

Technische Universität Berlin  
Institut für Technischen Umweltschutz  
Fachgebiet Kreislaufwirtschaft und Recyclingtechnologie  
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# **Bachelorarbeit**

## **Dynamic Material Flow Analysis for organic waste management in Python: An ODYM-based modelling approach**

vorgelegt von

Lukas Hoppe (399708)

Erste Prüferin: Prof. Dr.-Ing. Vera Susanne Rotter

Zweiter Prüfer: Albrecht Fritze, M.Sc.

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### **Selbstständigkeitserklärung**

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## Kurzfassung

Entscheidungsfindungen in allen Bereichen des Abfallmanagements im Einklang mit einer Kreislaufwirtschaft erfordern von Forschenden den Einsatz fortschrittlicher Systemanalysewerkzeuge. Die Materialflussanalyse (MFA) ist eine Methode, die ermöglicht, wertvolle Einblicke in Materialsysteme und deren Komponentenverteilung zu gewinnen. Die MFA-Community ist immer noch auf der Suche nach innovativer Software für die Durchführung dynamischer Analysen und komplexer Unsicherheitsbewertungen. ODYM ist ein kürzlich veröffentlichter, Python-basierter Ansatz, um einen angemessenen Rahmen für die dynamische Modellierung bereitzustellen, der die Anforderungen der Community erfüllt. In dieser Arbeit wurde das Potenzial von ODYM, speziell für das Management von organischen Abfällen, untersucht. In diesem Bereich wird die Abfallbehandlung häufig mithilfe biologischer Prozesse durchgeführt, welche mit herkömmlichen MFA-Methoden wie Flussberechnung mit Transferkoeffizienten nicht immer ausreichend beschrieben werden können. Eine fallstudienbasierte Modellierungsvorlage wurde entwickelt, um die Eignung von ODYM für die Durchführung dynamischer MFA mit Monte-Carlo-Simulation, einschließlich der gleichzeitigen Berücksichtigung von organischen Abfallströmen und enthaltenen Elementen, zu demonstrieren. Der quelloffene und modulare Aufbau von ODYM ermöglichte die Integration eines Modells für den Abbau erster Ordnung zur besseren Beschreibung von biologischen Prozessen und eine erste Methodik für interaktive Sankey-Diagramme zur generellen Erweiterung des ODYM-Ansatzes. Eine ausführliche Dokumentation des Arbeitsprozesses wird zur Verfügung gestellt, um die dynamische MFA für das Management von organischen Abfallströmen für Forschende zugänglicher zu machen.

## Abstract

Decision-making in all fields of waste management in line with a Circular Economy requires researchers to make use of advanced system analysis tools. Material Flow Analysis (MFA) is a method that enables obtaining valuable insights into material systems and their component distribution. The MFA community is still in search of innovative software for performing dynamic analysis and complex uncertainty evaluation. ODYM is a recently published Python-based attempt aiming at the establishment of an adequate dynamic modelling framework to satisfy the community's needs. For the thesis, the potential of ODYM specifically for organic waste management was investigated. In this field, treatment options often involve biological processes which cannot always be sufficiently described with conventional MFA methods like flow calculation with transfer coefficients. A case-study-based modelling template was developed to demonstrate ODYM's suitability for performing dynamic MFA with Monte-Carlo-Simulation, including simultaneously tracing organic waste flows and contained elements. The open source and modular design of ODYM allowed the integration of a first order model approach to better describe biological processes and a suggestive methodology for interactive Sankey diagrams to extend the original framework. Detailed documentation of the working process is provided to make dynamic MFA in the context of organic waste management more accessible for researchers.

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## List of abbreviations

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Abbreviation	Definition
CE	Circular Economy
FOMP	First Order Model Process
HOMFA	Handbook of Material Flow Analysis
MCS	Monte-Carlo-Simulation
MFA	Material Flow Analysis
NMC	Number of Monte-Carlo runs
ODYM	Open software framework for DYnamic Material systems
STAN	subSTance flow ANalysis
TC	Transfer coefficient

# 1 Introduction

The Circular Economy (CE) concept has grown to be one of the EU's main strategies to achieve climate neutrality by 2050 (European Commission, 2020a). Considering various definition approaches, Geissdoerfer et al. (2017) specify CE as “a regenerative system in which resource input and waste, emission, and energy leakage are minimized by slowing, closing, and narrowing material and energy loops” (ibid., p. 759). The European Commission lists food production and nutrient deployment as key product value chains (European Commission, 2020a), making appropriate management of organic waste streams an essential factor of its CE approach. Initiating circularization of material flows that helps shift toward a more sustainable economy requires an in-depth understanding of the considered supply chain structures and their interconnectedness with the ecosystem (Murray et al., 2017).

A frequently used method that allows a structured examination of defined systems regarding their input and output flows, processes, and stocks is Material Flow Analysis (MFA) (Graedel, 2019). The main goal of MFA is to obtain a data-driven model to improve system management, providing useful insights for successful decision-making (Brunner & Rechberger, 2016). As an illustration, Betz et al. (2015) used MFA to investigate food waste origins in the food service industry, providing information regarding relevant process sectors to be optimized for effective food loss reduction. Originally only able to describe static systems, research progress over the last 30 years made dynamic approaches in MFA a well-established research field (Brunner & Rechberger, 2016). Enabling investigation of system changes over time as well as making predictions on future developments, dynamic MFA has the potential to be even more helpful in making goal-oriented decisions compared to the static approach (Laner & Rechberger, 2016).

Waste treatment systems, especially those using biological processes, are subject to constant fluctuation due to changing waste input streams and process-related variations (Urtnowski-Morin et al., 2021; Vergara & Tchobanoglous, 2012; Zabaleta et al., 2020). Thus, choosing a dynamic MFA approach might improve the alignment of organic waste management with CE goals.

A highly popular tool for performing MFA is STAN (*subSTance flow ANalysis*) (Brunner & Rechberger, 2016). In addition to mathematical calculations, it allows plotting results via Sankey diagrams. However, consideration of complex time dependencies and differentiated uncertainty evaluation of processes cannot be performed with this software (Bornhöft et al., 2013; Laner et al., 2014; Pauliuk & Heeren, 2020). To provide a more suitable approach for dynamic MFA, Pauliuk & Heeren (2020) introduced ODYM as a Python-based modelling framework. The *Open software framework for DYnamic Material systems* has been published under permissive license along with detailed documentation, enabling researchers with a programming background to adapt the software for specific purposes (ibid.).

In this spirit of open science, the thesis explores ODYM's potential to serve as a modelling framework to develop an extended user-friendly modelling template for describing and investigating treatment systems in organic waste management via dynamic MFA. A subdivision into the following derived objectives is made:



## **Objective 1**

*Introduction of MFA as a concept and presentation of the importance of a dynamic MFA approach in waste management. Highlight challenges peculiar to organic waste treatment. Explain the benefits and drawbacks of current state-of-the-art MFA software (STAN and ODYM) and examine their applicability as a decision-making help in the given field. Introduce the programming language Python, as it is used in ODYM.*

## **Objective 2**

*Exhibit the suitability of a case-study-based modelling template for organic waste management using ODYM. Evaluate the user-friendliness and adaptability of the template.*

Considering the defined objectives, the thesis is structured as follows: chapter 2 (p. 3) covers the state of the science described in Objective 1. Chapter 3 (p. 15) lists all theoretical and practical methodologies that have been applied. Chapter 4 (p. 18) introduces the developed template as well as case study modelling results. The functioning of the code and the suitability of this approach will be discussed in chapter 5 (p. 22), followed by a conclusion in chapter 6 (p. 31).

## 2 Background

### 2.1 Material Flow Analysis (MFA): terminology and procedure

MFA is the study of material flows, stocks, and the inducing processes (Brunner & Rechberger, 2016). These components are not considered in isolation, the object of investigation is the system composed of them (Graedel, 2019).

MFA is built on the mass balance principle, which states that the system's input must equal its output (Laner & Rechberger, 2016). Considering the mass balance principle as its origin, MFA had its starting point already 2000 years ago in ancient Greek philosophy (Brunner & Rechberger, 2016). The wide application of mass balancing started in 1900, resulting in the development of MFA with application in various areas (Brunner & Rechberger, 2016). Having transformed so comprehensively within the course of history, the modern approach of MFA as a method aimed at the provision of reliable data on societal material distribution is specified as a field that emerged in the 21<sup>st</sup> century (Graedel, 2019). It is a common approach in various scientific disciplines like environmental management and engineering, industrial ecology, resource and waste management, and anthropogenic metabolism (Brunner & Rechberger, 2016). Due to this widespread application, the language around MFA is not consistent, which aggravates communication between researchers (ibid.). In this thesis, the terminology is based on Baccini & Brunner (1991) as presented in the *Handbook of Material Flow Analysis* (Brunner & Rechberger, 2016) and is introduced along with more details on methodology using the following example (see Figure 1):

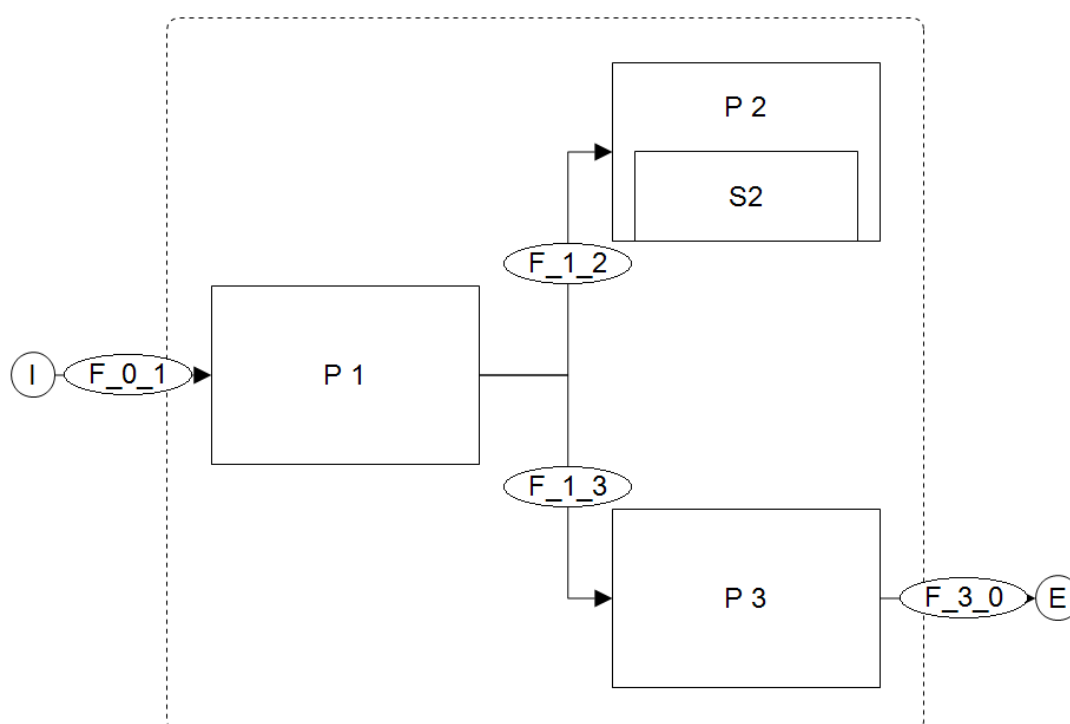


Figure 1: Exemplary Material Flow Analysis system (done with STAN)

The system, delimited from the environment by a system boundary in space and time, consists of the processes P1, P2 and P3, their relationship specified by flows. Flows can be entering (import:  $F_{0\_1}$ ) or leaving (export:  $F_{3\_0}$ ) the system boundary, or they can occur within the system between processes (input/output:  $F_{1\_2}$ ,  $F_{1\_3}$ ). Flows typically have the unit  $t\cdot year^{-1}$  or  $kg\cdot s^{-1}$ , fluxes are flows over cross-section (e.g. unit  $t\cdot year^{-1}\cdot capita^{-1}$ ). The system can be investigated on substance or good level. Substances can be elements (e.g. carbon) or molecules (e.g. nitrous oxide) and they make up goods (e.g. waste). Substances and goods are summarized under the term material. In processes, materials can be transported, transformed, or stored. The storage of mass within a process is defined as stock (see S2 in P2). To enable simplicity and accuracy at the same time, subsystems may be defined. Summarizing processes within a subsystem allows clearly arranged presentation of large systems while maintaining the option to look deeper into certain system aspects. The most important parameters to specify the allocation of materials to certain flows are transfer coefficients (TCs). In the example system, P1 has no stock and due to the mass balance principle,  $F_{0\_1}$  must equal the sum of  $F_{1\_2}$  and  $F_{1\_3}$ . If 60 % is assigned to  $F_{1\_2}$  and 40 % to  $F_{1\_3}$ , transfer coefficients would be 0.6 and 0.4. (Brunner & Rechberger, 2016)

MFA procedure consists of several steps (see Figure 2):



Figure 2: MFA procedure flow chart (based on (Laner & Rechberger, 2016; based on (Brunner & Rechberger, 2004))

It is recommended to start with a rough outline and successively make improvements until an advanced and informative model is obtained. During the analysis, it might be necessary to go back to previous steps to make refinements and adjustments. The MFA results should be checked for reliability since the used data, derived from measurements, literature, and estimations, are always subject to uncertainty. Building up the quantitative model is usually done with MFA software, two of which (STAN and ODYM) will be discussed in chapter 2.3 (p. 10) in more detail. (Brunner & Rechberger, 2016)

