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bioDYM: Dynamic material flow analysis for biogenic carbon management and CDR strategy assessment

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Abstract: Carbon management and the assessment of Carbon Dioxide Removal (CDR) strategies in the circular economy require dynamic material flow analysis (dMFA) tools capable of tracking and forecasting the complex and circular system behavior of heterogeneous carbon flows, stocks, and process dynamics over time. To fill a gap in capable and accessible tools, we present bioDYM, a flexible and open source dMFA software. On the basis of the ODYM framework, bioDYM enables low-code system modeling through the combination of stocks, flows and processes calculated with a modular system solver. Originally focused on biogenic carbon systems, bioDYM has evolved into a fully functional general-purpose dMFA software. Custom-built process logics allow the modeling of specific carbon transformation pathways such as multipool first-order decay processes and dynamic stock modeling with Weibull lifetime distributions. A Monte Carlo engine propagates parametric uncertainty. A scenario engine enables scenario comparisons within a single simulation. Results are accessible through an interactive dashboard.
We demonstrate bioDYM via a wheat straw carbon management case study (1,000 km², Germany, 2025–2125) and compare three application pathways: direct incorporation (DI), pyrolysis and incorporation (P&I) and use of construction material (CM). By 2125, the system removes 8,817 Gg C from the atmosphere, retained as stable biochar (P&I = 4,721 Gg C), long-lived construction products (CM = 3,687 Gg C) and decomposing soil organic carbon (DI = 409 Gg C). Monte Carlo analysis (n = 5,000) and scenario analysis prove the dominant influence of carbon stability and product lifetime on long-term CDR performance.

1 INTRODUCTION

Carbon (C) is a fundamental element for natural and anthropogenic systems. It is essential, e.g., for nutrition, construction and biobased/fossil energy systems. Organic, mineral, gaseous and dissolved carbon constantly transition between large carbon stocks - the atmosphere, lithosphere, pedosphere, hydrosphere and biosphere - forming the global carbon cycle. The accumulation of carbon in the atmosphere is the major driver of climate change. To decrease the speed of this development, the objectives of carbon neutrality and net zero by 2050 were formulated in the Paris Agreement in 2015 (United Nations Climate Change, 2016). For carbon neutrality, negative emissions are crucial (Don et al., 2024) and require carbon dioxide removal (CDR) strategies. CDR strategies are a "cluster of technologies, practices, and approaches that remove and sequester carbon dioxide and durably store the carbon in geological, terrestrial, or ocean reservoirs, or in products" (IPCC, 2023). Sequestration refers to the process of increasing the carbon content of a carbon pool other than the atmosphere (IPCC, 2001). Carbon sequestration in soils describes the "process of transferring C from the atmosphere into the soil through plants or other organisms, which is retained as soil organic carbon (SOC) resulting in a global C stock increase of the soil" (Don et al., 2024). The carbon stability of SOC reflects the degeneration of biomass in the soil (Gross et al., 2024; Kpemoua et al., 2024). The CDR taxonomy lists, among other methods, improved forest management, soil carbon sequestration and the use of biochar as a land-based biological method for carbon storage on a timescale of decades to centuries (IPCC, 2023).

Material flow analysis (MFA) is an established methodology in industrial ecology for environmental system analysis (Graedel, 2019) (Brunner & Rechberger, 2017). On the basis of the conservation of mass (Input = Output + ΔStock), the MFA evaluates defined material flows and stocks within a system defined in space and time. Process-specific transfer coefficients (TCs) determine the partitioning of material flows. MFA can be used in a descriptive manner for a quantitative assessment, e.g., material turnover, and in an explorative manner, aiming to understand the governing processes.

The dynamic MFA (dMFA) extends these principles from a static model with constant flow rates to a dynamic model where the dimension of time forms a system variable (Brunner & Rechberger, 2017, 2020; Müller et al., 2014). It allows the modeling of dynamic systems over time and the forecasting of the effects of strategies and actions in the future. Additionally, modeling of time-dependent processes becomes possible with its introduction into the balancing process by the in-use stock and its lifetime distribution (Deng et al., 2023).

The potential of the dMFA for complex environmental system analysis is partly hindered by the accessibility and functionality of the available software. The commonly applied MFA software STAN offers a graphical user interface (GUI) for system design but is mostly applied for static analysis even when basic dynamic capabilities are available. A special feature is the integrated data reconciliation, which is of high-value for explorative MFAs, where the combination of several pieces of information is needed. Many other dMFA tools have been developed over the last decade, employing dynamic (Bertram et al., 2017; Müller et al., 2014) or probabilistic modeling procedures (Lupton and Allwood, 2018) or both combined (Bornhöft et al., 2016) to advance the MFA and overcome its inherent shortcomings, i.e., lack of data, uncertainty and inability of the static MFA to forecast stocks (Graedel, 2019).

The python-based "Open software framework for DYnamic Material systems" (ODYM) provides a flexible framework for the creation of complex dMFAs in six-dimensional (6D) systems, including the following dimensions: time (t), region (r), process (p), good (g), material (m) and

element (e). Each system variable is defined by a set of aspects (e.g., time, age cohort, material). ODYM is a toolkit of modules intended to balance rigidity and flexibility, allowing researchers to select the required aspects and variables for their study. It sets the foundation for a large set of interoperable MFA datasets (Pauliuk and Heeren, 2020). Various researchers have used ODYM for dMFAs in the fields of metals (Pedneault et al., 2022), plastics (Schmidt et al., 2026) and biomass (Gingrich et al., 2025). One important type of ODYM adaptation is flodym, developed by the PIK Potsdam (Dürrwächter et al., 2026). It focuses on flexibility, simplicity and versatility by reducing dimension adaptation effort, dimension management and predefined standard methods. Nevertheless, its own system definition in Python is needed.

As CDR strategies operate over long time periods, time-dependent stock and flow changes must be considered. Therefore, dMFA can be a valuable assessment tool for CDR strategies, as it can provide insight, e.g., into the quantity and efficiency of carbon sequestration processes. For example, Aryapratama and Pauliuk, 2019 researched the amount of biogenic carbon within the built environment in Indonesia and timber use pathways in Germany (Wang and Haller, 2024). Three representative dMFA tools, STAN, ODYM, and flodym, which span the GUI-to-code accessibility spectrum, are compared in Table 1 to identify functional gaps relevant to biogenic CDR strategy assessment.

Table 1: Gap description of available dMFA software for the assessment of CDR strategies. Three different software programs with the capabilities required for accessible CDR strategy assessment are compared. Compared are STAN 2.7, the ODYM framework and the flodym.

Capability	STAN	ODYM	flodym
System Definition	GUI	Python	Python
Programming Required	No	Yes- Advanced	Yes - Reduced
Time Dimension	Dynamic - (With effort)	Dynamic	Dynamic
Multielement tracking	Substance Level	6 D Systems	Yes - basic
Circular flow handling	No	Manual decoupling	Manual decoupling
First Order Decay	No	No	No
Dynamic Stock Modeling	No	Yes	Yes
Uncertainty Quantification	Yes- Data Reconciliation	No - but possible	No - but possible
Scenario Analysis	No	No - but possible	No - but possible
Visualizations	Sankey	No - Extension required	Yes - basic Visualizations

STAN provides an accessible GUI-based interface but is limited in functionality, precluding the modeling of temporal stock dynamics and decay processes. ODYM and flodym both support dynamic modeling and DSM but require system definitions in Python code, limiting adoption among practitioners without programming expertise, and neither provides biomass-specific process modules for organic matter decomposition. Across all three tools, first-order decay process logic, integrated scenario analysis, and automated handling of circular material flows are absent.

To address these gaps in existing dMFA tools, this study presents “bioDYM - biogenic Dynamic Material Systems Model”, a python-based software for dMFAs, with a focus on biogenic CDR strategy assessment. We addressed the following objectives:

1. Development of accessible and modular dMFA software capable of complex multielement calculations based on the low-code bioDYM workflow.
2. The development and integration of custom biomass-specific process logics capable of simulating multipool first-order decay processes.
3. The demonstration of bioDYM through a case study focused on wheat straw CDR strategies, comparing long-term sequestration performances in pathways differing in carbon stability and product lifetime.

2 METHODS: Architecture and workflow

bioDYM is Python software built upon the ODYM framework and uses its tested modules, mass balance and data structure definitions as a foundation. While ODYM provides a powerful toolkit, bioDYM uses and extends these tools with biomass-specific modules and a modular system solver to create functional dMFA calculation software. bioDYM allows users to create flexible dMFA systems within predefined bioDYM system dimensions. It is built as a two-dimensional system (time (t) × elements (e)) but with the option of creating a fictional "multielement" structure capable of modeling complex product, component and material flows. bioDYM reduces the number of ODYMs dimensions and flexibility as a trade-off for accessibility. The tool's operation follows the three-step workflow displayed in Figure 1. The first conceptual version of bioDYM was developed as a bachelor thesis (Hoppe, 2022). Portions of the current bioDYM Python codebase were developed with the assistance of Claude (Anthropic) and Gemini (Google). All software was reviewed, tested, and validated by the authors.

