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Product-related CO_2 Allocation in Manufacturing: Handling Operational Variability, Exceptional Events, and Process Changes

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Abstract

Product-related CO_2 values are increasingly required in manufacturing, but direct attribution of production emissions to individual products can create distorted Product Carbon Footprint (PCF) values under real operating conditions. Machine failures, scrap, material losses, fluctuating quantities, changing product mixes, or process changes such as new electricity mixes or photovoltaic systems can strongly affect product-level results.

This paper proposes an allocation-oriented approach for product-related CO_2 calculation in manufacturing. It decomposes production-related PCF contributions into materials, consumables, energy use, maintenance, asset and infrastructure shares, and waste treatment and defines allocation strategies for products, batches, product types, accounting periods, and future periods. A forecast-and-reconciliation mechanism compares expected and actual emissions and distributes deviations through correction factors. A gDEZ-based data foundation provides the energy-related accounting context, while an exemplary BaSyx-based deployment illustrates how allocation choices, calculation inputs, correction parameters, and traceability information can be represented in Asset Administration Shells for adaptable PCF calculation.

Keywords: Product Carbon Footprint, carbon accounting, emission allocation, Asset Administration Shell, Digital Twin

1 Introduction

1.1 Motivation

Manufacturing companies are increasingly required to quantify and reduce product- and production-related carbon footprints due to regulatory, economic, and customer-driven pressures [1–3]. Product-related CO_2 values are relevant for sustainability reporting, customer communication, regulatory compliance, and the identification of operational improvement potentials. However, the accurate tracking and calculation of emissions remains challenging, as numerous factors have to be considered: Products are manufactured through multiple heterogeneous production steps. Machines process large numbers of products, may require setup activities, consume energy and auxiliary materials, generate waste, and can fail unexpectedly. Some products do not pass quality gates, and only a fraction of rejected parts may be recycled, which itself requires additional energy and resources. A product-related CO_2 footprint calculation therefore needs to account for all relevant contributions in a transparent and traceable manner.

In this paper, we describe a straightforward CO_2 footprint calculation approach based on Digital Twins and the Asset Administration Shell (AAS). Existing approaches to carbon accounting in manufacturing often focus on electricity-related emissions, site-level emission factors, or corporate reporting. Such approaches are necessary, but insufficient for product-related decision-making. A product-level perspective requires a more detailed consideration of how CO_2 contributions arise during production and how they should be assigned to product instances, or batches. This is especially relevant in discrete manufacturing, where production orders, machines, tools, and intermediate products can often be identified individually, while not every environmental burden can be causally assigned to a single product.

1.2 Problem Statement

The Product Carbon Footprint (PCF) of a manufactured product can be understood as the sum of the PCFs of all input products or intermediate products plus the additional CO_2 contributions caused by the considered manufacturing step. In practice, manufacturing companies face the challenge that some sources of carbon emissions, such as consumables, machine-related impacts, maintenance activities, setup efforts, or waste treatment, have to be distributed across a larger number of products. Since such emissions can only be allocated to products that are known or expected at the time of calculation, this often requires assumptions about future production quantities. These assumptions may change due to market demand, production planning updates, or unexpected short-term events.

A naive attribution of production-related emissions directly to the products currently being manufactured can therefore lead to distorted PCF values. For example, if a machine fails after only a few produced parts, assigning the full failure-related burden to those parts would result in unrealistic product-level CO_2 values. Similar distortions can occur in the case of unplanned maintenance, scrap, rework, material losses, fluctuating production quantities, changing product mixes, or process changes such as the installation of photovoltaic systems, a changed electricity mix, or the introduction of new machines and tools. These situations are not rare exceptions in industrial practice; they are part of real production systems. Product-related CO_2 calculation therefore requires allocation mechanisms that are precise enough to support traceability, but robust enough to avoid misleading outliers.

To address this gap, this article extends our previous work on accurate emission factors for production sites [4], which introduced a green Digital Energy Twins (gDEZ) -based representation of production activities, energy sources, energy storage systems, consumers, and forecasted grid carbon intensities for time-resolved carbon accounting in manufacturing. That work focused on determining accurate and forward-looking emission factors for production sites and on representing the required data through Asset Administration Shells and is revisited in Section 5. The present article retains this foundation because product-related CO_2 allocation depends on reliable, source-specific, and temporally resolved emission data. However, the scientific focus is shifted from determining emission factors to allocating production-related emissions to products under real manufacturing conditions. In particular, this paper addresses how emissions from energy use, materials, consumables, maintenance, assets and waste can be assigned to product instances, batches, product types, accounting periods, or future production when operational variability, exceptional events, and process changes would otherwise distort product-level PCF values. We therefore describe an accounting approach that handles events and changes in manufactured product quantities and thereby enables the proper treatment of unexpected operational situations. We discuss how the number of manufactured products can be considered in the allocation process and illustrate the software infrastructure required to operate the AAS as a technical foundation for digital product twins.