Initially, the problem and the goal of the research are defined. Subsequent selection of relevant goods, substances, processes, and the definition of a system boundary leads to the build-up of a qualitative model. To quantify material flows and stocks within the system, available input data is then inserted into the model. (Brunner & Rechberger, 2016)

Depending on the scope of the data, MFA provides several subsequent calculation options (ibid.):  
**1)** Unknown quantities can be computed by balancing the system. In the case of the exemplary MFA system in Figure 1 (p. 3),  $F_{1\_2}$  could be calculated if  $F_{0\_1}$  and  $F_{1\_3}$  are available, which then could be used to calculate  $TC_{1\_2}$  by dividing  $F_{1\_2}$  by  $F_{0\_1}$ . **2)** If certain aspects of the system are overdetermined and the system is solvable, data can be reconciled to better fit the model. All measured and estimated data are to some extent occupied with uncertainty, which needs to be taken into account. The import flow  $F_{0\_1}$  could be a set value without uncertainty. If the sum of the mean values of  $F_{1\_2}$  and  $F_{1\_3}$  is not equal to  $F_{0\_1}$  and uncertainty values are given for these flows,

they can be adjusted to fulfil the mass balance principle. **3)** An overdetermined system can also be checked for result consistency. If  $F_{1,2}$  is calculated as described for calculation option 1) and  $TC_{1,2}$  is also given but they do not match, it might be necessary to check the input data as well as the performed calculations. **4)** Uncertainty evaluation of the analysis results and the underlying data is an essential step in MFA, ensuring its reliability. Using normal distribution by specifying mean values and their standard deviation for data is common to be applied in scientific practice (Limpert & Stahel, 2011). However, this assumption is not always reasonable, since it can lead to the calculation of negative mass flows or TCs (Laner et al., 2014). Limpert & Stahel (2011) demonstrate the suitability of the log-normal distribution for published scientific data in various fields like medicine, biology, physics, and soil science. The authors of the examined studies used the normal distribution, leading to less meaningful results than Limpert & Stahel did by applying the log-normal distribution (ibid.). They concluded by asking the question: “Has the normal distribution become too normal?” (Limpert & Stahel, 2011, p. 6). Moreover, more specific variants like Weibull, exponential, or gamma distribution may be used to refine uncertainty characterization, while the log-normal approach may replace the often less adequate normal distribution as an approximation standard (ibid.).

Using uncertain input data inevitably leads to uncertain results, a consequence that can be quantified by “uncertainty propagation” (Zhang, 2021). In MFA, Monte-Carlo-Simulation (MCS) is frequently used to assess the effects of data uncertainty on the model results (Brunner & Rechberger, 2016). MCS includes random sampling of all input variables according to their probability density function and running the simulation with the obtained values to see how they influence the outputs (Zhang, 2021). Computer-based random number generation is well tested and considered to be pseudo-random, since the underlying algorithms are usually reproducible (Harrison, 2010). For each run in the MCS, a new set of pseudo-random values for all variables with uncertainty is provided and results are collected afterward (ibid.). Approximated probability density functions of output results can be generated by analysing the simulation outcome afterward (Raychaudhuri, 2008). To determine the number of simulation runs that should be done, it is a common procedure to choose a number of runs, and then check if the mean and standard error of the results change significantly with additional model runs, or if the scale of deviation is acceptable (Lerche & Mudford, 2005). But there are also more advanced methods to estimate the number of runs before starting MCS (ibid.). (Brunner & Rechberger, 2016)

In general, MFA can be subdivided into a static and a dynamic approach (Brunner & Rechberger, 2016). Static MFA describes a system snapshot-like at a specific time, while the dynamic MFA allows model analysis over time (Laner & Rechberger, 2016). The latter approach emerged in the 1990s and is mostly used for stock investigation and creating development scenarios (Laner & Rechberger, 2016). For stock calculation, there are two common approaches (see Figure 3, p. 6 for the case of a building material).

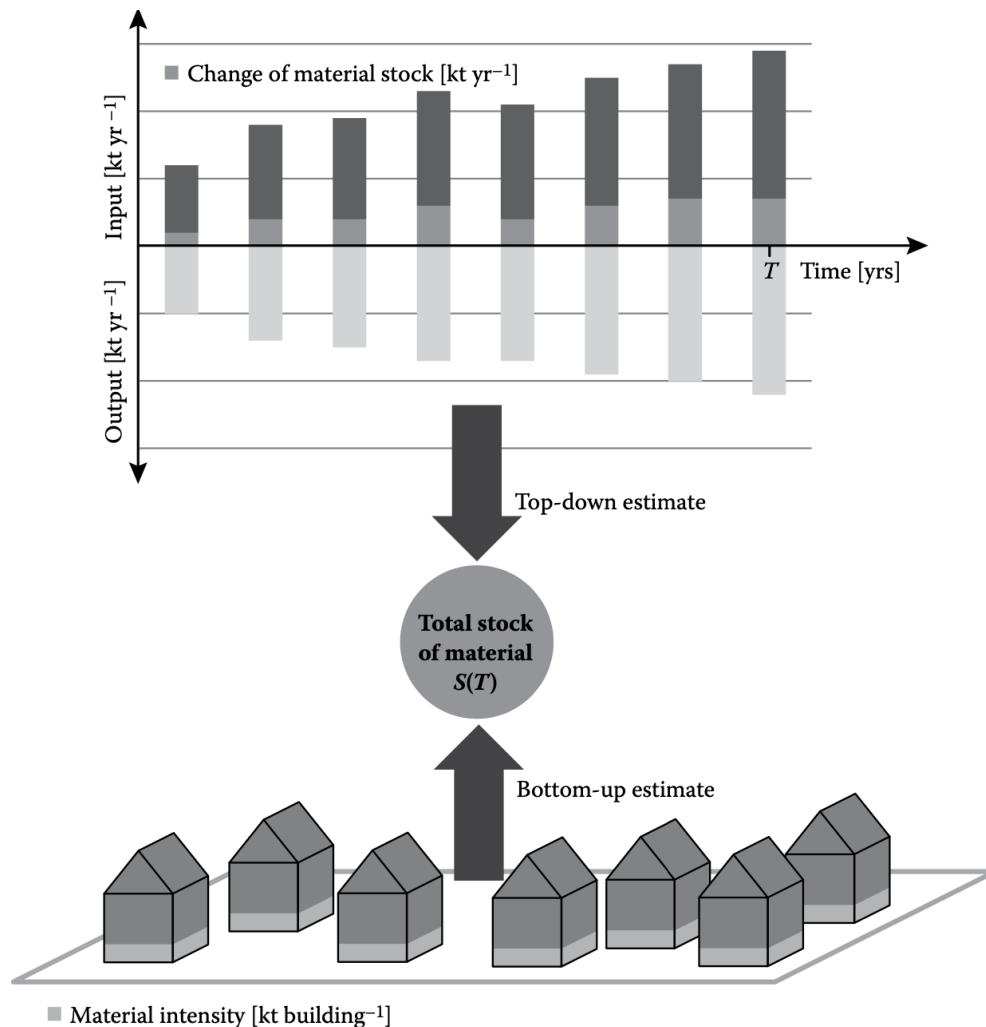


Figure 3: Top-down and bottom-up stock estimation using the example of material in buildings ((Laner & Rechberger, 2016) based on (Brunner & Rechberger, 2004))

The top-down method, frequently used in dynamic stock modelling, balances in- and output flows over time, generating stock changes for specific years (Brunner & Rechberger, 2016). Due to the lack of actual output data, making use of lifetime functions is a common method to be applied in dynamic stock modelling (ibid.), for example, for modelling different scenarios of end-of-life passenger cars accumulation in China (Chen et al., 2015). If all in-stock material has the same likelihood of leaving the stock at a specific time, leaching coefficients can be used (Voet et al., 2002), for instance, for metal leaching in landfills (Laner & Rechberger, 2016). In static MFA, the bottom-up estimation is preferred, in which stock is calculated at a specific time by considering all material sources within the system. (Brunner & Rechberger, 2016)

Although dynamic MFA has received growing attention from the research community in the past 30 years, Brunner & Rechberger (2016) conclude that static MFA will remain relevant. It is often sufficient to apply static analysis to describe a system and to grasp its basic characteristics in a resource- and data-efficient way. Furthermore, it can be used as a basis for dynamic MFA. (ibid.)

The final step in the MFA procedure includes the illustration and interpretation of results (Brunner & Rechberger, 2016). Sankey diagrams are typically used to display the analysis outcome (Graedel, 2019). The quantity size of a flow is proportional to the width of the displaying arrows, colours can

be used to show additional characteristics of the system (ibid.), including different flows (e.g. (Hoogzaad et al., 2019)), the composition of the flows (e.g. (European Commission. Joint Research Centre., 2017)) and uncertainty of data (e.g. (Lupton & Allwood, 2018)). Sankey diagrams stand out as a comprehensible yet profound method to present MFA results to different audiences like industries and governments. Figure 4 shows the analysis results of the anaerobic digestion of switchgrass as Sankey diagram (Niu et al., 2015). The researchers tracked nutrient amounts and distribution of carbon (C) and nitrogen (N) within the process (the proportion of nitrogen is too small to be visible). They concluded that the process is inefficient due to significant amounts of carbon in biogas residues, which can be easily understood by looking at the diagram (ibid.). (Brunner & Rechberger, 2016)

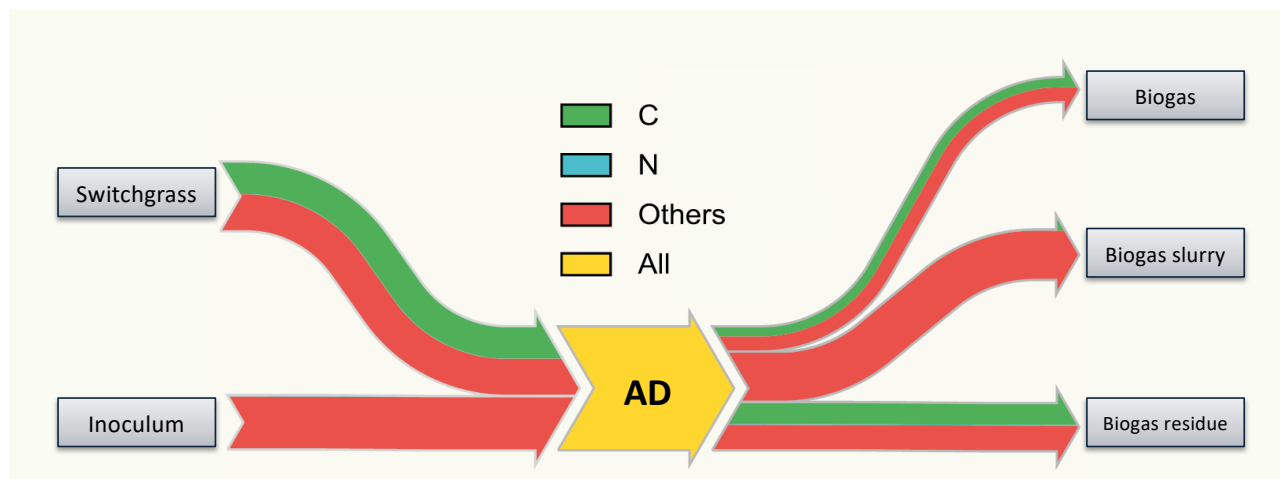


Figure 4: Sankey diagram of an anaerobic digestion process of switchgrass (modified) (Niu et al., 2015)

For decision making, MFA must be combined with other methods that allow evaluation of the obtained results in terms of conduciveness to the set goal (Brunner & Rechberger, 2016). MFA gives insight into process flows and stocks, but whether their arrangement in the current system structure (or in planned scenarios) is beneficial or not is out of its scope (ibid.). Thus, it is common to combine MFA with methods of risk assessment and economic analysis, applying, for example, life cycle assessment, which complements the analysis-derived system information with assigned environmental effects. (ibid.; Laurent et al., 2014)

The scope of MFA is variable (Brunner & Rechberger, 2016). A single process (e.g. (Niu et al., 2015) for anaerobic digestion) or a system containing several processes (e.g. (Fisher et al., 2017) for sulfur flows in wastewater treatment plants) may be investigated, but also material flows within countries (e.g. (Alagha et al., 2022) for marine plastic flows in Qatar) or intergovernmental unions (e.g. (European Commission. Joint Research Centre., 2018) for different metal flows in the EU-28) can be assessed. On an even broader scale, MFA may help uncover the connection between anthropogenically induced material flows and natural cycles (e.g. (Rauch & Pacyna, 2009) for global metal cycles) (Graedel, 2019). However, MFA depends on the quality of input information, and it has been frequently emphasized that the supply of reliable data is one of the major challenges for MFA research (Brunner & Rechberger, 2016; Graedel, 2019). Increasing the usability of the MFA approach requires the development of openly available and standardized databases for relevant input data (Brunner & Rechberger, 2016). Although dynamic approaches have been explored in MFA

research for 30 years, another challenge remains the lack of established software for dynamic MFA (see chapter 2.3, p. 10) (Pauliuk & Heeren, 2020).

## 2.2 Application of MFA in waste management

Appropriate waste management is a complex field intended to preserve conditions that benefit the health of humans and the environment, enable resource efficiency as well as cultivate aftercare-free disposal practices to avoid imposing problems on future generations (Allesch & Brunner, 2015).