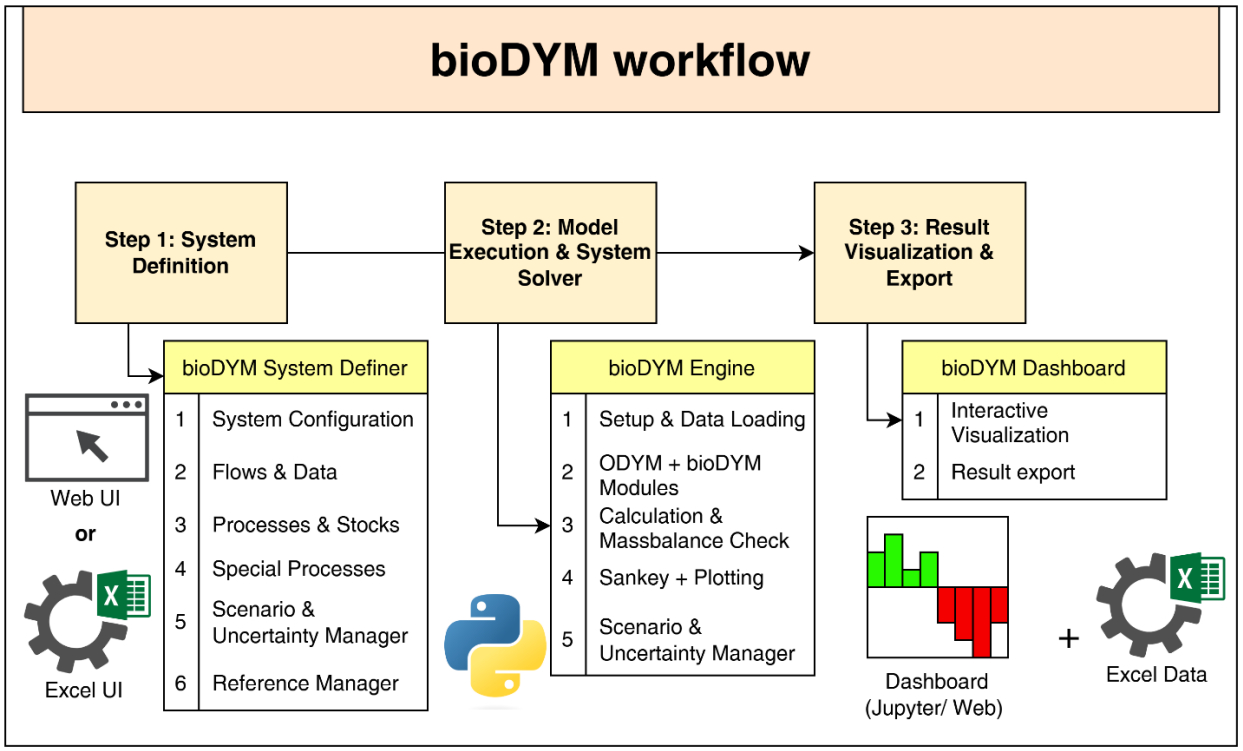


Figure 1: bioDYM workflow overview. The bioDYM framework operates in three sequential steps. Step 1 (System Definition): the user defines the complete model in the bioDYM System Definer (bioDYM-SD), available as either a structured Microsoft Excel workbook or a browser-based Web UI. Both interfaces provide six configuration sections: (1) system configuration, (2) flows and data, (3) processes and stocks, (4) special processes, (5) scenario and uncertainty managers, and (6) reference managers. Step 2 (Model Execution & Solver): the bioDYM Engine loads the bioDYM-SD, executes the ODYM and bioDYM-specific calculation

modules, performs process-level mass balance checks, and runs the Scenario and Monte Carlo Uncertainty Manager. Step 3 (Result Visualization & Export): the bioDYM Dashboard provides an interactive visualization environment, deployable as a Jupyter notebook or browser-based Web Dashboard, with structured result Excel export.

2.1 System Definition via the bioDYM System Definer

dMFA modeling frameworks such as ODYM and flodym require users to implement systems directly in python. We developed the bioDYM-System Definer (bioDYM-SD), a structured Microsoft Excel workbook that allows complete system definition, parameterization and module configuration. As an alternative, bioDYM includes the bioDYM SystemDefiner app, a browser-based configuration interface that guides users through the definition of model scope, processes, flows, and parameters without direct spreadsheet access. All system parameters, such as processes, flows or TCs, are defined within a single file, eliminating the need for Python interaction during system setup. The approach intentionally separates the data from the engine and supports reproducibility, since only the configuration file is required to model a system.
The bioDYM-SD is structured into six sections: *Section 1 "Model Configuration"* defines the timeframe of the system (years), the element hierarchy (e.g., material, water content, dry mass and total carbon content) and calculation settings (definition of scenarios, MC settings). *Section 2, "Processes & Stocks,"* enters processes and defines the individual process logic and the use of static/dynamic TCs, stocks and initial stocks. *Section 3 "Flows & input data"* allows flows to be entered, connecting them to processes, flow composition (based on defined elements) and dynamic flow quantity. *Section 4 "Advanced models"* contains parameter sheets for the DSM and FOD modules. *Section 5, "Scenario & Uncertainty Management,"* defines parameters for scenarios and uncertainty parameters for Monte Carlo sampling. *Section 6, "Reference Manager,"* delivers a reference system to increase transparency. The bioDYM-SD automatically generates unique parameter IDs for every data point. Click-boxes, code lists, drop-down menus, data validation, locked cells and color coding allow an accessible user experience. The bioDYM Engine requires only the file path of bioDYM-SD configuration file to execute the model.

2.2 Model calculation via the bioDYM Engine

The bioDYM Engine is the computational core for data loading, computing and calculation. Central is the selection of a "Process Logic" for every process. The "Process Logic" call the specific calculation logic defined in separate python modules. Table 2 provides an overview of currently implemented process logics. By combining process logics, users can configure systems of varying complexity from simple static flow networks to systems that integrate dynamic stocks or organic decomposition.

Table 2: Description of process logics implemented within the bioDYM Engine.

Process Logic	Function	Application
Input/Output	Sink or source	Material Input/Output of the system
Splitter	Distribution of Inflows via TCs	Sorting, Distribution
Transformer	Changes element composition via TCs	Drying, Incineration
Passthrough	Unchanged Flows	Cosmetic processes

DSM	Dynamic Stock Modeling with age cohort tracking	Product Use-Phase, Product in Use
FOMP	First order mineralization process	Biogenic Decay, Soil organic carbon

2.2.1 System Modeling Solver

A central novelty of bioDYM is the modular system solver, which is able to integrate all process logics into a single fixed-point iterative algorithm. The solver processes the system year by year, iterating until all flow and stock values converge within a defined tolerance. This enables both the combination of arbitrary process logics and the resolution of circular material flows without manual decoupling. A topological process minimizes the number of iterations required for convergence in acyclic systems, whereas the fixed-point algorithm correctly manages genuine recirculation. A process-level mass balance check is executed at each time step and, upon completion, verifies the conservation of mass per process, element, and year. The modular architecture allows the addition of new process logics.

2.2.2 First-Order Mineralization Process (FOMP)

The applicability of MFA tools to biogenic systems is limited by their ability to model organic matter decay dynamics. The novelty of bioDYM is its built-in process logic for first-order decay (FOD). Biomass incorporated in the soil forms a dynamic stock that decomposes over time due to mineralization (Robertson and Paul, 2000). FOD models are often used to model biomass/carbon decay rates. A multipool FOD model allows the differentiation of fast and slow decay pools to describe the C mineralization kinetics of biomasses. A labile (fast) and recalcitrant (slow) decaying pool is described in equation 1 (Cayuela et al., 2010; Gregorich et al., 2017). According to (Woolf et al., 2021), this two-pool FOD model is required to extrapolate decay over centennial timescales.

$$C_{remaining}(t) = f_1 \times e^{(-k_1 t)} + (1 - f_1) \times e^{(-k_2 t)} \quad (1)$$

$$f_1 = \text{labile pool fraction}[\%]$$

$$k_1 = decay\ rate\ labile\ pool\ [yr^{-1}]$$

$$k_2 = decay\ rate\ \text{recalcitrant}\ pool[yr^{-1}]$$

$$t = time\ [yr]$$

bioDYM implements this FOD model within its First Order Mineralization Process (FOMP) process logic as an annual stock-flow balance. At each time step, the annual carbon inflow is first distributed into the labile and recalcitrant pools, and decay is calculated from the updated pool stock. The outputs are calculated and added to the overall system balance. Multiple FOMP processes with different pool parameters can coexist within a single system. The configurable pool fractions and decay rates allow the FOMP module to represent a wide range of biogenic materials.

2.2.3 Dynamic Stock Modeling (DSM)

Dynamic stock modeling (DSM) is a core method for tracking the accumulation and release of materials in in-use stocks over time (Müller et al., 2014). ODYM provides a DSM module, which was used, extended and implemented as process logic. Age cohort-specific material lifetime distributions are used to describe the lifetime of products (Pauliuk and Heeren, 2020). Each annual inflow cohort is tracked independently until outflow via a survival function. Four distribution

functions are natively supported to model the survival function: fixed, normal, lognormal and Weibull via bioDYM-SD.

The bioDYM DSM module extends standard age cohort tracking for element conservation. Each cohort has the full elemental composition (WC, DM, TC) defined at the time of inflow, preserving compositional changes over time. The iterative solver enables systems with real recirculation between the DSM processes and downstream flows. Multiple DSM processes with different multiple lifetime distributions can coexist within a single system.