1.3 Contributions and Paper Structure

Motivated by these challenges, this paper makes the following contributions:

- It introduces a component-wise product-related CO_2 calculation model for manufacturing, describing how PCF contributions arise from existing product PCF, added materials, process consumables, energy use, maintenance, asset and infrastructure use and waste treatment.
- It defines allocation strategies for assigning these contributions to product instances, batches, product types, accounting periods, or future periods depending on causal plausibility, data availability, and the risk of distorted product-level CO_2 values.
- It proposes a carbon-account-based forecast-and-reconciliation mechanism that compares expected and actual emissions at the end of an accounting period and

distributes deviations through correction factors to avoid unrealistic PCF outliers while still reflecting persistent changes in the production system.
- It shows how the allocation method can be supported by a gDEZ-based representation of energy-related accounting data.
- It describes an exemplary BaSyx deployment that maps the proposed CO_2 allocation model to digital twins, repositories, registries, services, and documented calculation choices, thereby supporting traceability and adaptability for SMEs.

The remainder of this paper is structured as follows. Section 2 introduces the background, scope, terminology, and related work. Section 3 presents the proposed allocation-oriented approach. Section 4 formalizes the PCF calculation model and the calculation rules for the individual PCF components. Section 5 describes how the data and traceability requirements can be operationalized using a gDEZ representation. Section 6 presents an exemplary AAS/BaSyx-based operationalization of the proposed approach. Section 7 concludes the paper and outlines future work.

2 Background Knowledge

For the calculation of Product Carbon Footprints (PCF) and production-related carbon emissions, relevant standards, regulations, and methodological frameworks have to be considered. In this paper, the focus is on PCF calculation. This also requires a high-resolution accounting of electricity-related emissions at machine and order level, their aggregation into product carbon footprints, and their consistent embedding into the corporate greenhouse gas inventory, which is referred to as Corporate Carbon Footprint (CCF). Our proposed approach is therefore positioned in relation to key international standards and frameworks, including the GHG Protocol, ISO 14067, ISO 14040, ISO 14044, ISO 14064, ISO 14083, the GLEC Framework, ISSB S2, and the WBCSD PACT/Pathfinder Framework, as well as relevant EU regulations such as CSRD/ESRS E1, PEF/PEFCRs, CBAM, the EU Battery Regulation, and the ESPR/Digital Product Passport [5, 6]. The organizational carbon accounting perspective is aligned with the GHG Protocol Corporate Standard and Scope 2 Guidance [6, 7].

These standards and bodies of knowledge define principles, requirements, and reporting structures for carbon accounting and life cycle assessment. In particular, life cycle assessment principles and requirements are specified in ISO 14040 and ISO 14044 [8, 9]. However, the standards also leave methodological degrees of freedom that have to be addressed when applying them to high-resolution, production-related PCF calculation. The most relevant aspects for the approach presented in this paper can be summarized as follows:

- The use of time-resolved, for example hourly, grid emission factors can improve operational control and production planning, but requires careful aggregation and reconciliation for annual external reporting.
- The allocation of overhead emissions requires transparent and causally motivated allocation drivers, such as energy use, processing time, machine time, production volume, or capacity utilization, and should be accompanied by sensitivity analyses.

- The treatment of self-generated electricity, electricity storage, power purchase agreements, and certificates requires explicit rules to avoid double counting and to distinguish location-based and market-based Scope 2 accounting.
- The limited coverage of some product categories by Product Environmental Footprint Category Rules (PEFCRs) or Product Category Rules (PCRs) requires documented methodological choices to support transparency and comparability.

2.1 Corporate vs. product perspective

It is important to distinguish between the corporate and the product perspective of carbon accounting. The Corporate Carbon Footprint (CCF) follows an organizational accounting logic, for example according to the GHG Protocol Corporate Standard, and classifies emissions into Scope 1, Scope 2, and Scope 3 categories. Scope 1 covers direct emissions from sources owned or controlled by the company, Scope 2 covers indirect emissions from purchased or acquired energy, and Scope 3 covers other indirect emissions along the upstream and downstream value chain. In contrast, the Product Carbon Footprint (PCF) follows a product life-cycle perspective, for example according to ISO 14040, ISO 14044, and ISO 14067, and is not subdivided into scopes.