MFA is common to be applied in waste management and serves different purposes (Brunner & Rechberger, 2016):

### 1) Application in waste analysis as an alternative to direct analysis

Since MFA enables the investigation of flows on good and substance levels, this approach is useful for investigating the amount and composition of waste simultaneously. Direct analysis (also known as “sample and sort”) is often inefficient, requiring many working hours and expensive equipment. MFA can bypass direct analysis either by market product analysis or analysis of products of waste treatment (see Figure 5).

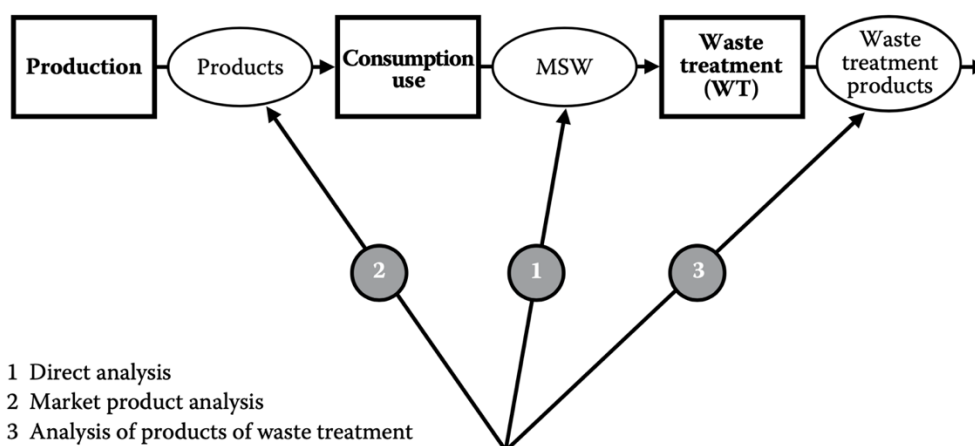


Figure 5: Methods of Municipal Solid Waste analysis ((Brunner & Rechberger, 2016) from (Brunner & Ernst, 1986))

Market product analysis allows a simple and quick estimation of waste generation using production data. It is predestined for scenario development, as production data is generated before products are classified as waste. Thus, waste flows can be predicted by considering production inflow into society consumption and the lifetime of products. This method is used by the US EPA (US EPA, 2002). In addition to production statistics, also sales data can be used, as done by Steubing et al. (2009) for computer waste generation in Chile. (Brunner & Rechberger, 2016)

Analysing waste treatment products takes advantage of an inherent objective of waste treatment systems, that is: sorting material. Therefore, output flows are usually better characterized than unsorted waste. If the input and output mass is known and treatment residues are characterized, the waste composition can be calculated via MFA. This approach has been frequently used for waste incineration treatment systems. (Brunner & Rechberger, 2016)

## 2) Application in waste management decision-making

MFA allows analysing and visualizing the current system situation. Results can be used to identify problems (as done in the above-mentioned case of the inefficient anaerobic digestion process of switchgrass by (Niu et al., 2015)), serve as a basis for scenario assessment, either to compare different treatment systems (e.g. (Padeyanda et al., 2016) for different food waste treatment options for Daejeon Metropolitan City, Korea) or make predictions regarding future developments (e.g. (Lederer et al., 2021) for demolition waste generation in the building sector of Vienna, Austria). Additionally, MFA proves as valuable when it comes to system transparency since the underlying mass balance principle prevents unintentional or deliberate negligence of certain flows in the course of the system processes (e.g. hazardous emissions) (Allesch & Brunner, 2015). With its dynamic approach, MFA might help notice problems building up before they become too critical (e.g. the future build-up of lithium-ion battery waste from electric vehicles (Richa et al., 2014)).

Even if not much data is available, which will lead to highly uncertain results, formulating different scenarios with regard to their likelihood is helpful. The goal of a successful MFA is not coming close to eliminating uncertainty, but achieving as much cost-effective reliability as needed, so that results can be used as a well-founded basis in decision-making. Due to its relative simplicity, making MFA the basis of interdisciplinary communication can be very beneficial. Its results, presented with the help of visualization tools like Sankey diagrams, can be understood and discussed by various societal fields like politics, the general public, science and industry (Allesch & Brunner, 2015). (Brunner & Rechberger, 2016)

A literature review by Allesch & Brunner (2015) of 83 publications, applying MFA as decision support in waste management, revealed that most studies performed the analysis on substance level (50 %). 25 % evaluated systems on good level and the remaining 25 % considered both levels. Common waste types to be investigated are mainly Municipal Solid Waste and electronic waste, but also construction and demolition, biological, plastic, and industrial waste. 47 % of the publications aimed at assessing the performance of existing systems, followed by comparing different treatment options (20 %), analysing systems for subsequent qualitative interpretation or as a basis for evaluation methods like life cycle assessment (13 %) and scenario analysis or predictions (20 %). Interpretation of MFA results focused on resource potential, environmental effects, and energy performance. A wide variety of system scales was investigated, ranging from cities to countries to global contexts. The study demonstrates the importance of MFA for various intents of decision-making in waste management. (Allesch & Brunner, 2015)

Closing material cycles to enable resource efficiency and protection of human and environmental health requires trustworthy tracking of hazardous compounds in waste, that is meant to be used as a resource in a Circular Economy (CE). CE requires information both on the amount of potentially recyclable products of waste treatment systems as well as composition regarding valuable substances (e.g. phosphorous in organic waste components for fertilizer use) or hazardous substances that hinder recycling (e.g. cadmium in MSW). Furthermore, workers of treatment facilities can be protected by considering where critical concentrations and emissions of hazardous substances occur within the process. Against the background of CE, the boundary between waste and resource management blurs, which broadens the scope for CE researchers from formerly waste-specific areas to increasingly integrated life cycle and resource-based considerations of



anthropogenically used materials. In short, MFA supports appropriate waste management by providing information on the waste composition and supporting data-based decision-making regarding development scenarios. It is a valuable tool to improve waste management in the context of CE. (Brunner & Rechberger, 2016)

In waste management, studying the treatment of organic wastes via MFA remains a challenge. Organic waste treatment often involves biological processes like composting or anaerobic digestion (Zabaleta et al., 2020). Due to their complexity and dependency on specific process conditions, like temperature, pH, and water content (ibid.), they are subject to significant fluctuations (e.g. (Yu et al., 2021), (Jie Wei et al., 2016)). Moreover, waste generation may vary in quantity and composition over time (Vergara & Tchobanoglous, 2012). To address the significance of time-dependent process variations, organic waste management requires adequate dynamic MFA tools (Urtnowski-Morin et al., 2021). Also, TCs, which are MFA's main concept to describe material distribution within systems, cannot always sufficiently describe complex processes (ibid.). A solution might be integrating more specific models into the MFA framework to describe processes within the system that exceed the applicability of TCs (ibid.). Urtnowski-Morin et al. (2021) presented the suitability of integrating a first-order model and more specific process models as improvement of MFA for the case of anaerobic digestion, suggesting the adoption of this approach in other fields of waste management.

## 2.3 MFA Software

### 2.3.1 STAN

In 2006, the Technical University of Vienna in cooperation with Inka software released the first version of STAN ("subSTance flow ANalysis") (TU Wien, 2022a). Today, freely available as version 2.7.101 with over 20.000 registered users (ibid.), it is the most popular tool in the MFA community (Brunner & Rechberger, 2016). STAN is frequently used in waste management (TU Wien, 2022b) and allows the performance of MFA according to the Austrian standard ÖNORM S 2096 (ASI Austrian Standards International, 2005), which regulates the application of MFA in waste management (Brunner & Rechberger, 2016).

Performing MFA with STAN follows the same pattern as the general MFA procedure described by (Brunner & Rechberger, 2016) (discussed in chapter 2.1, p. 3) (ibid.). The tool provides a graphical interface to develop the model by adding processes, flows, system boundaries, and text fields (Cencic & Rechberger, 2008). Both good and substance levels can simultaneously be handled, and subsystems can be defined (Brunner & Rechberger, 2016). After system definition, flow values, mass fractions, stock values, TCs, or other linear relations can be used as input data (ibid.). Data uncertainties can be taken into account by specifying standard errors (e.g.  $100 \text{ t}\cdot\text{year}^{-1}$  with a standard error of  $\pm 10 \text{ t}\cdot\text{year}^{-1}$  or 10 %), resulting in normal distribution functions (ibid.), which have limited significance in relation to reality (see chapter 2.1, p. 3) (Laner et al., 2014). Other probability distributions cannot be applied (ibid.). Given the system definition and input data, STAN can generate model results by means of data reconciliation, calculation of unknown data (if possible), and uncertainty evaluation using error propagation (Brunner & Rechberger, 2016). Results are displayed as Sankey diagrams, integrated into the graphical interface (see Figure 6, p. 11) (ibid.). Data can be imported from and exported to Excel (ibid.).

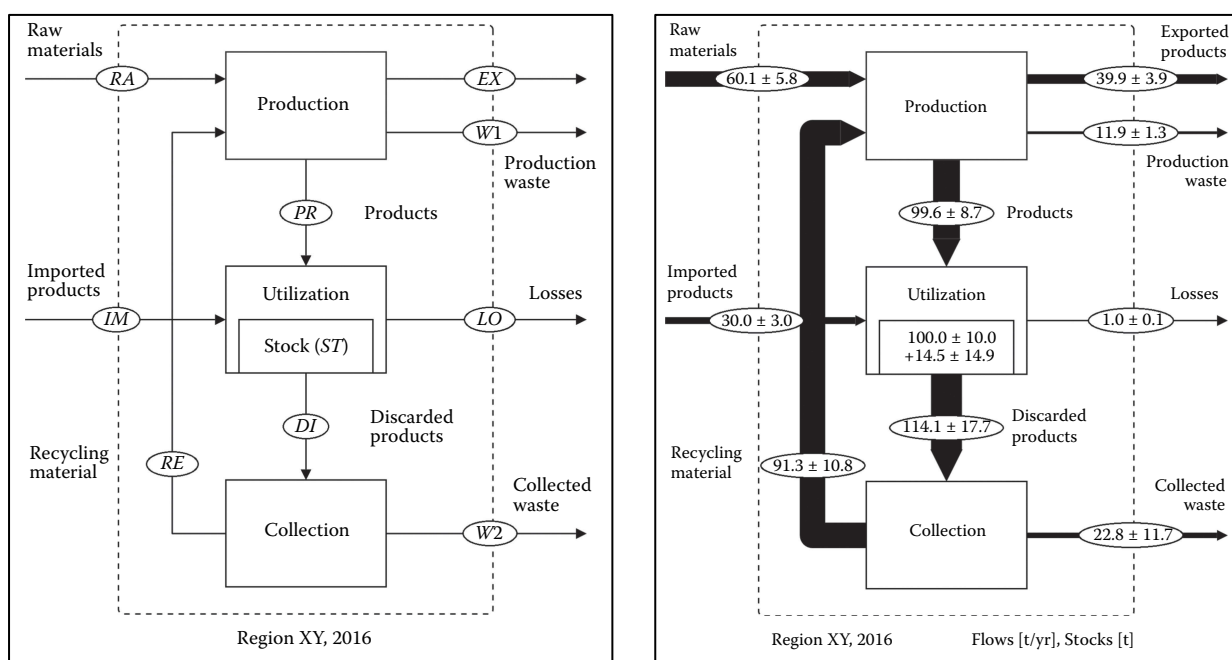


Figure 6: Graphical model (left) and Sankey diagram of results (right) of an exemplary system in STAN (Brunner & Rechberger, 2016)

There is controversy regarding the question if STAN can perform dynamic analysis, resulting primarily from different definitions of dynamic MFA. The software allows system definition for different time steps. Stocks from previous periods are added to the current, which the developers call a dynamic approach (Cencic & Rechberger, 2008). However, it is not possible to assess systems based on continuous functions (e.g. first order decay) (ibid.), which prevents the calculation of complex dynamic stock behaviours (Bornhöft, 2017). Stock behaviours that cannot be studied with STAN can be as simple as the example given by Bornhöft (2017), in which material stays in stock for several periods and is released at a specific rate per year afterward. Depending on the use case, researchers **1**) used the period function as dynamic MFA (e.g. (Bonnin et al., 2012)), **2**) used the period function and modelled the dynamic stock manually with subsequent entry of specific results into STAN (e.g. (Bornhöft, 2017)), **3**) used STAN to calculate the steady-state situation and then applied the obtained results (e.g. TCs) in dynamic MFA in Excel (e.g. (Pivnenko et al., 2016)) or other tools (e.g. (Kawecki et al., 2021)).

STAN is an accessible and freely available program for performing fundamental aspects of MFA. It is a well-established tool within the MFA community and has been applied in many scientific projects. Still, it has limitations regarding dynamic analysis and advanced uncertainty evaluation.

### 2.3.2 ODYM

In an approach to provide a solution for the problems that researchers face with popular MFA software like STAN, Stefan Pauliuk & Niko Heeren released the *Open software framework for DYnamic Material systems* (ODYM), written in the programming language Python, in 2020 (Pauliuk & Heeren, 2020). It has not been extensively applied in published literature and due to the lack of independent reviews, the presentation of ODYM in this chapter is mainly based on the paper of the developers. A general search in Google Scholar and a more specific search in the

“Journal of Industrial Ecology” revealed only a few papers that mention or use ODYM, most of them with the software developers as main- or co-authors.

The main motivation for the development of the tool was to establish a modelling framework for data-intensive investigation of complex problems, taking advantage of the intrinsic simplicity of MFA (Pauliuk & Heeren, 2020). ODYM only requires the fulfilment of the mass balance principle and the provision of suitable model data, within this framework, many aspects of systems can be explored. With ODYM, different materials, substances, regions, and periods can be simultaneously and dynamically investigated, while enabling advanced uncertainty evaluation of modelling data. (ibid.)