2.2.4 Scenario Manager

Creating explorative scenarios often requires formally copying an entire system or work-intensive input manipulation. The bioDYM Scenario Manager allows the manipulation of any parameter of the baseline scenario to explore its impact on the overall system. Users define parameter substitution (multiply, replace, addition) rules that systematically modify selected parameters across defined scenarios. Each scenario runs the complete bioDYM solver, ensuring that all module interactions are captured in the outputs. Any numerical parameter in bioDYM-SD, including flow quantities, transfer coefficients, DSM lifetimes and FOMP decay rates, can be manipulated. A mass balance check for each scenario is implemented. The results are aggregated and passed directly to Dashboard for visualization and export.

2.2.5 Monte Carlo (MC) simulation engine

Addressing uncertainty and thus model validity with MC simulation in MFA development is highlighted by (Pauliuk and Heeren, 2020). A Monte Carlo (MC) simulation is used as a methodology to address system parameter uncertainty. It samples parameter values from user-defined probability distributions. bioDYM integrates this capability into the calculation engine. Defined in bioDYM-SD, four distribution functions are offered (normal, lognormal, uniform, and triangular). For each MC sample, the complete bioDYM solver is executed, ensuring that parametric uncertainty propagates through all module interactions and circular flows. Any numerical parameter, including flow quantities, transfer coefficients, DSM lifetimes, and FOMP decay rates, can be designated as uncertain. Parameter normalization prevents unintended parameter combinations, for example, in TCs. When user-defined Min/Max bounds are specified for all TCs in a group, rejection sampling additionally ensures that normalized values remain within the defined parameter ranges. Flow quantities can be defined as uncertain parameters by specifying an operation (set, multiply, or add), a distribution, and start/end year bounds, enabling uncertainty in time-varying inputs. Beyond quantifying output uncertainty, running a mass balance check across all MC realizations simultaneously serves as structural model validation. The results are aggregated as histograms and passed to Dashboard for visualization and export.

2.3 Visualization and export via bioDYM Workflow and Dashboard

Existing dMFA frameworks provide limited integrated visualization capabilities, requiring users to build their own routines. The bioDYM Dashboard, a Jupyter Notebook environment, serves as the GUI and provides a structured, reproducible workflow for result verification, visualization and export.

bioDYM provides two deployment modes for the same notebook. The "*bioDYM-Workflow*" is the standard Jupyter Notebook, which includes detailed diagnostics and results. The "bioDYM-Dashboard" is a simplified browser application via Voilà (Renou et al., 2019), which renders all interactive controls without exposing code cells, enabling nontechnical stakeholders to explore the results.

An automated system flow chart confirms the integrity of the defined system. Process-level mass balance diagnostics help identify violations of the conservation of mass principle per process, element and year. A hierarchical element composition check flags cases where the sum of sub elements deviates from the parent element. Verified results are accessible through a set of interactive visualizations. A dynamic Sankey diagram provides a multielement system-wide overview of mass flows in any selected year. Interactive plots display the evolution of processes, stocks and flows. Scenario comparisons are visualized as side-by-side plots of stocks and flows. The results of the Monte Carlo simulation are presented as histograms of probability distributions. The layout of all the figures can be controlled via a central control function and exported as PNG or SVG files. The system results, KPI dashboards, Monte Carlo outputs and Sankey data are exported as structured Excel files for further analysis via eternal MFA visualization tools such as (Structural Collective, 2025).

2.4 Application of bioDYM: Case study Wheat Straw potential for CDR strategies

bioDYM`s modular architecture, process logic and analytical tools create a versatile assessment tool for CDR strategies. This is demonstrated by a complex case study on the potential of wheat straw (WS) to create stable carbon sinks by combining different processes (FOMP, DSM) with a scenario engine and a Monte Carlo simulation within a single system. The objective was to compare the CDR potentials of three wheat straw application scenarios: 1. Direct Incorporation, 2. Pyrolysis & Incorporation, and 3. Construction Material. The research question is as follows: which approach can store the largest amount of carbon after 100 years?

The system is defined as part of the global carbon cycle by including carbon transport from the atmosphere via the biosphere to the pedosphere and back to the atmosphere, modeling the impact of durations of biogenic carbon on global carbon stocks. The system covers the cultivation, harvest, collection, treatment, use and end-of-life of WS. The entire biomass is sourced from the atmosphere (P0) or from the water & nutrient cycle (P1). Gaseous mineral carbon (CO_2) from the atmosphere is the source of biogenic carbon through its transformation into biomass by photosynthesis. Water, nutrients and all other noncarbon components are sourced from P1, forming a water and nutrient cycle. To allow tracking of the net change in the atmosphere and the environment, both are assumed to be stocks, with an unlimited material supply. Therefore, both stocks start with a value of 0, allowing a negative value to display the cumulative net mass removal by the system over time. To describe WS flows, a multielement system is modeled, consisting of material (biomass), water content (WC), dry matter (DM), and total carbon (TC) in a three-level hierarchy, as displayed in Figure 2.

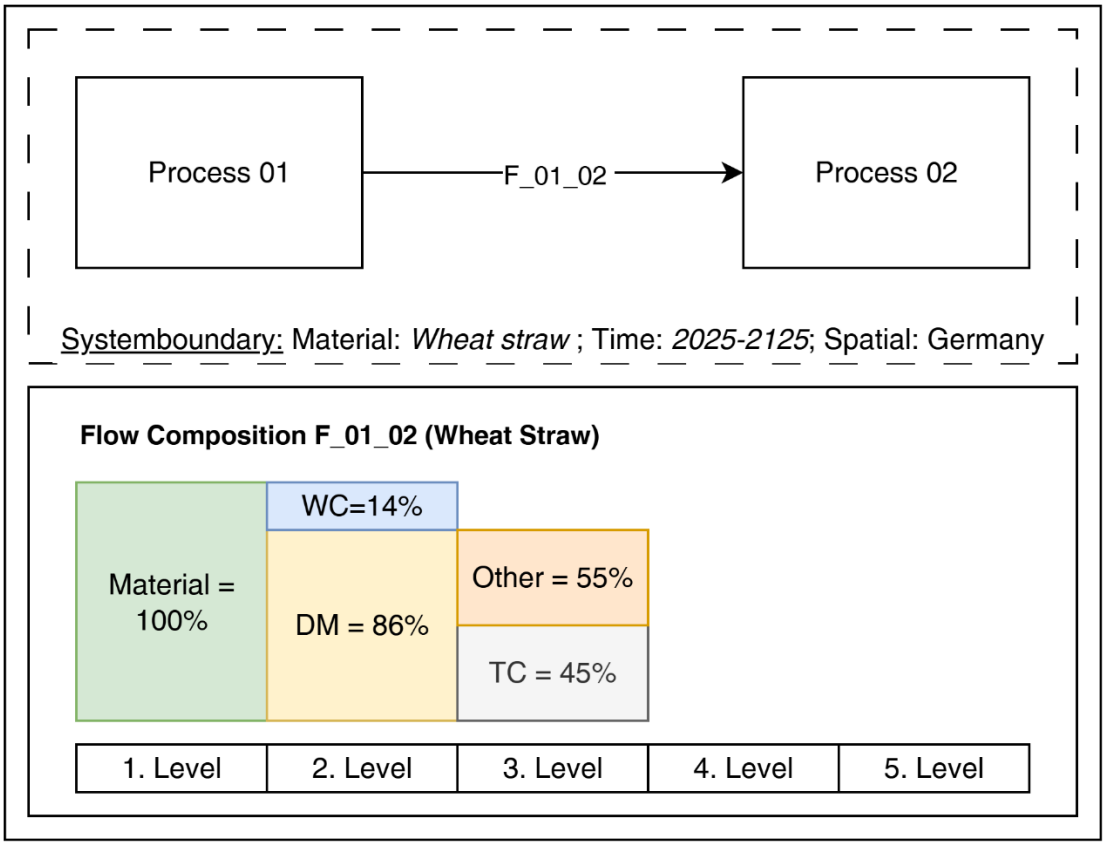


Figure 2: *bioDYM multilevel material composition structure illustrated with the wheat straw case study flow F_01_02. The upper panel shows the general MFA system structure with processes, flows, and system boundaries. The lower panel shows the three-level element hierarchy: material (Level 1) is partitioned into water content (WC, 14%) and dry matter (DM, 86%); DM is further partitioned into other dry mass (55%) and total carbon (TC, 45%). All the element levels are tracked independently throughout the simulation .*

The system models the biogenic carbon dynamics of a WS economy in Germany over a 100-year horizon (2025-2125) over a reference area of 1,000 km² (100,000 ha). The processes, flows and system boundaries are shown in Figure 3. The input forecast is based on the annual yield of wheat in Germany from 1990-2024. The mean wheat yield was 7.32 Mg/ha, with a standard deviation of 0.57 Mg/ha. A long-term trend of +0.25% yield increase per year is, on the basis of linear regression, is included in the flow forecast (DeSTATIS, 2025a, 2025b). A separate Python script uses these assumptions to calculate the wheat yield forecast until 2125.

Wheat ready for harvest should have a WC of 14% (LLG, 2020; Wiersma and Ransom, 2021), resulting in a DM of 86%. For the entire wheat plant without roots, an average TC of ~ 45% DM was assumed (grain 45.0%, straw 45.7%, chaff 42.6%) (Raimanova et al., 2024). The grain-to-straw ratio is assumed to be 47.6:52.4% (LLG, 2020).