The approach presented in this paper considers emission contributions that may correspond to all three scopes from a corporate accounting perspective. Direct process emissions, fuel combustion, refrigerant losses, or other emissions from company-owned or controlled production assets are relevant for Scope 1 accounting. Purchased electricity, heat, steam, or cooling are relevant for Scope 2 accounting. Upstream contributions from input materials, consumables, purchased components, services, capital goods, or waste treatment may be relevant for Scope 3 accounting. From the product perspective, which is relevant for PCF calculation, these contributions are not treated as scope categories, but as life-cycle contributions that have to be assigned to products, batches, product types, or accounting periods.

The core contribution of this paper is a calculation and allocation approach for production-related CO_2 contributions at the level of machines, production steps, and orders. Particular emphasis is placed on the calculation and product-level attribution of direct production-related emissions, which correspond to Scope 1 from the corporate perspective. In addition, electricity-related emissions are represented in a way that is consistent with Scope 2 corporate reporting and can be attributed to the manufacturing stage of the PCF. Upstream emissions that have already been assigned to input products, intermediate products, materials, or consumables are included as life-cycle contributions of the PCF, while their possible relevance for Scope 3 corporate accounting is preserved.

This paper does not propose a new method for corporate Scope 3 accounting. Instead, Scope 3-related contributions, such as embodied emissions of purchased materials, consumables, machines, tools, or infrastructure, are used as input data where required for product-level allocation. The methodological contribution lies in the transparent calculation, allocation, and updating of production-related emission contributions in discrete manufacturing, with a particular focus on direct emissions and their consistent integration into PCF calculation and CCF-compatible reporting structures.

2.2 Related Work

Existing work provides several foundations for product-related CO_2 accounting in manufacturing. Smolek et al. [10] propose a bottom-up method for aggregating product footprints during manufacturing. Their approach already addresses the allocation of resource consumption from production, logistics, energy systems, buildings, and auxiliary systems to batches or individual products. It also considers situations such as setup, standby, ramp-up, and multi-output production.

Standardization-oriented frameworks, such as the Pathfinder Framework [11] and the Catena-X PCF Rulebook [12], provide guidance for PCF accounting, data exchange, system boundaries, allocation, waste treatment, transportation, electricity, primary data shares, and data quality. These frameworks are important for harmonizing PCF calculation and exchange across companies. However, they remain comparatively generic with respect to operational allocation logic inside production systems, where emissions have to be assigned to concrete products, batches, machines, orders, or accounting periods under changing production conditions.

Digital-twin-based approaches further show how PCF-relevant data and calculation models can be represented in manufacturing environments. Winter [13] integrates PCF calculation, uncertainty, data quality, and provenance into Digital Master and Digital Twin concepts. Balduf et al. [14, 15] use Green Digital Twins and Asset Administration Shells to model activity data and calculate gate-to-gate PCFs depending on the digitalization degree of the production system. Trusted data space approaches extend this perspective towards sovereign cross-company PCF data exchange [16].

Complementary review work highlights practical barriers for industrial PCF assessment, especially for small and medium-sized enterprises. These barriers include methodological complexity, insufficient data availability, and inconsistent software support [17]. Uncertainty-focused studies show that system boundaries, activity data, emission factors, allocation methods, and scenarios are major sources of PCF uncertainty. They also highlight that methods such as Data Quality Indicators, Monte Carlo simulation, and sensitivity analysis are commonly used to assess the reliability of PCF results [18].

Despite these contributions, existing work provides limited guidance on how product-related CO_2 values should be allocated under operational variability, exceptional events, and persistent process changes. Examples include machine failures, unplanned maintenance, scrap, rework, material losses, fluctuating production quantities, changing product mixes, new production patterns, or changes in the energy supply. These situations are highly relevant in discrete manufacturing, where production systems are dynamic and not all environmental burdens can be causally assigned to individual product instances at the time they occur.

Our work addresses this gap by proposing a component-wise calculation logic, suitable allocation levels, and forecast-based correction mechanisms for production-related PCF values. The approach supports the transparent handling of operational events and changes in production quantities and is illustrated by an exemplary implementation based on the Asset Administration Shell and Eclipse BaSyx.

3 Proposed Approach

This article proposes an integrated approach that documents gDEZ with calculation rules for individual factors that contribute to a PCF, and an account-based distribution to enable an even distribution of carbon emissions among products, and to handle unexpected events at the same time. A gDEZ exists for all assets with a Digital Twin, i.e. production orders, machines, meters, energy sources, storage systems, products, and resources that are represented by an AAS. This enables time-resolved carbon accounting for production-related energy consumption. This digital representation makes it possible to capture machine-specific consumption, grid electricity, self-generated electricity, storage behavior, and temporally varying emission factors in a traceable form.