According to Pauliuk & Heeren (2020), the unavailability of appropriate, adaptable software led to the situation that MFA is applied by using various practices. This prevents researchers from working together successfully. Thus, ODYM provides a uniform data format to better facilitate cooperation between research teams. Enabling adaptation and at the same time providing a standardized modelling framework requires establishing a delicate balance between what the authors call “flexibility” and “rigidity”. In order to clearly structure the large number of possible system aspects, the software provides a structure that determines how information has to be inserted into the model database. (Pauliuk & Heeren, 2020)

ODYM is published as Free and Open Source Software (FOSS) (ibid.), which allows the reuse of the code within the scope of its license conditions (Manabe et al., 2014; Open Source Initiative, n.d.). While sometimes the provision of software packages with different FOSS licenses complicates the reuse (Manabe et al., 2014), ODYM is published exclusively under the MIT permissive license (Pauliuk & Heeren, 2020). It grants permission to “[...] deal in the Software without restriction, including without limitation the rights to use, copy, modify, merge, publish, distribute, sublicense, and/or sell copies of the Software, and to permit persons to whom the Software is furnished to do so [...]” (Open Source Initiative, n.d.). The only condition is to indicate the copyright notice along with the permission notice (ibid.). In contrast to popular MFA software like STAN, this allows researchers to adapt the software to fit their specific needs. In addition to allowing modification of the framework, ODYM’s modular programming structure is even intentionally designed to support adaptation (Pauliuk & Heeren, 2020). Modular software consists of different parts that are at least to some extent independent of each other (Dennis, 1975). They can be combined as needed to address a particular problem, without having to change the code or make use of all software modules (ibid.). Modularity also enables combining software modules with independently written code to modify and extend the provided program (ibid.). To serve as a tool to solve different scientific problems in various fields, modularity must be considered while writing the code (Kang et al., 2012), which has been done in the case of ODYM (Pauliuk & Heeren, 2020). Thus, modularity enables not just considering only the parameters and model aspects that are relevant but also adapting the framework, like adding a first-order model for biological processes that cannot always be described by the use of TCs, as suggested by Urtnowski-Morin et al. (2021).

Other features of ODYM are automatic consistency and mass balance checks. More specific explanations regarding essential features as well as ODYM’s modelling structure will be provided in chapter 5.1 (p. 22), based on the template version developed for this thesis. (Pauliuk & Heeren, 2020)

The software code with explanations along with extensive documentation in form of a Wiki and exemplary tutorials can be accessed via a GitHub repository (Pauliuk & Heeren, 2022). Tutorial No. 5. demonstrates ODYM's suitability for performing extensive dynamic MFA by modelling the global passenger vehicle fleet in 2017, considering the period 1990–2017, 130 countries, relevant processes, and various materials (like steel, Al, plastics, ...) (ibid.). For the calculation, integrated dynamic stock modelling functions are used, which allow the determination of the stocks with the help of lifetime functions (ibid.). The example also includes a Monte-Carlo-Simulation (MCS) for evaluating the uncertainty regarding the material content and the lifetime of the vehicles (ibid.). Nonetheless, ODYM does not provide a built-in procedure for MCS, this part of the analysis must be manually programmed depending on the specific use case (Pauliuk & Heeren, 2020). In addition, built-in options for visualization of model results via Sankey diagrams have also not been implemented yet (ibid.). Finally, due to the lack of a graphical user interface, ODYM requires programming skills for its usage.

ODYM is a recently published approach to facilitate dynamic MFA of complex systems. It provides a framework for the analysis as well as tools for dynamic stock modelling. The software is free and open, allowing researchers familiar with Python to fit the software to their needs, such as adding specific process models, advanced uncertainty evaluation, and MCS. Although there are other Python MFA tools (e.g. PYMFA 2.1 (Thiébaud, 2019) or DPMFA (Bornhöft, 2017)), ODYM stands out as an approach designed for adaptation as an open science tool.

## 2.4 Programming in Python

Python is a prevalent programming language, which was released in 1991 (Lubanovic, 2014). Today, it is used in various fields like data science, artificial intelligence, game development, and scientific research (Rolon-Mérette et al., 2020). Users range from private individuals to scientists to employers at companies like Google, YouTube, or Netflix (Lubanovic, 2014; Rolon-Mérette et al., 2020). Python is free and open source, running on all common operating systems (Windows, Mac, Linux, Ubuntu) with low computational power demand (Rolon-Mérette et al., 2020).

Compared to other programming languages, its structure is considered to be easy to learn (Lubanovic, 2014). Besides being accessible, a highly beneficial aspect regarding Python's potential is the large and active community of users (Rolon-Mérette et al., 2020). The Python online community provides support for all levels of programmers in the entirety of the field:

**1)** There are large numbers of **tutorials**, many of them free, in the form of text documents, online courses, and videos to begin programming, but teaching material is also provided for complex and more specific topics (e.g. machine learning for medical data (Bloice & Holzinger, 2016)) (Rolon-Mérette et al., 2020).

**2)** Programmers can make use of previous efforts by using ready-to-use **software** or pre-written code ("**packages**"), targeting programming procedures common to many different application fields (ibid.). For example, if one would like to access data from a Microsoft Excel spreadsheet for a Python project, there is no need to write the whole code to do so, one can use, for instance, the package `pandas` (McKinney & Team, 2015). Instead of having to start from scratch by developing an interface between Excel and Python, one can conveniently use the `pandas` formula `read_excel('Example.xlsx')` to import data from a spreadsheet into a Python project.

With `pandas`, users can handle analysis and manipulation of databases like Microsoft Excel directly in Python (ibid.). Further popular Python packages in scientific research are `NumPy` (array calculation for efficiently processing large sets of data), `SciPy` (statistics, optimization, ...), and `SciKit` (machine learning) (Lubanovic, 2014).

**3)** Python developers can provide and ask for support in various **online forums**. Reusing software snippets from web pages, tutorials, and forums, also known as Amethodical Snippet Remixing, is a common practice in software engineering (Philip et al., 2012). However, recent studies raised awareness of potential quality and security issues, advising researchers to be careful with using code snippets found on the popular forum Stack Overflow (Bafatakis et al., 2019; Rahman et al., 2019). Another very helpful tool is GitHub (Yang et al., 2017). While forums are dominated by Q&A discussions, the social coding website is intended to allow sharing code and exchanging ideas about it (ibid.). Combining repository characteristics with interaction tools capable of tracking, discussing, and resolving software issues, GitHub enables software development as a collaborative effort (Ma et al., 2017).

Writing and running Python code requires suitable development environments, like text editing requires software like Microsoft Office Word or OpenOffice (Rolon-Mérette et al., 2020). Anaconda is a program that provides tools for scientific programmers (ibid.), with the most common packages being pre-installed (others can be added) (ibid.). One offered tool is Jupyter Notebook (Randles et al., 2017). It contains cells, that can display code, code outputs, and text, which makes it suitable for providing ready-to-use code with explanations in a transparent way, allowing gradually building up the tool with consecutive code blocks in a document-like style (Kluyver et al., 2016; Mendez et al., 2019; Rolon-Mérette et al., 2020).

An increasing quantity of data requires researchers to make use of adequate software to investigate scientific research questions (Kadiyala & Kumar, 2017). Python and associated tools like Anaconda, GitHub, and Jupyter Notebook offer a suitable environment for scientific programming.

## 3 Materials and Methods

### 3.1 Theoretical Methodologies

#### 3.1.1 Literature Research

The work process was initialised by extensive literature research regarding MFA in general, its significance for waste management, and MFA software. The *Handbook of Material Flow Analysis* (HOMFA) (Brunner & Rechberger, 2016) served as an entry point for the research. It offers a comprehensive and detailed overview of MFA and associated engineering fields (e.g. waste management), MFA methodology, and practical case study applications to provide an extensive and at the same time practical manual for engineers (ibid.). The research was then expanded by using the snowballing method. The HOMFA refers to various research literature, which was systematically checked for other relevant references. The procedure was analogously applied multiple times for resulting publications (“snowballing”) (Rosert, 2009). For important sub-topics (e.g. statistics, Sankey diagrams), more specific literature was consulted. To further specify the requirements for MFA in organic waste management and the current state of research, systematic online research on specific topics complemented the snowballing procedure. To emphasise the relevance of the presented scientific background, example studies are cited that apply the described methods. They have been found via keyword online search.

In combination with studying papers where STAN has been used as a research tool, HOMFA’s chapter on the software is used to introduce the tool. The presentation of ODYM is mainly based on the associated publication (Pauliuk & Heeren, 2020).

In the further course of the thesis, the obtained state of the science is linked to the developed ODYM-based modelling script to discuss the applicability of the thesis’ template in the field.

### 3.2 Practical Methodologies

The template was developed on a MacBook Pro (Early 2015) with a 2,7 GHz Dual-Core Intel Core i5 Processor, 8 GB 1867 MHz DDR3, macOS Monterey Version 12.2.1.

#### 3.2.1 Jupyter Notebook

Jupyter Notebook version 6.4.11 has been used to write the code. Also, the modelling template is provided as a Jupyter Notebook.

#### 3.2.2 Case study

To present the features of the template, a case study system was modelled (see Figure 7, p. 16). It includes agricultural wheat production, subsequent treatment of residues (wheat straw), and the effect on the atmosphere, surface water, and aquifer and soil. The aim was to obtain information on the impact of the application of agricultural residue treatment products as soil conditioner on the carbon stock of the soil. Incorporation of crop residues and the use of treatment products like compost can help reduce carbon losses of soils and thus, ensuring soil fertility (Tiefenbacher et al., 2021). As discussed in chapter 2.2 (p. 8), CE requires waste management to also study more resource-based topics increasingly. Therefore, not only waste treatment, but also the application of

process products as a potential resource for agricultural use is covered. For the analysis, the system is investigated on good (biomass from agricultural production) and substance level (carbon) and is dynamically modelled for the years 2020 until 2040.

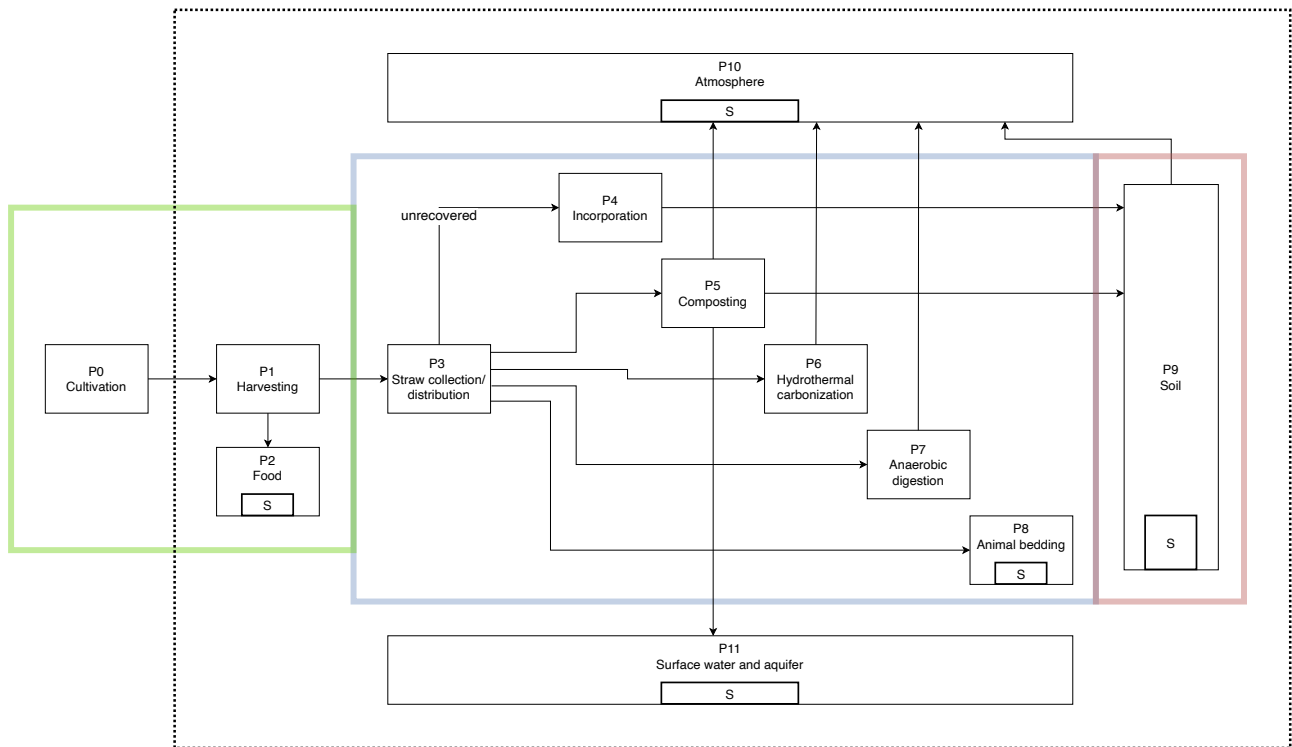


Figure 7: Case study MFA system including agricultural production (green), waste treatment (blue), and sequestration processes of soil conditioner products (red)

The carbon sequestration processes in the soil are calculated with a first order decay model according to Cayuela et al. (2010) based on Robertson & Paul (2000):

$$C_{remaining}(t) = f \cdot \exp(-k_1 t) + (100 - f) \cdot \exp(-k_2 t) \quad (1)$$

Organic matter consists of a wide variety of substances with different properties and carbon mineralization behaviours (Taneva et al., 2006). To address these variations, this type of modelling usually distinguishes between different pools that degrade with distinct decay rates (ibid.). In Equation 1,  $f$  is the fraction of carbon of the fast turnover pool,  $k_1$  is the decay rate parameter for the fast turnover pool,  $k_2$  is the corresponding parameter for the slow turnover pool,  $t$  is the process time in days (Robertson & Paul, 2000). The data for wheat straw is obtained from Cayuela et al. (2010):

Table 1: Sequestration formula data for wheat straw (Cayuela et al., 2010)

Residue type	$f$ [%]	$k_1$ [day <sup>-1</sup> ]	$k_2$ [day <sup>-1</sup> ]
Wheat straw	4.8	0.1975	0.0027

To keep the case study simple, other biological processes like anaerobic digestion and composting are described with TCs. Additionally, it is assumed that only the sequestration leads to soil outflows, the remaining fractions of the good accumulate as stock without any emissions. Also, the compost outflow is considered to have the same sequestration behaviour as the unprocessed wheat straw. Known input data are good and carbon imports from the cultivation, TCs for all processes (except soil carbon sequestration processes), and standard deviation of all given values (2 % for flows, 5 % for TCs and first order model parameters). Import flow and TC data can be viewed in Annex A (p. 39).