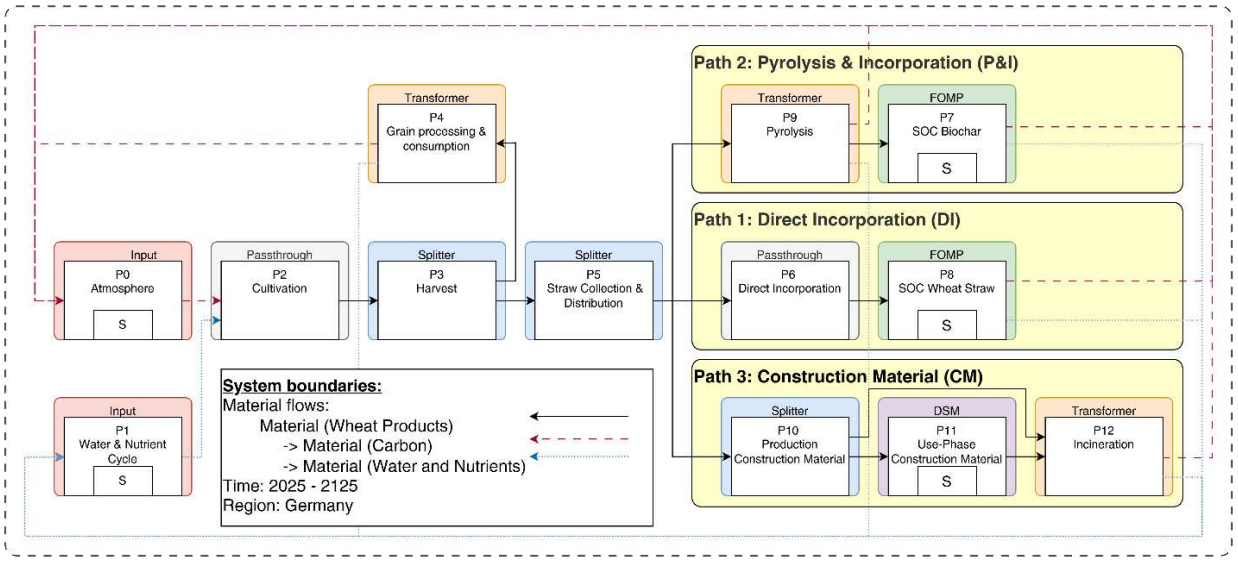


Figure 1: *bioDYM system diagram of the wheat straw CDR strategy case study (Germany, 2025-2125). The system comprises 13 processes (P0-P12) and 5 stocks, organized into three end-use pathways, indicated within yellow frames: Path 1 - direct incorporation (DI), Path 2 - pyrolysis & incorporation (P&I), and Path 3 - construction material (CM). Boundary processes P0 (Atmosphere) and P1 (Water & Nutrient Cycle) represent the system interfaces with the global carbon cycle and the nutrient and water cycles. Process logic types are color-coded: input (red), Passthrough (gray), splitter (blue), transformer (orange), first-order mineralization process (FOMP) (green), and dynamic stock modeling (DSM) (purple). Three material flow types are distinguished: wheat product flows (black, solid), carbon flows (red, dashed), and water and nutrient flows (blue, dotted).*

The collected wheat straw is distributed equally across three end-use pathways (1/3 each): direct incorporation (DI), pyrolysis and incorporation (P&I), and construction material (CM).

- **Direct incorporation (DI):** 100 % of the biomass is incorporated into the soil. Wheat straw has high cellulose, hemicellulose and lignin contents (Zhang et al., 2016). A baseline lignin content of 18 % is defined as the recalcitrance pool (Beuel et al., 2020). Since wheat-straw-specific multipool parameterizations are limited, average straw decay rates from the long-term meta-analysis by (Cai et al., 2018) are applied, who reported labile $k1$= 15.95 yr^{-1} and recalcitrant $k2$ 0.05 yr^{-1} (averages across six straw types, including wheat, fitted to a three-pool model and collapsed to the two pools).
- **Pyrolysis & Incorporation (P&I):** The pyrolysis process temperature highly influences the carbon yield of biochar production (Sanei et al., 2025). At 600°C, a WS biochar yield of 28.9 % (Sedmihradská et al., 2020) with a carbon content of 65 % (Liu et al., 2018; Woolf et al., 2021) was used as a baseline. The remaining carbon is emitted, together with water and volatiles such as gas and liquid. Biochar is highly stable, with a recalcitrance pool often defined as 99.4 % (Woolf et al., 2021). The recalcitrance decay rate $k2$ was reported to be 0.00252 yr^{-1}(Kuzyakov et al., 2014).
- **Construction Material (CM):** The CM pathway routes straw into the production of CM, with production losses, as three building-material subtypes via DSM. Each annual cohort is described by a Weibull-distributed service lifetime (k = 2.5): Straw-Roof (λ = 28 a, 30%), Straw-Insulation (λ = 45 a, 30%), and Straw-Structural (λ = 56 a, 40%), on the basis of Kaesberg and Scharmer (2024). At the end of life, the material is assumed to be incinerated, returning carbon to the atmosphere.

To demonstrate bioDYM's scenario manager, a policy scenario (Wheat Straw Application Stop 2075) is implemented in which TCs in the collection and distribution process (P5) are switched in 2075 from equal distribution to 100% routing to DI. Consequently, after 50 years, no new wheat

straw feeds the paths P&I and CM. This mid-simulation TC change should model a realistic program discontinuation: new biochar production and construction stop, whereas previously accumulated stocks (SOC Biochar, Use-Phase CM) continue to evolve independently without new inputs. The scenario tests whether a 50-year CDR program generates long-lasting carbon sequestration and demonstrates bioDYM's ability to evaluate time-dependent changes within a single continuous simulation. Uncertainty in the baseline scenario is assessed through Monte Carlo simulation (n = 5,000 runs). The full parameterization, MC uncertainty ranges, and sources are provided in Table SI-1.

3 RESULTS

bioDYM is published as open-source software under the MIT License (Version 1.2.1: GitHub: JScholz-tech/Biodym_JS; Zenodo: (Scholz et al., 2026)), with a citable versioned release, automated test suite, user documentation and developer guide. Table 3 summarizes bioDYM's capabilities and displays how it fills gaps, highlighted in the introduction. A full function-level detail is provided in Table S2. The ODYM framework provides the process-flow-stock foundation; the remaining components represent bioDYM-specific contributions. The system architecture follows an integrated three-step workflow: the bioDYM-SD provides a structured system configuration; the bioDYM Engine executes calculation, scenario, and uncertainty analyses; and a Voilà-based interactive Dashboard enables result exploration without code interaction. Detailed documentation, a user manual, and tutorial case studies support first-time users.

Table 3: Overview of bioDYMs' capabilities and key functions. The feature that is based on ODYM and which feature is a custom bioDYM addition are indicated.

Capability	bioDYM	Notes
System definition	bioDYM-SD (Excel or App)	No Python required
Programming required	No	Installation + File path only
Process logic system	6 configurable types	Input/Output, Splitter, Transformer, Pass-through, DSM, FOMP combinable in one solver run
Time dimension	Yes, Dynamic	Year-by-year iterative solver
Multielement tracking	Yes, configurable hierarchy	Material, WC, DM, TC; Freely adaptable to any other composition
First-order decay module	Yes, FOMP (two-pool FOD)	Per-process configurable pool fractions and decay rates
Dynamic stock modeling	Yes, DSM (age-cohort)	Normal, Lognormal, Weibull, Fixed distributions
Circular flow handling	Yes, fixed-point iterative solver	Convergence within each time step
Scenario analysis	Yes, integrated scenario engine	Replace, multiply, add rules; no code change
Uncertainty quantification	Yes, integrated MC	4 distribution types, most parameters
Visualization	Yes, Plotly + Dashboard	Sankey, stocks, flows, MC histograms, scenario comparison

Result export	Yes, structured Excel	Results, KPI dashboard, MC outputs
Open source/License	MIT Zenodo DOI	Reproducible from bioDYM-SD alone

3.1 Case study results and bioDYM capabilities

This case study analyses the carbon sequestration potential of three wheat straw treatment paths over a 100-year period (2025-2125). The bioDYM SD configuration file is available as S3. In total, the modeled wheat straw system extracts ~63 million Mg C from the atmosphere as biomass. By the year 2125, approximately 14% of this (8,817 Gg C) is retained as SOC and construction material.

3.1.1 System Definition and Circular Flow Simulation

The wheat straw system consists of 13 processes, 5 stocks, and 5 process logic types (splitter, transformer, FOMP, DSM, and pass-through) and covers a timeframe of 100 years. It is fully configured within bioDYM-SD. bioDYM's fixed-point iterative solver (Section 2.2.1) resolves the inherent circular system of the carbon cycle, in which mineralized carbon from soil decomposition and end-of-life incineration continuously returns to the atmosphere without requiring manual decoupling of subsystems-a structural limitation of conventional dMFA frameworks.

