treatment waste can be simulated. This includes generation and concentrations of the gases hydrogen and methane, which are interesting both for the power production, but also for the fire protection and environment. Furthermore, the whereabouts of carbon, nitrogen, and sulfur in the different phases of composting and digestion or fermentation can be ascertained.

The SimuCF model is based on stoichiometric equations for principal reactions of the aerobic and anaerobic metabolism. Only a few mathematical equations from empirical determinations or physical laws were used. Correction factors were partly integrated as alterable assumptions. They concern the air-water saturation including withdrawal of saturated air from the system, the temperature, the oxygen, and the nutrient availability.

The developments of curves of the substances are determined with priority by correlations, which lead to a time-discrete process (iteration). The result is an expandable simulator routine with the substantial values of the biological waste treatment and their emissions.

In the future, the simulation program SimuCF is to be used for the composting, digestion or fermentation, and combined processes at real plants. Validation of the program will continuously take place. The use in education is possible and SimuCF can be reduced for it. Extensions and specializations are possible in further versions through programming.

## 6. List of Abbreviations

EEG	Renewable Energy Sources Act
EU	European Union
IWA	International Water Association
VI	Virtual Instrument
DM	dry weight or matter
oDM	organic dry weight or matter
WM	wet weight or matter
L	Liter
mg	milligram
kg	kilogram
Mg	megagram
m	meter
m <sup>3</sup>	cubic meter
vol.	volume
d	day
°C	degree of Celsius

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