Analysis results should be displayed as Sankey diagrams and uncertainty evaluation is to be performed via Monte-Carlo-Simulation (Number of Monte-Carlo runs (NMC) = 10,000) with log-normal distribution of all input data as approximation standard. The case study input data are arbitrarily chosen and are only meant to demonstrate the template procedures. The open source vector graphics editor Inkscape (Inkscape Project, 2022) has been used for post-processing Sankey diagrams for presentation purposes (see Figure 9, p. 19), as suggested by Pauliuk & Hasan (2017).

### 3.2.3 Documentation

Documentation of the tool is provided using four methods:

**1)** The MFA procedure flowchart, introduced in chapter 2.1 (see Figure 2, p. 4), is used to present and explain the different modelling steps since the template has been structured in line with the flowchart. This part of the documentation can be found in the discussion chapter 5.1 (p. 22).

**2)** Unified Modeling Language (UML) provides different tools and methods, that are meant to support analysis, design, and implementation of software (Object Management Group, 2017). It is not a programming, but a frequently applied graphical modelling language, used in all steps of software development (Seemann & von Gudenberg, 2006). For this thesis, a UML use case diagram was developed to illustrate which features of the template are inherent to ODYM and which are customized extensions. The UML figure can be accessed in the results chapter 4 (p. 18) with further explanations in the discussion chapter 5.1 (p. 22).

**3)** Practical notes on how to use and adapt the tool can be found directly in the modelling template as comments.

**4)** A graphical and abbreviated interpretation of the explanations of documentation method 1) is provided to offer a structural overview as quick-start guide for the template. It is included in Annex C (p. 44) and in the GitHub repository of the biODYM modelling template (see results chapter 4 (p. 18)).



## 4 Results

The biODYM modelling template adapts ODYM for performing dynamic MFA in organic waste management. The results of the developing process are available via a GitHub repository (<https://github.com/lukashpe/biODYM-modelling-template>). It includes the following files:

- biODYM modelling template as Jupyter Notebook
- Excel input data template
- biODYM quick-start guide
- Copy of the original ODYM as of 20<sup>th</sup> of June 2022
- Case study modelling results of biODYM as Excel export
- Case study modelling in Excel to confirm biODYM results

biODYM is, like ODYM, published under the permissive MIT license, allowing users to use, adapt and distribute the template without restrictions (see chapter 2.3.2, p. 11). biODYM is capable of:

- Dynamic analysis with time-dependent transfer coefficients and input data
- Simultaneous investigation of good and substance level
- Integration of biological first order model processes (FOMPs)
- Monte-Carlo-Simulation (MCS)
- Export of MFA results to Excel
- Interactive Sankey diagrams

The added features (first order model, MCS, interactive Sankey diagram, Excel export) are directly included in the template. Figure 8 presents the UML use case diagram of biODYM.

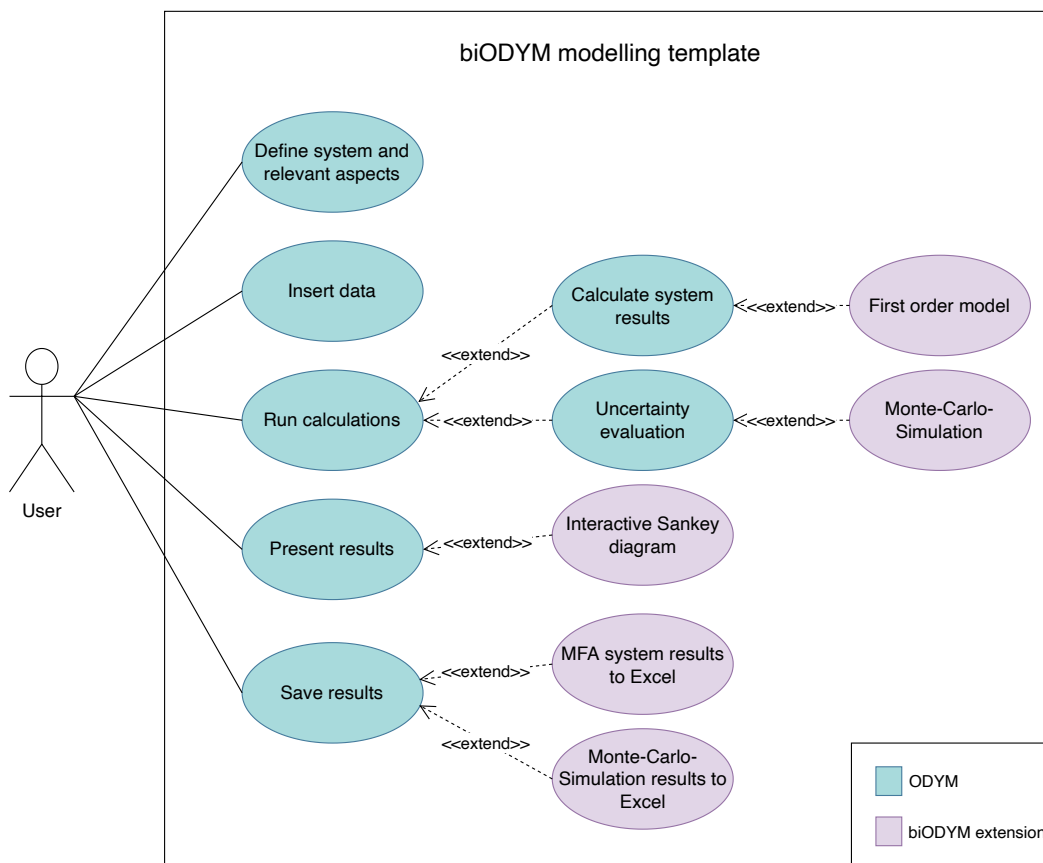


Figure 8: biODYM modelling template UML use case diagram

The structure of the template follows the general procedure of ODYM and is inspired by the tutorials provided along with the ODYM package. biODYM includes modelling a case study system that presents the used ODYM functions as well as the added features (see chapter 3.2.2, p. 15). Here, only figures for carbon are displayed, total results can be accessed in the modelling template:

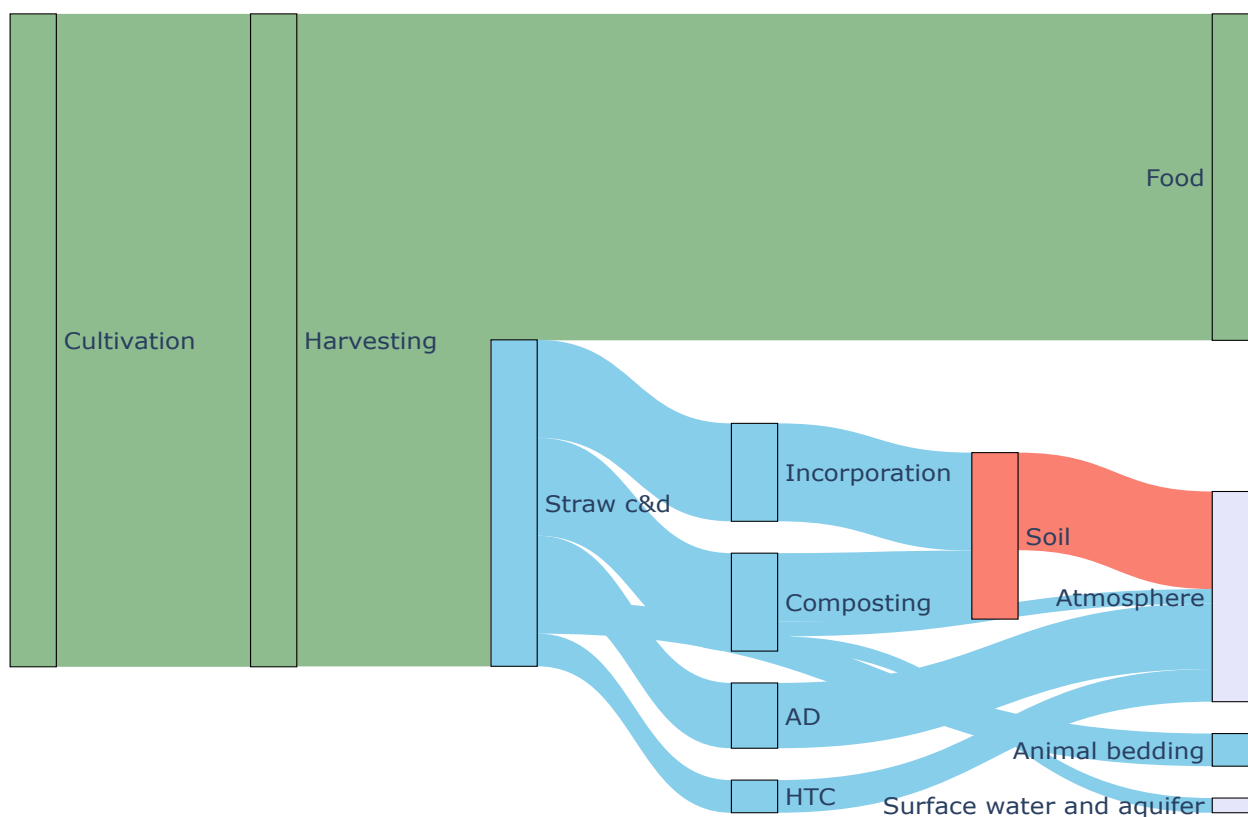


Figure 9: Screenshot of interactive Sankey diagram on carbon level for the year 2021 (modified)

Figure 9 shows a screenshot of the interactive Sankey diagram on carbon level for the year 2021. In the notebook, a slider is used to switch between years. Figure 9 has been modified on vector basis, so that the output flows of the “Harvesting” process do not overlap. From “Straw c&d” on, overlapping cannot be avoided without taking up significantly more space for the diagram system structure. With the interactive Sankey diagram in the template, however, each flow can be clearly characterised: hovering with the cursor on a flow, it is highlighted, and its source and target process and the mass values are displayed.

MCS (Number of Monte-Carlo runs (NMC) = 10,000) results are shown in Figure 10–Figure 13 for the carbon inflow to (Figure 10 & Figure 11, p. 20) and the stock in (Figure 12 & Figure 13, p. 21) the soil. The simple plot displays all model runs as separate lines, whereas the violin plot shows mean values (white dots with orange line), data ranges (whiskers), upper and lower quartile (black boxes), and probability density functions (“violin body”).