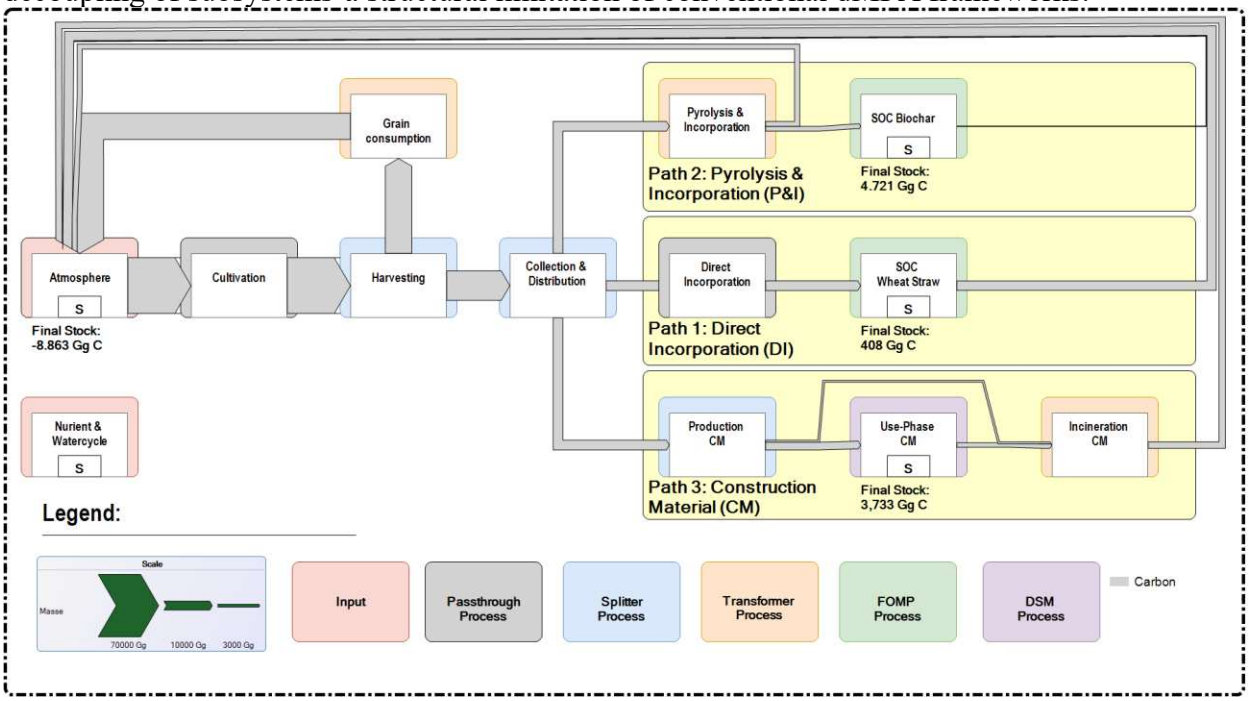


Figure 4: *System Sankey diagram of the wheat straw carbon management case study (cumulative flows, 2025-2125). Carbon flows are shown as cumulative totals over the 100-year simulation period for three end-use pathways: Path 1 - direct incorporation (DI), Path 2 - pyrolysis & incorporation (P&I), and Path 3 - construction material (CM). Process color coding follows the bioDYM process logic classification (see legend): input/output (pink), pass-through (gray), splitter (blue), transformer (orange), FOMP (green), and DSM (purple). The final stocks displayed within each pathway represent the cumulative carbon retained at 2125: SOC Wheat Straw (DI: 408 Gg C), SOC Biochar (P&I: 4,721 Gg C), and Use-Phase CM (3,687 Gg C). The negative atmosphere stock (−8,817 Gg C) reflects net cumulative carbon removal from the atmospheric boundary over the simulation period.*

Figure 4 presents the cumulative carbon balance over the simulation period (2025-2125) as a Sankey diagram, with equal distributions across the three scenarios (33% each). Return flows to the atmosphere are color-coded by scenario (DI: yellow; P&I: red; Construction: dark green), making the circular carbon pathways traceable within the diagram.

Over 100 years, the system extracts a cumulative 8,817 Gg C from the atmosphere (net stock change, shown on the left). The three pathways retain markedly different carbon fractions: P&I stores 4,721 Gg C as biochar; the CM use-phase retains 3,687 Gg C in the building stock; and DI retains only 409 Gg C, which is approximately one-tenth of the P&I outcome. The simulation of FOD (FOMP), anthropogenic use-phases (DSM), and circular atmospheric exchange within a single solver run demonstrates bioDYM's capacity to assess carbon systems that existing dMFA tools require to be solved as separate, manually coupled subsystems.

3.1.2 Biogenic decay in the soil with the FOMP module

BioDYM's FOMP module models organic matter decomposition as a discrete two-pool first-order decay process at each time step (Section 2.2.2). FOMP tracks the accumulation and mineralization of SOC, enabling direct comparisons of pathways with fundamentally different carbon stability profiles.

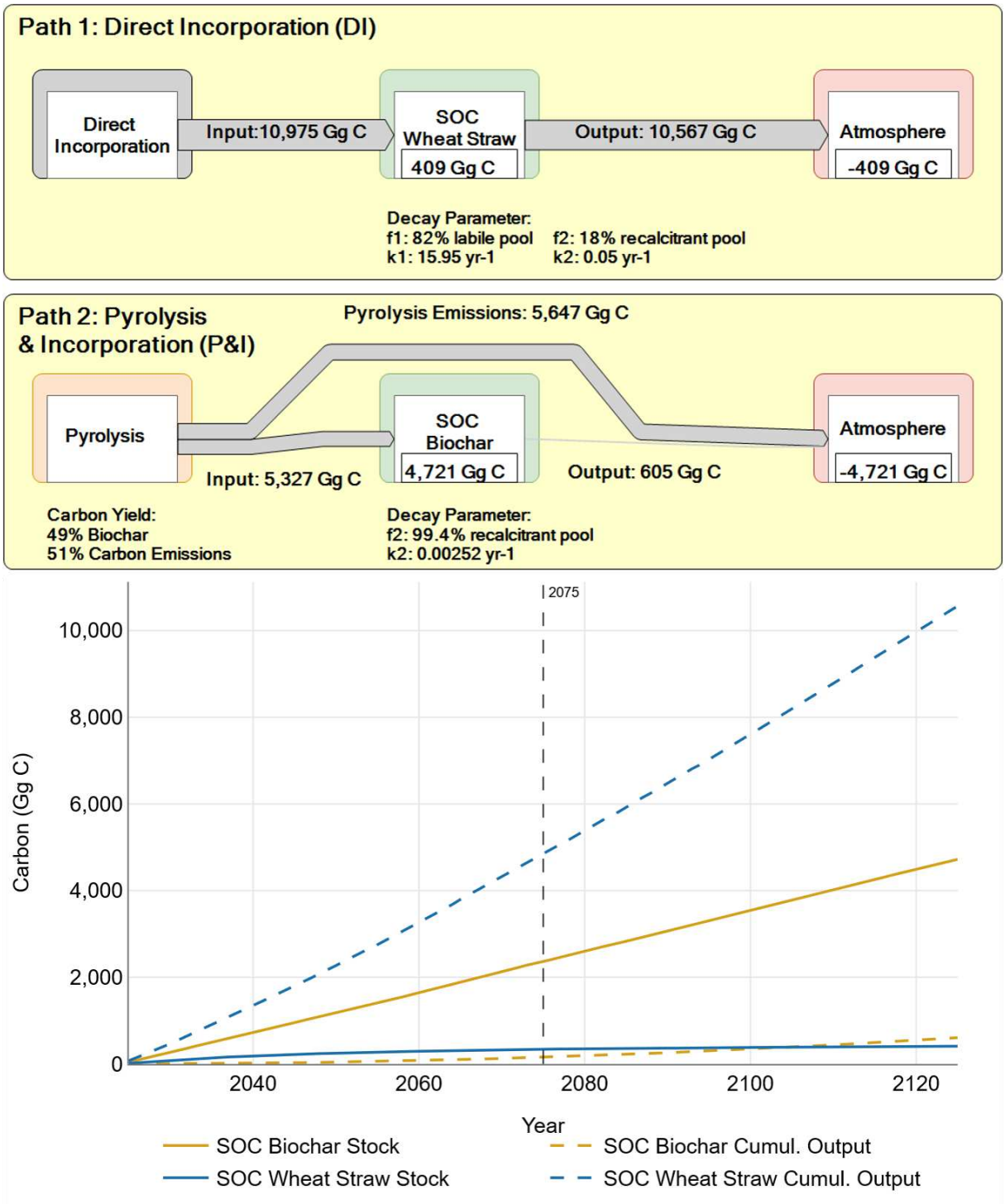


Figure 5: *FOMP process flows and cumulative SOC stock trajectories for the direct incorporation (DI) and pyrolysis & incorporation (P&I) pathways (2025-2125). The upper panels show the cumulative carbon balance of each FOMP process as Sankey diagrams in 2125: cumulative carbon input, retained SOC stock at 2125, and cumulative output returned to the atmosphere boundary. The decay parameters applied in the FOMP model are displayed per pathway: both use a two-pool model (DI = f_1 = 82% labile, f_2 = 18% recalcitrant; k_1 = 15.95 yr^{-1}, k_2 = 0.05 yr^{-1}); P&I approximates mostly a recalcitrant pool (f_2 = 99.4%; k_2 = 0.00252 yr^{-1}), reflecting the high carbon stability of the biochar. The P&I pathway includes 51% carbon loss as pyrolysis emissions, resulting in a net biochar carbon input of 5,327 Gg C from a gross straw carbon input of 10,975 Gg C. The lower panel shows the SOC stock trajectories and emissions modeled by the bioDYM FOMP module: SOC Biochar (P&I, yellow) accumulates continuously over the simulation period, whereas SOC Wheat Straw (DI, blue) approaches a dynamic equilibrium.*

Figure 5 shows the two-pool model structure for DI and P&I, including the pyrolysis carbon yield split (49% TC retained as biochar). The figure presents the resulting SOC stock trajectories over the full simulation period (2025-2125). DI reaches a steady state within approximately 20 years, with annual mineralization nearly equaling annual input, producing a final stock of only 408 Gg C. P&I, with a recalcitrant fraction of 99.4%, produces a continuously growing stock of 4,721 Gg C by 2125, with no steady state reached within the simulation horizon. The results demonstrate that carbon stability is a more important parameter for long-term sequestration than is the quantity of pure carbon input. P&I delivers half of the DI's carbon to the soil yet stores eleven times more carbon after 100 years.