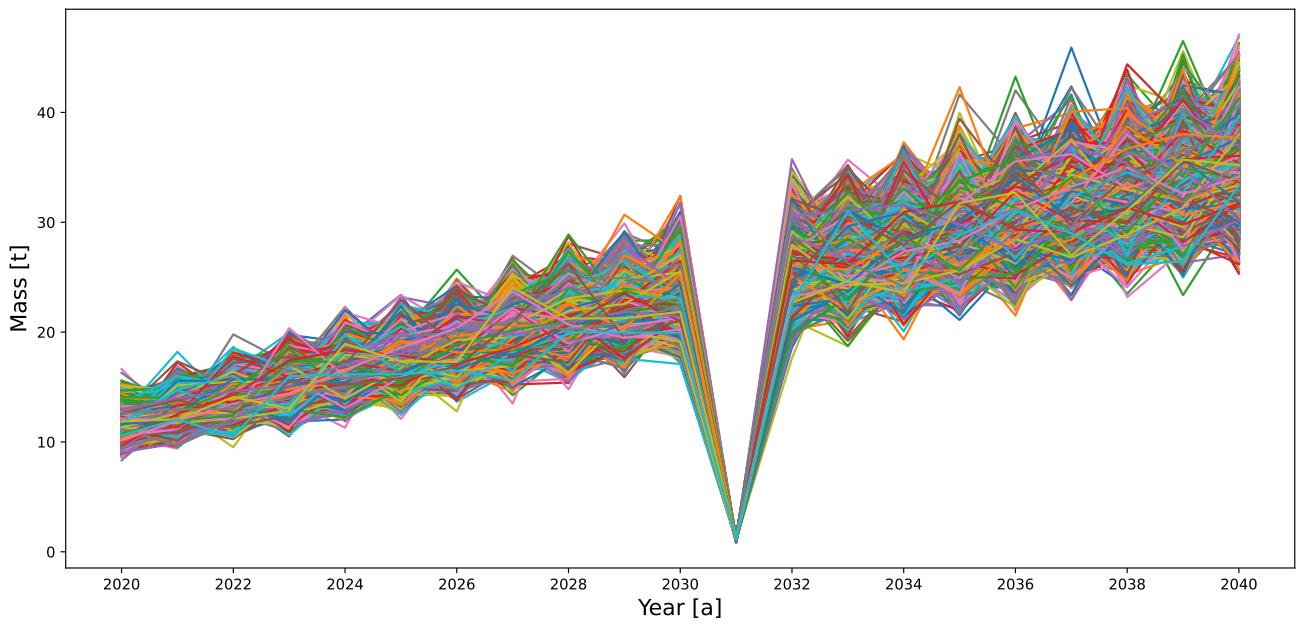


Figure 10: Plot carbon inflow to soil (NMC =10,000)

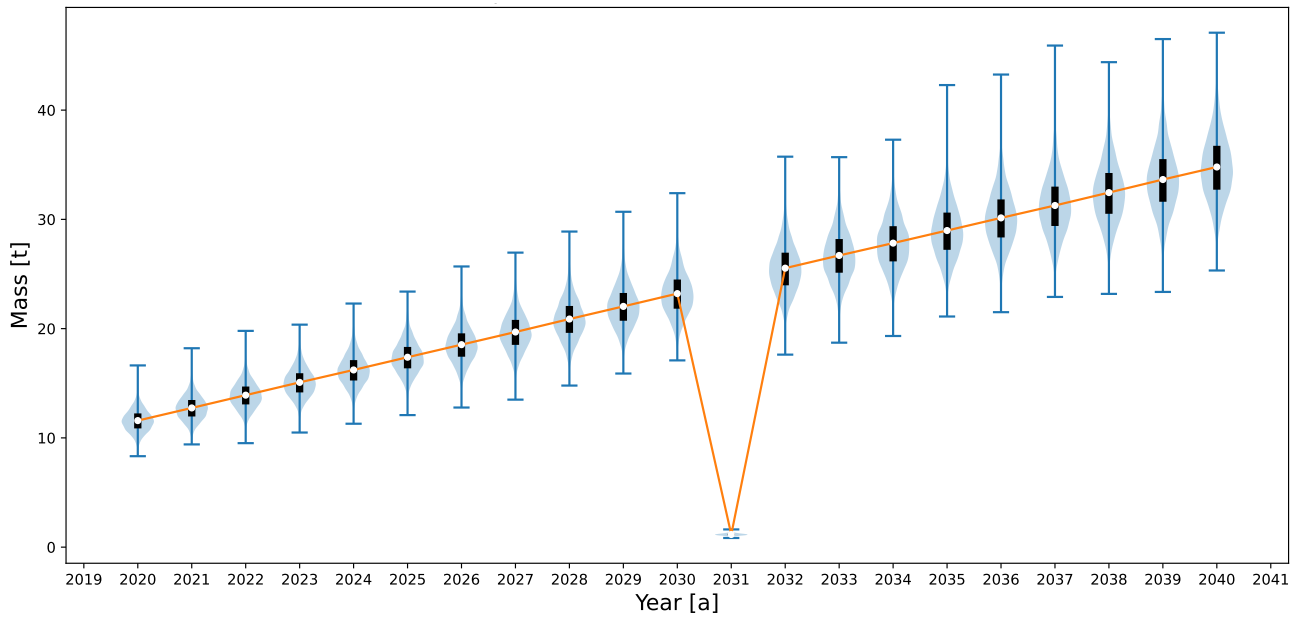


Figure 11: Violin plot carbon inflow to soil (NMC = 10,000)

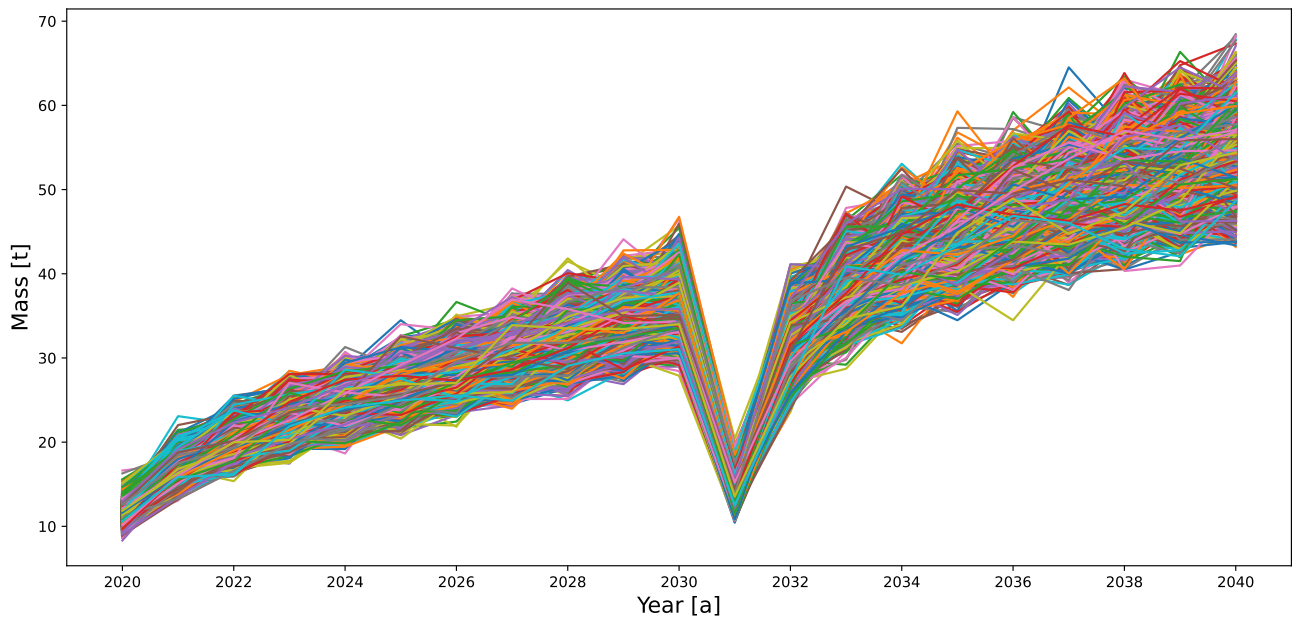


Figure 12: Plot carbon stock in soil (NMC = 10,000)

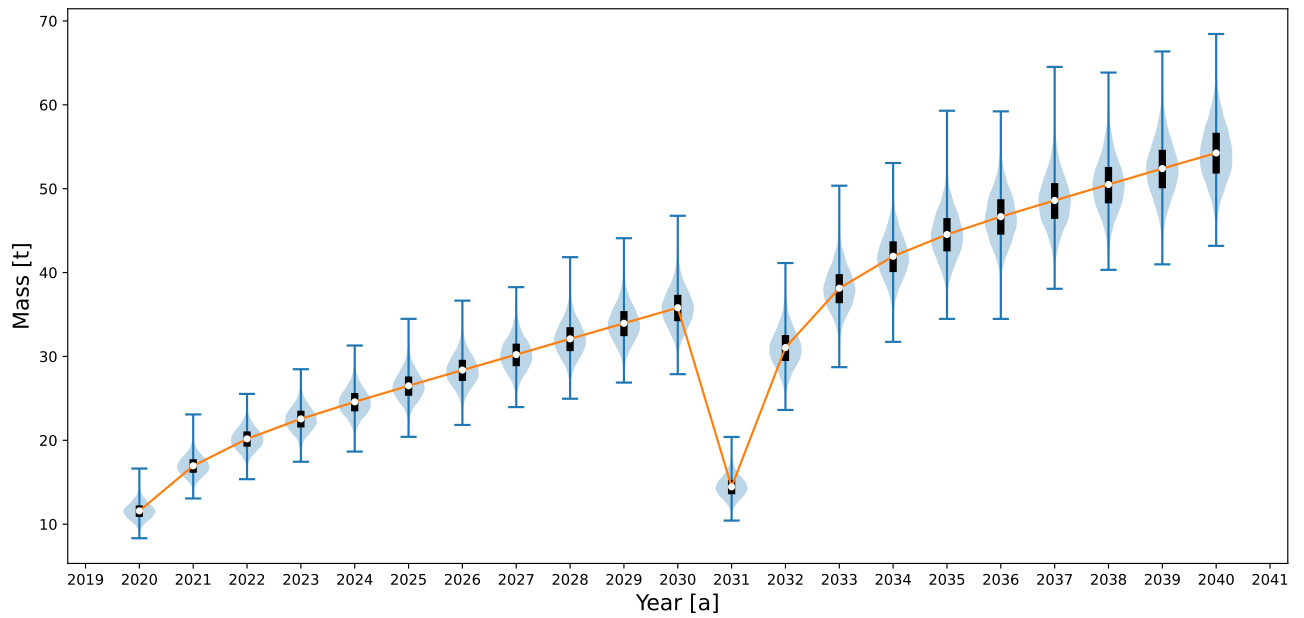


Figure 13: Violin plot carbon stock in soil (NMC = 10,000)

## 5 Discussion

### 5.1 How does the biODYM modelling template work?

The template presents essential features of ODYM and is complemented by specific biODYM extensions. The extensions are directly written into the notebook and not woven into the ODYM code or provided as a separate package, the latter two options being the usual coding style. This is done to enable simple modification and to visualize their structure without having to look at class or function files. Also, the extensions are not developed enough to be used as a separate Python package, since they need to be modified for different use cases. It is, for example, not possible to use the integrated Sankey diagram option as simple as the `pandas` formula `read_excel('Example.xlsx')` (see chapter 2.4, p. 13). There is a one-line formula `sankey_diagram_results(flows_Values_loop, element)` but it requires input data that has been processed by manual coding (for details see template section 4.2). Programming general Python packages or professional software is an enormously complex and lengthy process considered to be out of the scope of this thesis. The extensions are practical and working means to explore ODYM's potential for adaptations, including specific ones (first order model) but also suggestion stimuli for general improvements for future versions of the framework (interactive Sankey diagrams).

The developing process of biODYM was based on the ODYM tutorials provided in the GitHub repository of the tool (Pauliuk & Heeren, 2022). In fact, the template could be thought of as another ODYM tutorial addressing more specific functions helpful for organic waste management, but also suggesting general improvements. Due to the framework's modular design, looking through various tutorial application cases enabled easy adoption of procedures to biODYM and modifying them to fit the case study's needs. Especially starting steps, like defining the system, setting a modelling period, and choosing relevant system aspects, usually include the same initiating routines. Presenting the intended data structure in the tutorials also made transparent at which points and how extensions can be included. The developers themselves sometimes added calculation steps that have not been implemented yet into ODYM as inherent features (e.g. MCS in Tutorial No. 5.). The detailed documentation including the introduction paper (Pauliuk & Heeren, 2020), a Wiki page, tutorials, and detailed explanations enabled a straightforward working process for this thesis, making ODYM a prime example for open science.

In the background on MFA terminology and procedure chapter 2.1 (p. 3), the MFA procedure flow chart (see Figure 2, p. 4) has been introduced and is now used to explain what the template does stepwise. It should be noted that ODYM is a large modelling framework with many functions (see chapter 2.3.2, p. 11). Here, only the features included in the bioODYM modelling template are explained. Nevertheless, other ODYM features can be implemented if needed. In the original flow chart, the steps were deliberately unnumbered to emphasise the iterative character of MFA. For reasons of clarity, numbers are given for them in the following section:

#### 0 Problem and goal definition/Load packages

Problem and goal of the study must be defined before starting the analysis with biODYM. For the case study, this has been done in the materials and methods chapter 3.2.2 (p. 15). Instead, the template starts with an introduction, and the first coding cell loads ODYM and its required packages

as well as additional packages that were used for the adaptations. A local copy of ODYM as of the 20<sup>th</sup> of June 2022 is loaded (included in the biODYM repository) to assure that the template keeps working even after major updates on the original version. Still, it is unlikely that changes will affect the general functions of ODYM to this extent and the original framework may be used just as well. Furthermore, the framework requires the following packages:

- `sys`
- `os`
- `pandas`
- `matplotlib.pyplot`
- `pickle`
- `pylab`

Additional packages are:

- `matplotlib.ticker` (*plotting*)
- `plotly.graph_objects` (*interactive Sankey diagram*)
- `ipywidgets` (*interactive Sankey diagram*)
- `xlsxwriter` (*results export to Excel*)
- `scipy.stats` (*MCS*)

## 1 Definition of system and relevant aspects

In this section, the qualitative model is developed. The model period, relevant goods and substances, processes, flows, stocks, and stock changes are defined. The outcome could be likened to the graphical model of STAN (see Figure 6 (left), p.11). Instead of graphical symbols, ODYM uses lists, tables, dictionaries, and arrays to store information. System aspects (for the case study time and element) are stored in an index table. Each component (process, flow, stock) is defined by specific attributes: Processes receive an ID and are stored in a list, the IDs are then used to define where flows and stocks occur. Indices, referring to the index table, indicate the dimensions (time and/or element dependence). In the template, goods and substances are both called elements. Flows and stocks along with their attributes are stored in separate dictionaries `FlowDict` and `StockDict`. At the end of the section, a value array filled with zeros as placeholder according to the given dimension is assigned to each flow, stock, and stock change. For the case study, the arrays have the shape (21, 2), corresponding to the number of analysis years and elements (total biomass and carbon) (see Figure 14, p. 24). They are used to store and compute results in the further course of the analysis.

Component values and corresponding calculations are completely built upon arrays, and the considered system aspects define their dimension. For instance, if additionally, three different regions, applying the same treatment process, should be compared in the MFA, the dimension of the arrays would be (21, 3, 2). The index table would then list time, region, and element as system aspects.

```
array([[0., 0.],
       [0., 0.],
       [0., 0.],
       [0., 0.],
       [0., 0.],
       [0., 0.],
       [0., 0.],
       [0., 0.],
       [0., 0.],
       [0., 0.],
       [0., 0.],
       [0., 0.],
       [0., 0.],
       [0., 0.],
       [0., 0.],
       [0., 0.],
       [0., 0.],
       [0., 0.],
       [0., 0.],
       [0., 0.]])
```

Figure 14: Exemplary empty array for the case study dimensions

The ODYM data structure is responsible for its analytical power. When the system is defined, any calculations can be performed with Python coding. The modelling framework is not limited to a given set of calculation functions (like e.g. STAN). Results must only fit the ODYM data structure at the end of the calculations. The user is free to explore the whole range of Python's potential. Admittedly, this also challenges user-friendliness, which will be further discussed in the next chapter 5.2 (p. 27). Pauliuk & Heeren (2020) consider ODYM's data structure the most relevant novelty for the MFA community.

## 2 Data input into model

Given data is imported from the Excel template. In the case study, import flows on both levels, TCs on both levels, and relative standard deviation for all values are given. Standard deviation is specified by default values defined in the sheet "relSTD\_default" but can be manually changed for individual flows and stocks. The data import is followed by inserting the data into ODYM's data structure. Input data is assigned into a parameter dictionary `ParameterDict` and empty value arrays get created analogously to the procedure for `StockDict` and `FlowDict`. In addition to values, the relative standard deviation is also stored. The Excel template and the code that facilitates the import can be modified to fit other research questions.

After defining the system and inserting input data into the model, ODYM enables an automatic consistency check, which checks if dimensions have been used consistently and if flows have been assigned only to existing processes. This feature allows definition errors to be found quickly. The absence of a graphical user interface makes it more difficult to develop the qualitative model, the consistency check is a way to compensate for this complication.

At this point, the qualitative MFA system is defined, and an ODYM-compliant memory of all input data has been created. In the next step, analysis results are calculated.

### 3 MFA Calculations

Calculations start with computing results that do not depend on first order model processes (FOMPs). In the case study, all flows (except  $F_{0\_1}$ , which is given and directly inserted into `FlowDict`) are calculated via TCs:

$$F_{y\_z} = F_{x\_y} \cdot TC_{y\_z} \quad (2)$$

The arrays of flows and the TCs are combined via the Hadamard product, which allows the multiplication of same dimension matrices according to the scheme:

$$\begin{array}{ccc} & & \xrightarrow{\text{Elements}} \\ \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \\ a_{31} & a_{32} \\ \dots & \dots \end{bmatrix} \cdot \begin{bmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \\ b_{31} & b_{32} \\ \dots & \dots \end{bmatrix} = \begin{bmatrix} a_{11} \cdot b_{11} & a_{12} \cdot b_{12} \\ a_{21} \cdot b_{21} & b_{22} \cdot b_{22} \\ a_{31} \cdot b_{31} & a_{32} \cdot b_{32} \\ \dots & \dots \end{bmatrix} \quad \downarrow \text{Years} \\ F_{x\_y} & TC_{y\_z} & F_{y\_z} \end{array} \quad (3)$$

This is very practical and is applied throughout ODYM. Calculations don't have to be repeated for each element and year, they are performed simultaneously.

Other formulas for flow computing can be applied, depending on the input data. If, for instance, TCs on good level are known, but only mass fractions  $x$  on substance level are given, the flows  $F$  for substances could be calculated via:

$$F_{substance} = F_{good} \cdot x_{substance} \quad (4)$$

Another option that has been applied frequently in the ODYM tutorials (Pauliuk & Heeren, 2022) is dynamic stock modelling with lifetime functions (see chapter 2.1, p. 3). The Excel template only presents the first option via TCs, but other approaches like those mentioned can be integrated.

In the case study, annual stock changes ( $dS(t)$ ) correspond to the difference of inflow ( $F_i(t)$ ) to outflow ( $F_o(t)$ ), the actual stock is then calculated by summing up all stock changes:

$$dS(t) = F_i(t) - F_o(t) \quad (5)$$

$$S = \sum dS(t) \quad (6)$$

The calculations of FOMPs are separated from the standard ODYM procedure. The associated parameters are stored in a separate dictionary `BioParameterDict`. Values and uncertainties are inserted manually into the notebook and not imported via the Excel template. The goal behind this approach is not to intervene with ODYM's complex structure and obstruct it in any way. After calculating the part of the system independent of FOMPs, the standard ODYM procedure is put on pause, a new model is defined with separate practices to calculate FOMPs and the results are fitted to ODYM's data structure and then the ODYM procedure is continued. This technique can be applied to any number of FOMPs in a system. The first order model is also built upon array calculations.



Extensive looping through each year and element to apply the exponential function is more intuitive, but very inefficient. With regard to the MCS (where calculations are run 10,000 times), a fast approach had to be chosen. The first order exponential function is used to calculate the relative course of the decay process through the years ( $d_{year}$ ), which can then be used for all cohort inflows  $F_{ic}$ . The computation follows:

$$\begin{array}{c} \text{Cohort-Years} \\ \xrightarrow{\hspace{1.5cm}} \\ \text{Years} \downarrow \begin{bmatrix} F_{i1} & 0 & 0 \\ F_{i1} & F_{i2} & 0 \\ F_{i1} & F_{i2} & F_{i3} \end{bmatrix} \wedge \begin{bmatrix} d_1 \\ d_2 \\ d_3 \end{bmatrix} = \begin{bmatrix} F_{i1} \cdot d_1 & 0 & 0 \\ F_{i1} \cdot d_2 & F_{i2} \cdot d_1 & 0 \\ F_{i1} \cdot d_3 & F_{i2} \cdot d_2 & F_{i3} \cdot d_1 \end{bmatrix} \end{array} \quad (7)$$

$F_{i1}$  is the inflow into the FOMP in year 1 and the first column of the result array represents the first order decay of this inflow cohort.  $F_{i2}$  is the inflow in year 2, which is not yet present in year 1, thus, the decay process starts in year 2 with  $d_1$ . In the case study, summing up each row of the result array leads to the total stock of the process in each year, since the applied exponential equation (Equation (1), p. 16) represents the share of remaining carbon during the sequestration process. However, this calculation approach is not limited to stock calculations. For instance, a first order model that represents emissions could also be used (e.g. first order model for methane emissions from landfills (Towprayoon et al., 2019)). Summing up array rows would then represent the annual emission outflow of the process.

In the case study, after computing the soil stock and stock change for each year, Equation (5) (p. 25) is rearranged to obtain the outflows:

$$F_o(t) = F_i(t) - dS(t) \quad (8)$$

Results are then inserted into `StockDict` and `FlowDict`.

Before the MCS is done, ODYM provides an automatic mass balance check that reports the balance dimension and all absolute balancing errors per process. For the case study, the balance dimension is (21 time steps, 12 processes, 2 elements) and no significant errors are reported (specified are only balancing errors with an order of magnitude smaller than  $10^{-12}$  due to computer hardware arithmetic (Python Software Foundation, 2008)).

The MCS in essence repeats all the preceding calculations but introduces another dimension: according to the given standard deviation and, assuming a log-normal distribution for each parameter, 10,000 pseudo-random values are drawn. The dimension of the arrays is now (10,000, 21, 2) and they are stored in separate MCS dictionaries. The calculations done to compute the initial results are then repeated but with the MCS dictionaries and flow and stock results (now also in the dimension (10,000, 21, 2)) are again separately stored. More specific distributions functions like Weibull or gamma distribution can be integrated into the template. The simulation closes by calculating the absolute standard deviation for all stock and flow values for the Excel export.

Building the code on array calculations, the complete MCS with generating pseudo-random values and repeating all calculations with three-dimensional arrays takes as much time as running the first discarded looping FOMP approach just once (on average around 5-9  $\mu$ s).

## 4 Presentation (+ Interpretation) of results

All flows and stocks can be plotted via simple plots. In the case study, the inflow into the soil and the stock development of the soil over the years on good and carbon level are plotted.

ODYM originally does not include procedures for integrated Sankey diagrams (Pauliuk & Heeren, 2020). The biODYM modelling template includes a first approach to provide an option for dynamic and interactive Sankey diagrams. The method makes use of ODYM's dictionaries and extracts all information needed to build the diagram. Then, the `ipywidget` package together with the `plotly` package is used to create plots that can be controlled with a slider to present annual results. Although there have been Python-based innovations for Sankey diagrams (e.g. hybrid Sankey diagrams (Lupton & Allwood, 2017)), the author is not aware of any published methods for interactive Sankey diagrams in Python. The developed approach is inspired by an application of the European Union's statistical office that visualises material flows within the EU as an interactive Sankey diagram (with many more details) (European Commission, 2020b). In its current version, the interactive Sankey diagram option of biODYM needs to be modified for other problems (more elements, comparing regions, ...), but the general procedure could be applied to any MFA problem. Further developed and refined, it could be implemented into the ODYM framework as an easy visualization feature for MFA results in all fields.

MCS results are displayed as violin plots and simple plots of all model runs.

In a last step, MFA results of all flows and stocks are exported to Excel. Additionally, mean values and absolute standard deviation of the MCS are also exported as a separate file. Although ODYM provides exporting options, an individual method has been developed that fits the structure of the used Excel template.

Interpretation of the MFA results is not included in the template.

The case study calculations have been confirmed by calculating the MFA in Excel by hand. Profound model validation and extensive testing are considered essential next steps.

## 5.2 Considerations on suitability

The thesis is meant to evaluate the suitability of ODYM to develop a user-friendly modelling template for the application in organic waste management. Thus, the question is not just if ODYM can be applied in the field but also how approachable and adaptable an ODYM-based modelling template is:

### 1. Application in organic waste management

The results show that ODYM is a thoughtful modelling framework, providing a profound data structure without hindering Python's immense potential for scientific programming. It combines two aspects, which Pauliuk & Heeren (2020) call "flexibility" and "rigidity", to allow complex material flow problems to be investigated in a well-defined and standardized MFA environment. For the application in organic waste management, ODYM's modular design allowed easy extraction of the needed features as well as adding an efficient first order model approach. Furthermore, interactive Sankey diagrams and a case-study-specific MCS have been included. Of course, the developed template does not nearly cover all possible scenarios for MFA in organic waste management. In particular, the input data is highly case-specific, making template adaptations inevitable. biODYM demonstrates

that ODYM can be applied in all steps of MFA that are usually supported by software and that a case study in the given field can be modelled dynamically. Describing a complex system, ranging from agricultural production to comprehensive organic waste treatment to modelling the application of products of the treatment processes as soil conditioner, ODYM's capability of handling complex problems has been demonstrated. Hitherto, the modelling framework has not been extensively tested independent of the developers in available scientific literature. The thesis delivers strong evidence of ODYM's potential to solve problems researchers encounter with popular software like STAN. Advanced uncertainty evaluation via MCS, using the log-normal distribution as an improved approximation standard compared to the normal distribution, as well as dynamic analysis are considered essential methods for MFA research. It has been shown that ODYM is a framework fully supporting these approaches.

The ODYM modelling framework is well defined, allows for complex dynamic MFA, and is open and even designed for adaptations and improvements, which makes it a highly suitable tool for organic waste management, but also possibly for any other field of application.