3.1.3 Carbon Storage in the Use-Phase with the DSM Module

BioDYM's DSM module tracks carbon stored in physical products through age–cohort accounting, assigning each annual cohort a lifetime drawn from a selected probability distribution (Section 2.2.3). This enables modeling of the delayed, distribution-driven carbon release from long-lived product stocks.

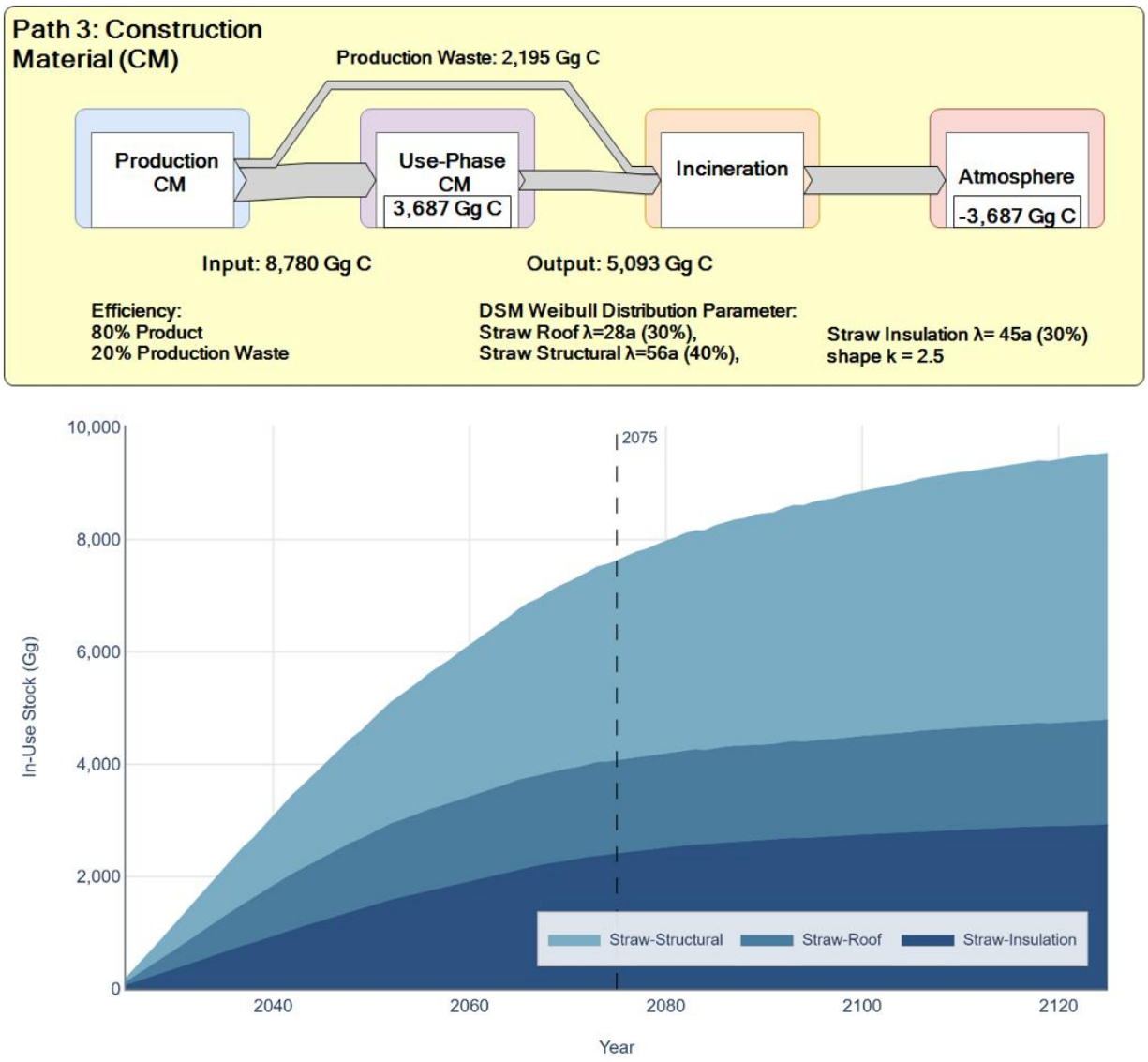


Figure 6: *DSM process age cohort carbon stock accumulation for the construction material (CM) pathway (2025-2125). The upper panel shows the cumulative carbon balance of the CM pathway as a Sankey diagram. Of the total carbon input (10,975 Gg C), 80% enters the use-phase stock via manufactured construction products (net input: 8,780 Gg C), whereas 20% is lost as production waste (2,195 Gg C) and enters direct incineration. The Use-Phase CM stock retains 3,687 Gg C at 2125. The lower panel shows the DSM stock evolution divided into three building material subtypes, each modeled with a Weibull lifetime distribution (shape k = 2.5): Straw-Structural (λ = 56 a, mean ≈ 50 a, 40% of input, light blue), Straw-Roof (λ = 28 a, mean ≈ 25 a, 30%, teal), and Straw-Insulation (λ = 45 a, mean ≈ 40 a, 30%, dark blue).*

Figure 6 presents the CM path results. The top panel shows the annual carbon flows through the Production CM and the Use-Phase DSM process; the bottom panel shows stock evolution by building subtype (2025-2125). Three subtypes contribute to a total carbon stock that grows continuously due to continuous straw inflow, reaching 3,687 Gg C by 2125. As early cohorts reach end-of-life and carbon returns to the atmosphere via incineration, the rate of stock accumulation decelerates, although the stock continues to grow throughout the simulation.

3.1.4 Scenario Comparison with the Scenario Manager

bioDYM's scenario engine implements time-specific transfer coefficient changes or flow quantity changes within a continuous simulation, maintaining accumulated stocks and flow history from prior periods (Section 2.2.4) running separate instances. Similarly, custom scenarios can be built to exploratively manipulate the baseline scenario.

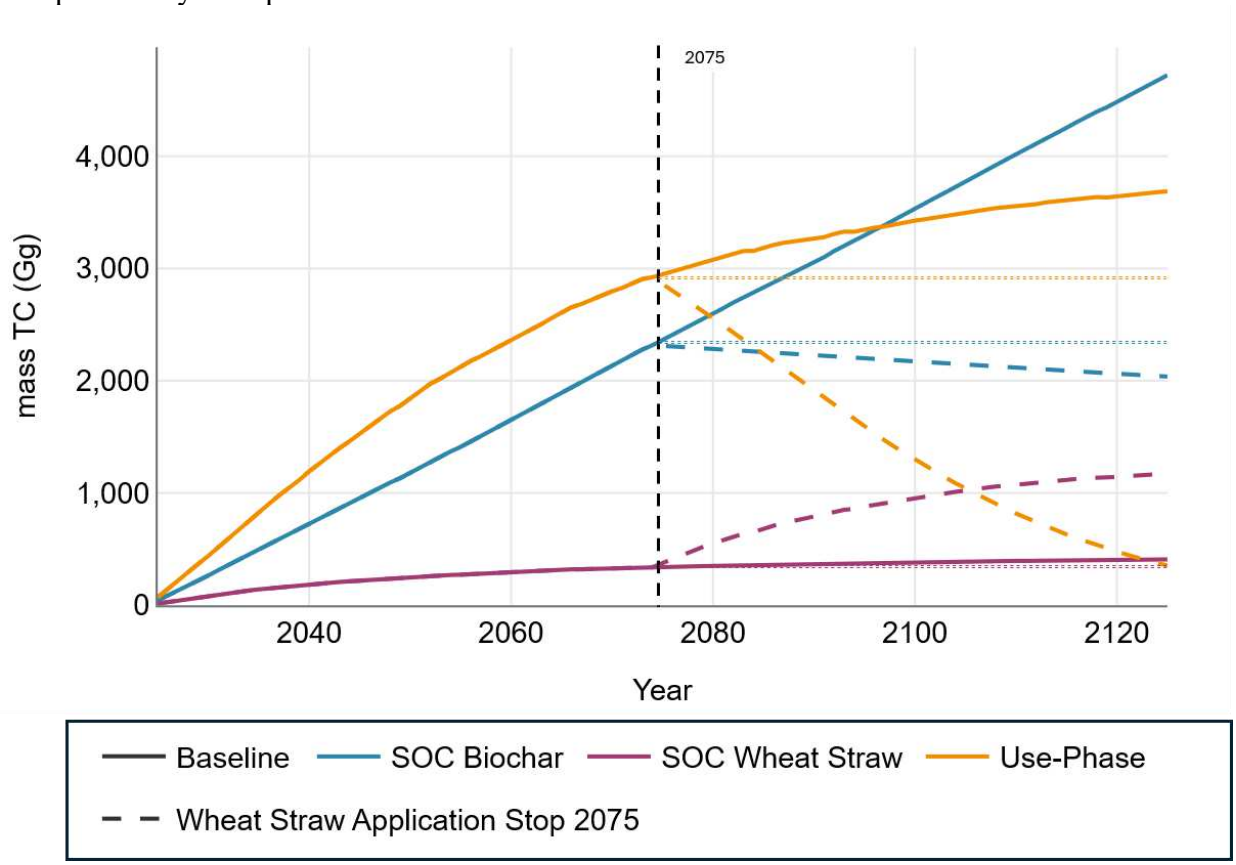


Figure 7: Carbon stock trajectories under the baseline and Wheat Straw Application Stop 2075 scenarios for all three pathways (2025–2125). The solid lines represent the evolution of the baseline stock (2025-2125). The vertical dashed line in 2075 marks the simulated application stop, resulting in cessation of straw supply to the CM and P&I pathways. The dashed lines represent post-2075 stock trajectories. The horizontal dotted lines indicate the stock level in 2075 for each pathway, which serves as a reference.