For the template, made-up values for the import flows and transfer coefficients were used. In order to demonstrate the applicability of the template using real-life data, the calculation was repeated with actual total wheat production data of Germany from 2019 until 2021 (Destatis, 2022). The soil conditioner potential of the waste treatment products was estimated, assuming that 50 % of the total wheat harvest was treated in the presented case study system. Considering the residue to product ratio of wheat (RPR = 1.75), as applied by Koopmans & Koppejan (1997), supplied by Bhattacharya et al. (1993), flows from the "Harvesting" process to the "Food" process (F\_1\_2 as wheat grain flow or product flow) and to the "Straw collection/distribution" process (F\_1\_3 as wheat straw flow or residue flow) can also be adjusted to more realistic data (see case study MFA system Figure 7, p. 16). Additionally, the total organic carbon content of wheat straw (TOC = 0.438) can also be used to refine the carbon substance level of the flows (Cayuela et al., 2010). Adopting the remaining data from the case study, the following violin plots for the potential carbon inflow to (Figure 15) and the stock in (Figure 16, p. 29) the soil are obtained:

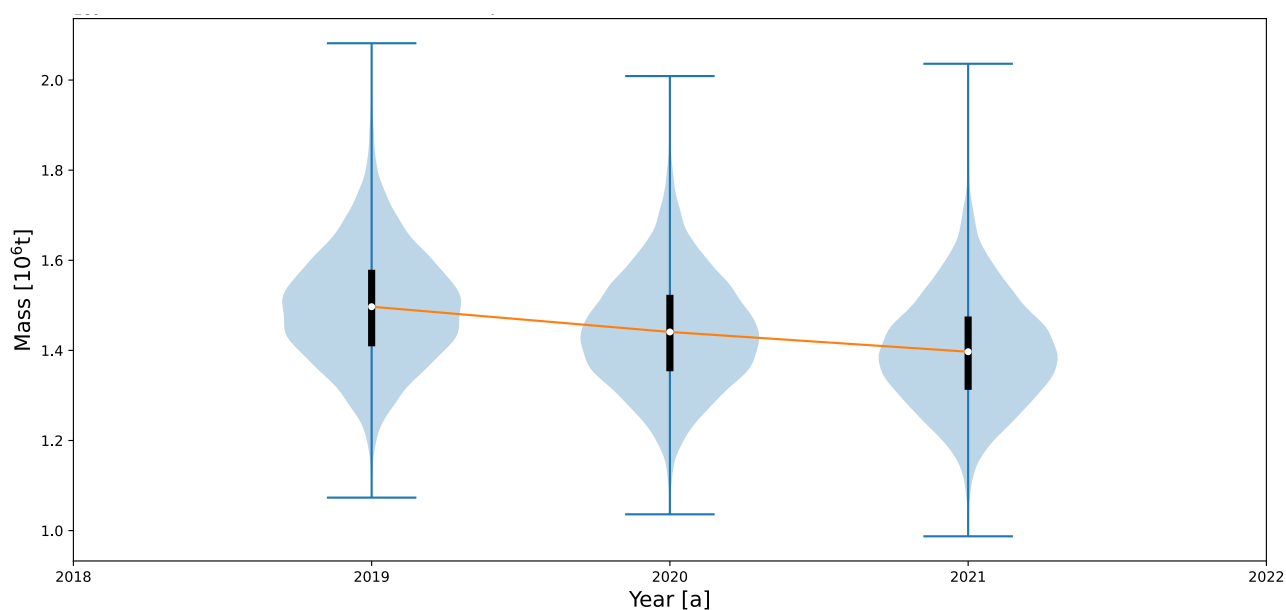


Figure 15: Violin plot carbon inflow to soil using adjusted data (NMC =10,000)

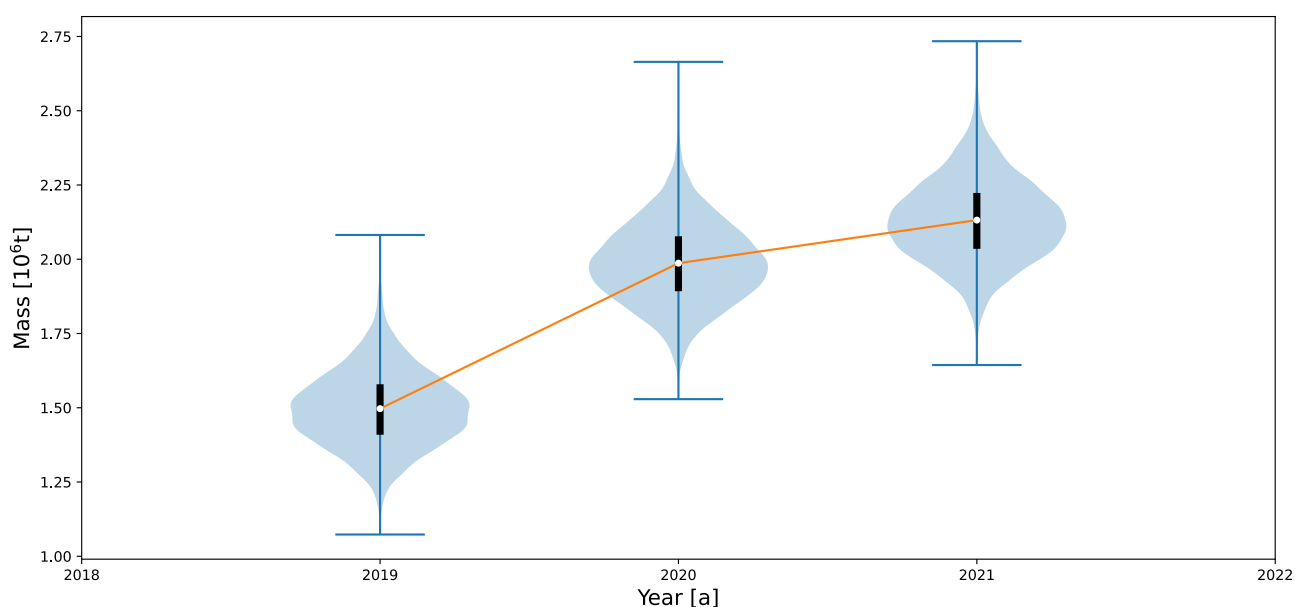


Figure 16: Violin plot carbon stock in soil using adjusted data (NMC = 10,000)

Import flows, TC data and associated calculations can be viewed in Annex B (p. 42). Although this example is still simplified and requires many assumptions (e.g. same carbon content of wheat grain and straw, transfer coefficients for material distribution in the waste treatment process still made-up), the procedure shows that the template is very flexible and can be used for real-life data.

## 2. User-friendliness

User-friendliness in the context of the thesis' aim includes two aspects:

- a. Simple adaptation of the template for similar purposes
- b. Handling of the template accessible for researchers without advanced Python knowledge
  - a. It has been discussed before that ODYM is designed for adaptation. The biODYM modelling template has actually been developed by combining modified code of the tutorials with customized programming products. Additionally, Jupyter Notebook is used, which is itself a comprehensible way to distribute code, and extensive documentation of the template is provided. Thus, the adaptability of the template for similar purposes is assessed to be high. It is not a tool that automatically delivers a ready solution when inserting any data, but it is an approach that presents procedures and capabilities of ODYM in the context of organic waste management, providing several practical extensions. Users who would like to apply biODYM are suggested to compare the offered features with their research requirements and determine if the case study calculations resemble the intended purpose. For instance, dynamically modelling other organic waste treatment systems including FOMPs, along with tracing certain substances while simultaneously keeping track of the good level and evaluating the uncertainty of the analysis via MCS can be performed with simple adaptation measures fitting the procedures to the researchers' needs.

If relevant features are missing, users can create their own case study template, taking advantage of biODYM and the explanatory notes of the development process and the ODYM

documentation. If the research includes, for example, comparing different facilities applying the same treatment process (e.g. anaerobic digestion described as FOMP) and evaluating efficiency differences, ODYM's feature of comparing regions could be applied, defining one region as a plant to be investigated (provided that each plant system consists of the exactly the same process flows). Comparing regions is subject of the ODYM Tutorial No. 3. (Pauliuk & Heeren, 2022), and with the help of biODYM and its first order model approach, a case study template for this case could be designed straightforwardly.

- b. Using and adapting the tool is assessed to be easy for researchers with advanced Python knowledge, and even for those with only basic Python or general programming skills. The accessibility for researchers without programming skills is ambiguous. The main reason for this is the lack of a graphical user interface, as it is implemented into STAN. The option to use buttons, input fields, and the drawing environment of STAN hides the programming procedures users are forced to interact with in software without an interface. Although adaptation procedures are considered to be good to learn, the mere absence of a graphical user interface may have a deterrent effect. It is hard to imagine framing ODYM in a tool that can be controlled with a graphical user interface without restricting its essential flexibility. Acknowledging the general accessibility of Python and the simplicity of ODYM compared to the complexity of the MFA problems that can be solved with it, researchers without programming knowledge may benefit greatly from working their way into the basics of scientific coding by investing a reasonable amount of time. Once ODYM's procedures have been understood, standardized dynamic analysis becomes accessible as a quick and profound MFA tool. If performing complex dynamic MFA is a frequent field of activity, the benefits of working with ODYM clearly outweigh the costs of learning how to handle the framework.

## 6 Conclusion

The biODYM modelling template has been developed to assess the option to perform dynamic MFA with ODYM in the field of organic waste management. The open science framework was extended by adding a first order model approach, a Monte-Carlo-Simulation, and a layout suggestion for interactive Sankey diagrams. To present the procedures, a case study was modelled. The template enables dynamic analysis with advanced uncertainty evaluation, providing essential features for advanced MFA studies that are not yet included in popular MFA software. Consequently, ODYM's suitability for the intended purpose is evaluated to be high.

The template presents a working process for adapting the framework for practical application as well as suggesting general and more specific extensions. This has not been done before independent of the developers in available scientific literature. Researchers can either directly apply biODYM or be inspired to create their own template if more features are needed. Documentation by means of practical comments in the code, visualization of the structure via UML use case diagrams, a quick-start guide and procedure explanations are meant to support easy usage of the template.

Dynamic MFA is a complex process and no implementable method for equipping the biODYM modelling template with a graphical user interface for a more intuitive and simple application has been found. Users always need to modify the code to fit it to their research questions and thus, programming knowledge or time to learn Python-basics to use ODYM-based dynamic MFA successfully is required. Future work should include extension refinement and exploring ways to better integrate them into the original modelling framework. Likewise, profound model validation, and extensive testing of the template should be performed. To further increase the availability of ODYM in organic waste management, further templates could be developed addressing additional application scenarios and use cases.

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## Annex A

### Case study input data

Table 2: Import data into system on biomass (good) and carbon level

Year	F_0_1 [t]	
	Biomass	Carbon
2020	100	50
2021	110	55
2022	120	60
2023	130	65
2024	140	70
2025	150	75
2026	160	80
2027	170	85
2028	180	90
2029	190	95
2030	200	100
2031	10	5
2032	220	110
2033	230	115
2034	240	120
2035	250	125
2036	260	130
2037	270	135
2038	280	140
2039	290	145
2040	300	150

Table 3: Case study transfer coefficients year 2020–2029 (same for biomass and carbon level)

Year	2020	2021	2022	2023	2024	2025	2026	2027	2028	2029
TC_1_2	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5
TC_1_3	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5
TC_3_4	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.3
TC_3_5	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.3
TC_3_6	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1
TC_3_7	0.2	0.2	0.2	0.2	0.2	0.2	0.2	0.2	0.2	0.2
TC_3_8	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1
TC_4_9	1	1	1	1	1	1	1	1	1	1
TC_5_9	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7
TC_5_10	0.15	0.15	0.15	0.15	0.15	0.15	0.15	0.15	0.15	0.15
TC_5_11	0.15	0.15	0.15	0.15	0.15	0.15	0.15	0.15	0.15	0.15
TC_6_10	1	1	1	1	1	1	1	1	1	1
TC_7_10	1	1	1	1	1	1	1	1	1	1

Table 4: Case study transfer coefficients year 2030–2040 (same for biomass and carbon level)

Year	2030	2031	2032	2033	2034	2035	2036	2037	2038	2039	2040
TC_1_2	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5
TC_1_3	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5
TC_3_4	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.3
TC_3_5	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.3
TC_3_6	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1
TC_3_7	0.2	0.2	0.2	0.2	0.2	0.2	0.2	0.2	0.2	0.2	0.2
TC_3_8	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1
TC_4_9	1	1	1	1	1	1	1	1	1	1	1
TC_5_9	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7
TC_5_10	0.15	0.15	0.15	0.15	0.15	0.15	0.15	0.15	0.15	0.15	0.15
TC_5_11	0.15	0.15	0.15	0.15	0.15	0.15	0.15	0.15	0.15	0.15	0.15
TC_6_10	1	1	1	1	1	1	1	1	1	1	1
TC_7_10	1	1	1	1	1	1	1	1	1	1	1



## Annex B

### **Adjusted input data for the MFA presented in the discussion chapter 5 (p. 22)**

Table 5: Import data into system on biomass (good) and carbon level (assuming treatment of 50 % of the total wheat production of Germany from 2019 until 2021 (Destatis, 2022) and using the total organic carbon content of wheat straw (TOC = 0.438) (Cayuela et al., 2010) for calculating the carbon flow)

Year	F_0_1 [t]	
	Biomass	Carbon
2020	11,531,300	5,050,709.4
2021	11,086,050	4,855,689.9
2022	10,729,600	4,699,564.8

Table 6: Transfer coefficients year 2019–2021 (same for biomass and carbon level, only TC\_1\_2 and TC\_1\_3 changed compared to the template's case study, see calculations in this Annex on p. 43)

Year	2019	2020	2021
TC_1_2	0.36	0.36	0.36
TC_1_3	0.64	0.64	0.64
TC_3_4	0.3	0.3	0.3
TC_3_5	0.3	0.3	0.3
TC_3_6	0.1	0.1	0.1
TC_3_7	0.2	0.2	0.2
TC_3_8	0.1	0.1	0.1
TC_4_9	1	1	1
TC_5_9	0.7	0.7	0.7
TC_5_10	0.15	0.15	0.15
TC_5_11	0.15	0.15	0.15
TC_6_10	1	1	1
TC_7_10	1	1	1

**Calculating adjusted transfer coefficients using residue to product ratio of wheat (RPR)**  
**(Bhattacharya et al., 1993)**

$$RPR = 1.75$$

$$RPR = \frac{F_{1_3}}{F_{1_2}} \quad (9)$$

Converting Equation (9) leads to Equation (10)

$$F_{1_3} = F_{1_2} \cdot RPR \quad (10)$$

TC<sub>1\_2</sub> can then be calculated according to:

$$TC_{1_2} = \frac{F_{1_2}}{F_{1_2} + F_{1_3}} \quad (11)$$

Combining Equation (10) and (11) lead to:

$$TC_{1_2} = \frac{1}{1 + RPR} \quad (12)$$

$$TC_{1_2} = 0.36$$

TC<sub>1\_3</sub> results to:

$$TC_{1_3} = 1 - TC_{1_2} \quad (13)$$

$$TC_{1_3} = 0.64$$

# Annex C

## biODYM quick-start guide