Figure 7 presents the TC stocks for all three pathways under two scenarios: Baseline (1/3 each, 2025–2125) and Wheat Straw Application Stop 2075 (TC switch to 100% DI at 2075). The vertical dashed line marks the switch year. The horizontal dashed lines indicate the pathway stocks in 2075. The three pathways respond fundamentally differently to the application stop. SOC biochar (P&I) declined by only ~11% between 2075 and 2125 after the input stopped (from 2,350 to 2,085 Gg C), confirming near-permanent biochar stability. The SOC wheat straw (DI) grows rapidly after 2075, as it receives 100% straw input, reaching 1,200 Gg C by 2125, which is three times the baseline value. Use-Phase CM (Construction) collapsed from 2,948 to 353 Gg C, as the accumulated building cohorts mostly reached the end of life without replacement.
This scenario demonstrates the relevance of carbon stability/product lifetimes for reliable carbon stocks. The scenario engine enables this multipath way policy comparison within a single simulation run.

3.1.5 Uncertainty Analysis with Monte Carlo Simulation

bioDYM's Monte Carlo module analyses parameter uncertainty through the complete system by executing the full fixed-point solver n times with independently sampled parameters (Section 2.2.5), verifying mass balance closure automatically for each run. Uncertainty is quantified simultaneously across all process logics, enabling direct comparison of parametric sensitivity across pathways within a single probabilistic simulation.

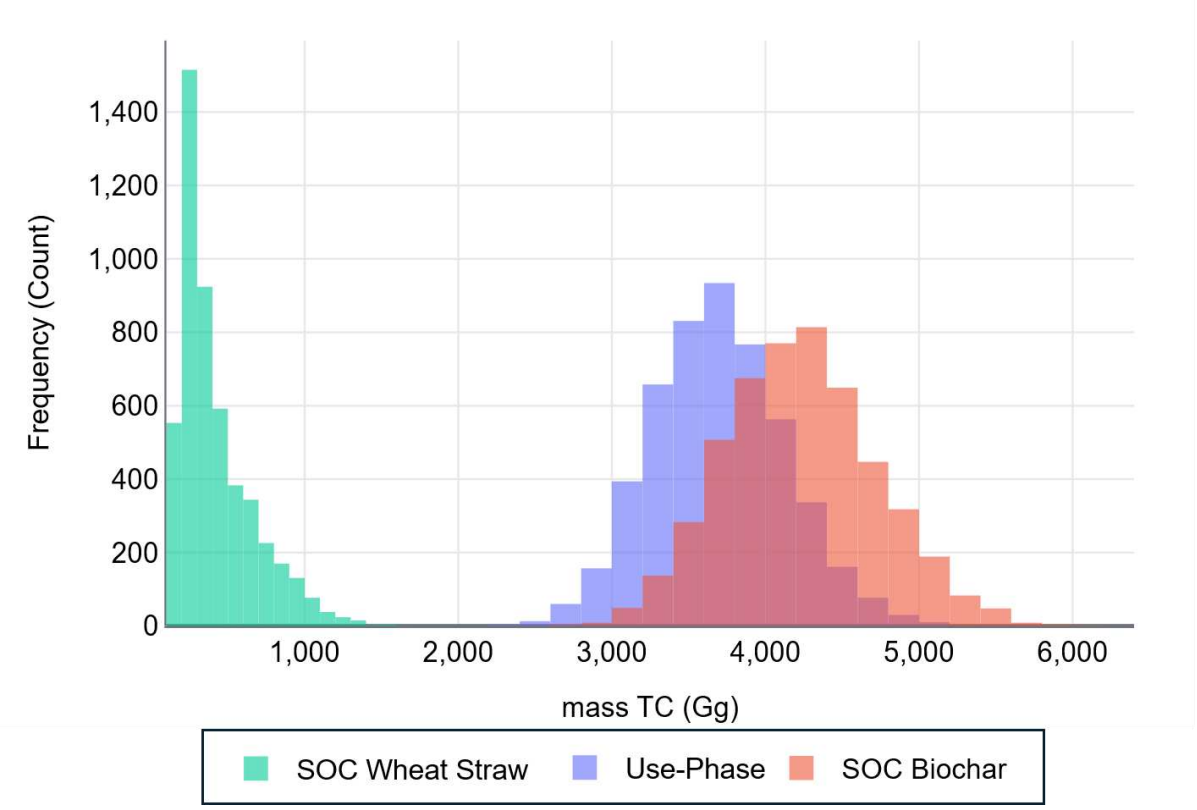


Figure 8: *Monte Carlo simulation results. Probability distributions of final carbon stocks at 2125 across all three pathways (n = 5,000 runs). Histograms showing the frequency distributions of the simulated carbon stock values at the end of the simulation period for the SOC Wheat Straw DI stock (green), Use-Phase CM stock (blue), and SOC Biochar P&I stock (orange). Parameters were sampled from predefined probability distributions defined in the bioDYM-SD: Wheat Straw System Input; pyrolysis TCs, FOMP decay rates (k_1, k_2) and pool fractions (f_1) for the DI and P&I pathways; and DSM input shares and lifetime scale parameters (λ) for the CM pathway.*

The total system results in a mean atmospheric stock of -8,341 Gg C (95% confidence interval [CI]: -10,272– -6,595 Gg C; coefficient of variation [CV] = 11%). All the researched uncertainties are listed in SI 1. Figure 8 presents the distribution of final TC stocks in 2125 across n = 5,000 runs for all three pathways. DI produces a strongly right-skewed distribution (median: 341 Gg C; 95% CI: 155–1,034 Gg C; CV = 58%): the long right tail indicates that favorable combinations of lignin content and decay rates yield substantially greater soil carbon stability, pulling the probabilistic mean (421 Gg C) above the deterministic baseline. The CM use phase yields the narrowest distribution (mean: 3,691 Gg C; 95% CI: 2,875–4,584 Gg; CV = 11%), reflecting that building-type inflow shares and Weibull lifetime parameters are well constrained relative to decomposition kinetics. P&I shows a similarly tight, nearly symmetric distribution (mean: 4,228 Gg C; 95% CI: 3,307–5,237 Gg; CV = 11%), confirming that the CDR potential of biochar is robust to parametric uncertainty in terms of biochar stability. Automated mass balance verification

across all 5,000 runs confirmed system closure and is validating bioDYM's MC framework for circular carbon systems.

4 DISCUSSION

bioDYM fills the gap between GUI-based tools such as STAN, which lacks dynamic and biomass-specific capabilities, and flexible but code-intensive Python frameworks such as ODYM and flodym, which require substantial programming expertise to configure systems. Its core contribution is making dynamic multielement MFA accessible to practitioners without deep programming knowledge and providing new modelling capabilities. It includes FOD, DSM, scenario analysis, uncertainty quantification and more. Three architectural choices distinguish bioDYM from its foundation, each carrying explicit trade-offs.

First-order decay is implemented as a native process logic within the iterative solver. In current dMFA practice, researchers applying mass flow models to biogenic carbon systems typically run decay calculations as separate models and combine outputs manually. When implemented as a two-pooled model, it can model complex biogenic decay. bioDYM removes the need to model these processes in different systems and combines them in a system-wide mass balance. A multipool model for landfill gas prognosis is also implemented.

The fixed-point iterative solver is built for modularity. This means that new additions for any type of dynamic process logic can be added to the calculation engine and integrated into the solver. This makes bioDYM an extendable foundation for future development in the field of CDR strategies as well as other fields of research.

The fixed-point iterative solver resolves circular material flows, an important feature for biogenic carbon systems or cascading utilization. A workaround in dMFA practice is to lag recirculation flows by one time step, introducing a systematic timing offset that accumulates silently over multiple simulation steps while the mass balance still nearly converges. bioDYM's solver converges circular dependencies within each time step, removing this source of systematic error from the model structure.

Other capabilities include simultaneous and extendible multielement tracking (e.g., material, water content, dry matter, and total carbon), which enables element-specific mass balance validation. Integrated Monte Carlo uncertainty quantification and scenario analysis, which lower the barrier from a programming task to a data-entry task. These capabilities would otherwise require separate model instances and manual result aggregation.

Acknowledged limitations arise directly from these design choices. bioDYM operates on a two-dimensional (time × element) matrix structure per process, with processes resolved sequentially by the iterative solver rather than as a tensor dimension. This reduces the six-dimensional framework of ODYM, limiting its application to single-region systems without product-type differentiation. No data reconciliation is provided: unlike STAN, bioDYM does not simultaneously adjust measured input values to satisfy mass balance constraints. Parametric uncertainty in flow quantities can, however, be defined via the MC module and propagated through the full system. Subsystems such as those in STAN are not supported; all processes share a single boundary and time axis, requiring manual coupling for multiscale analyses. Full use still requires Python installation and basic familiarity with Jupyter notebooks. Tracking errors in complex systems remains challenging, even when multiple types of control information and verification are implemented.

4.1 Case study: CDR potential of wheat straw

The case study demonstrated that carbon stability and product lifetime are the primary parameters for long-term CDR strategies. The quantity of carbon transferred into a stock is secondary. Despite receiving only one-third of the carbon input allocated to DI, P&I accumulates an 11 times larger pedosphere after 100 years (4,721 vs. 409 Gg C). The recalcitrant fraction impacts more than the carbon input quantity: P&I delivers half of the DI's carbon to the soil but stores eleven times more after 100 years. In the construction material scenario, carbon is sequestered in the anthroposphere for the duration of building service life, with release delayed decades before ultimately returning to the atmosphere.

The Wheat Straw Application Stop 2075 scenario reveals the differences between storage mechanisms. P&I stocks decline by only ~11% over 50 years after input ceases, confirming near-permanent biochar stability independent of continued supply. Construction stocks collapse by ~89 % as building cohorts reach end-of-life without replacement. This behavior supports the assessment parameter of CDR strategies: the impact of a CDR strategy depends structurally on the storage mechanism, not on the quantity of carbon transferred.

Several limitations limit this interpretation. The yield forecast assumes a linear +0.25 % annual trend; climate-driven yield changes are just partly captured within the MC. FOMP decay parameters are calibrated to a two-pool model averaged across straw types; structural uncertainty, such as the pool number, soil type effects, and climate-driven changes in decomposition rates, is barely addressed by the MC-Simulation and represents an unquantified additional source of uncertainty. Over century timescales, small differences in decay rates compound into order-of-magnitude differences in terminal stocks. The CM pathway models service lifetimes with a Weibull distribution (shape k = 2.5) across all subtypes, a standard assumption for building materials but one that ignores geographic and structural variability in actual product lifetimes. The Monte Carlo confidence bands quantify parametric uncertainty within the assumed model structure, and projections should be interpreted as scenario ranges rather than forecasts.

Finally, the results represent the carbon sequestration potential of wheat straw pathways in physical isolation, not a net climate benefit assessment. bioDYM provides no economic or social dimensions: the scenario engine models technically feasible pathways but cannot rank them by cost, social acceptance, or implementation feasibility. Combined applications with life cycle assessment and technoeconomic analysis are needed to evaluate overall climate impact and deployment viability. bioDYM is complementary to, rather than a substitute for, these tools.

4.2 Conclusions:

The modular architecture and the case study results establish bioDYM as a practical tool with several novelties for quantifying CDR strategies. Germany's total wheat cultivation area (~29,500 km²) is 29.5 times larger than the case study area, indicating a substantial national potential for biogenic carbon management to contribute to CDR targets(DeSTATIS, 2025a).

Three directions for future development are as follows: First, the modular solver architecture enables extension with additional process logics, such as biogas formation or anaerobic digestion, expanding bioDYM from a carbon management tool into a comprehensive planning system for biobased material cascades. Second, application with experimentally derived rather than literature-based parameters would deepen the empirical grounding of model outputs; decay experiments, landfill gas monitoring data, and building material surveys represent immediate data sources.

Third, user feedback and custom process logics will lead to the development of more general dMFA software.

bioDYM is available as an open-source tool (Scholz et al., 2025). It addresses a methodological gap in CDR strategy assessment where in which dynamic stock modelling, multielement tracking, and first-order decay have not previously been combined in a single auditable mass-balance system accessible to nonspecialist users.

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bioDYM, and this study was developed without external funding.

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720 **SUPPORTING INFORMATION**
721
722 **Supporting Information S1:** This supporting information provides an overview of all the defined
723 uncertainties of the system in the wheat straw case-study.
724

Path:	Process:	Description	Parameter	Value	Uncertainty	Source
general	None	Carbon input	F_00_01	100%	σ=10%	Assumption
general	None	Water & Nutrient input	F_01_02	100%	σ=10%	Assumption
DI	P8 SOC Wheat straw:	Recalcitrant fraction (lignin)	f2	18%	*U*(10.2%, 20%)	(Zhang et al., 2016) (Beuel et al., 2020)
DI	P8 SOC Wheat straw:	Labile decay rate	k1	15.95 yr^{-1}	*U*(10,20) yr^{-1}	(Cai et al., 2018)
DI	P8 SOC Wheat straw:	Recalcitrant decay rate	k2	0.05 yr^{-1}	*U*(0.01,0.09) yr^{-1}	(Cai et al., 2018)
P&I	P9 Pyrolysis:	Carbon Yield biochar	TC	49%	U(43%,50%)	(Liu et al., 2018; Woolf et al., 2021) (Sedmihradská et al., 2020)
P&I	P7 SOC Biochar	Recalcitrant fraction	f2	99.4%	*U*(84%, 99.4%)	(Sanei et al., 2025) (Woolf et al., 2021)
P&I	P7 SOC Biochar	Labile decay rate	k1	30 yr^{-1}	U(0.107,0.087) day^{-1}	(Kuzyakov et al., 2014).
P&I	P7 SOC Biochar	Recalcitrant decay rate	k2	0.00252 yr^{-1}	U(0.0012, 0.003) yr^{-1}	(Kuzyakov et al., 2014)
CM	P10 Production	Production efficiency	TC	80%	-	Modeling assumption
CM	P11 Use-phase	Shape factor	k	2.5		Assumption
CM	P11 Use-phase	Straw-roof inflow	DSM share	30%	U(20% - 40%)	Assumption
CM	P11 Use-phase	Straw-roof lifetime	λ	28 a	σ= 2.8a	(Kaesberg and Scharmer, 2024)

CM	P11 Use-phase	Straw-Structural inflow	DSM share	40%	U(30% - 50%)	Assumption
CM	P11 Use-phase	Straw-Structural lifetime	λ	56a	σ= 5.6a	(Kaesberg and Scharmer, 2024)
CM	P11 Use-phase	Straw-Insulation inflow	DSM share	30%	U(20% - 40%)	Assumption
CM	P11 Use-phase	Straw-Insulation lifetime	λ	45 a	σ= 4.5a	(Kaesberg and Scharmer, 2024)

Table (SI) 1: Uncertainty parameters defined for the Monte Carlo simulation

Supporting Information S2: This supporting information provides an overview of all the defined system uncertainties of the system.

Id	Feature Category	Feature	Description	Origin
1	System Architecture	bioDYM SystemDefiner	Structured Excel-based Template System for data input	BioDYM
			Browser-based web interface for system definition and configuration (FastAPI)	
		bioDYM Engine	Calculation, plotting, data loader engine	BioDYM
		bioDYM Dashboard	Jupyter Notebook as interactive UI (Voilà)	BioDYM
2	Core MFA Framework	Process-Flow-Stock Model	Material flow accounting with mass balance	ODYM
		Multi-Element Tracking	Simultaneous tracking of multiple elements (e.g. material, WC, DM, CC)	ODYM
		Time–Dynamic Simulation	Year-by-year material flow calculations	ODYM
		Mass Balance Validation	Automatic consistency checking	ODYM
3	Stock Modeling	Dynamic Stock Model (DSM)	Age-cohort based stock modeling with lifetime distributions	ODYM
		DSM Initial Stock Modes	Three modes: Zero, Decay, Cohort	BioDYM
		FOMP (First-Order Mineralization)	Organic matter decomposition modeling	BioDYM
		Initial Stock Engine	Flexible initial stock configuration	BioDYM
4	Process modeling	Process Types (5 types)	Splitter, Transformer, Input, DSM, FOMP, Flow Cap, BOM Assembler	BioDYM
		Transformer/Splitter	Composition-preserving/changing material splits	BioDYM
		Static/Dynamic TCs	Time-independent/dependent TCs	BioDYM

5	Flow Modeling	Hierarchical Elements	Parent–child element relationships (e.g., CC as % of DM)	BioDYM
		Flow Composition	Automatic flow composition checking	BioDYM
6	Visualization	Sankey Diagrams	Interactive flow visualization	BioDYM
		Flow Composition C	Stacked bar charts of element composition	BioDYM
		Mass Balance Error	Interactive error visualization by process	BioDYM
		Publication Themes	Named style presets (exploratory, JIE) for publication-ready figure export	BioDYM
7	Scenario Analysis	Scenario Manager	Multiscenario comparison framework	BioDYM
		Parameter Modification	TC and parameter adjustments per scenario	BioDYM
		Scenario Plots	Multiscenario comparison visualization	BioDYM
8	Data Management	YAML Configuration Mode	SystemDefiner exports YAML configs as alternative to Excel input	BioDYM
		Automatic Interpolation	Fills missing years in flow data	BioDYM
		Data Validation	Comprehensive input validation	BioDYM
9	Uncertainty Analysis	Monte Carlo Simulation	Probabilistic uncertainty propagation	BioDYM
		Distribution Sampling	Normal, uniform, triangular, lognormal	BioDYM
		MC Plots	Monte Carlo Simulation Visualization	BioDYM
		MC Mass Balance	Automatic MC consistency checking	BioDYM
10	Reporting & Export	Excel Results Export	Multisheet results with metadata	BioDYM
		Sankey Export	Batch export to HTML, JSON, CSV, and SankeyMatic formats	BioDYM
		KPI Dashboard	Key performance indicators calculation	BioDYM

Supporting Information S3: Case-Study configuration file, including references and assumptions.

Supplementary Files

This is a list of supplementary files associated with this preprint. Click to download.

- JIEWheatStrawfinal.zip