Building on this gDEZ-based foundation, the paper addresses the methodological problem of product-related CO_2 allocation. For this purpose, the PCF contribution of a manufacturing step is decomposed into relevant factors, including existing product PCF, added materials, process consumables, energy use, maintenance shares, asset and infrastructure shares and waste treatment. Each component is assigned to an appropriate allocation level, such as product instance, batch, product type, accounting period, or future period. In addition, special cases are classified to determine whether direct attribution, period-based averaging, forecast-based allocation, or correction over subsequent periods is appropriate. The resulting calculation model distinguishes between directly attributable contributions and contributions that should be allocated over batches, periods, or future production. In the CNC milling example introduced in the motivation, the incoming PCF of the aluminium blank and, where available, the measured energy consumption of a specific milling operation can be treated as directly attributable contributions. In contrast, contributions caused by tool wear, coolant replacement, maintenance activities, or scrap from an exceptional tool failure may have to be allocated over a batch, an accounting period, or future production to avoid distorted product-level PCF values.

The model further introduces a forecast-and-reconciliation mechanism. Expected production quantities and expected emissions are used for initial product-level allocation. At the end of an accounting period, the booked product-related emissions are compared with the actually measured emissions. Deviations are captured as residuals and distributed over subsequent periods through correction factors. In the milling example, this means that an unexpected tool failure is not assigned entirely to the few products processed at the time of the event. Instead, the corresponding residual can be distributed over subsequent products, while a persistent change, such as a permanently different energy demand or a changed electricity mix, is reflected in future PCF values.

The proposed approach is designed to support practical use in small and medium-sized enterprises (SMEs). It does not assume that all machines are fully instrumented or that all material and waste streams can be assigned to individual products with perfect accuracy. Instead, it supports different levels of data availability and allows companies to document which allocation drivers, correction factors, time windows, and data sources were used. This documentation is essential because PCF calculation

inevitably involves methodological choices. The objective is therefore not to eliminate such choices, but to make them explicit, consistent, and traceable.

In addition to the calculation model, this paper describes an exemplary deployment based on AAS and Eclipse BaSyx. The deployment demonstrates how gDEZ and the proposed CO_2 allocation model can be represented in a digital infrastructure and how the selected allocation choices can be documented for later inspection, auditing, and adaptation.

4 PCF calculation

A digital twin is composed of multiple submodels that represent different aspects of an asset or process, and support different use-cases. Our approach composes the carbon dioxide footprint of a discrete manufactured product from different factors, sources of CO_2 that are represented by variables. The product carbon footprint at the end of a production step is therefore the sum of the carbon footprint already associated with incoming products or intermediate goods and additional contributions from the production step:

$$\mathrm{Product}_{\mathrm{PCF}} = \sum_{i=1}^{n} \mathrm{PrdIn}_{\mathrm{PCF},i} + \mathrm{Mat}_{\mathrm{PCF}} + \mathrm{Cns}_{\mathrm{PCF}} + \mathrm{En}_{\mathrm{PCF}} + \mathrm{Mnt}_{\mathrm{PCF}} + \mathrm{Ast}_{\mathrm{PCF}} + \mathrm{Wst}_{\mathrm{PCF}} \tag{1}$$

- $\mathrm{PrdIn}_{\mathrm{PCF},i}$: Product carbon footprint of the i-th incoming or intermediate product or component that is incorporated into the product during the considered production step.
- $\mathrm{Mat}_{\mathrm{PCF}}$: Carbon footprint of additional materials that are added to the product during the production step, such as screws, coatings, or adhesives.
- $\mathrm{Cns}_{\mathrm{PCF}}$: Carbon footprint of process consumables or tools used during the production step, such as lubricants, oils, or coolants. These are consumed by the process but do not necessarily remain in the final product.
- $\mathrm{En}_{\mathrm{PCF}}$: Carbon footprint resulting from the energy consumed during the production step.
- $\mathrm{Mnt}_{\mathrm{PCF}}$: Allocated carbon footprint share of maintenance activities and materials or consumables required to keep the production process or the involved assets operational.
- $\mathrm{Ast}_{\mathrm{PCF}}$: Allocated carbon footprint share of the asset or assets required for the production step. This component accounts for the embodied carbon footprint of machines, handling systems, or infrastructure, allocated to the considered product according to a suitable allocation rule.
- $\mathrm{Wst}_{\mathrm{PCF}}$: Carbon footprint caused by the treatment, recycling, or disposal of waste generated during the production step.

4.1 Accounting and Leveling

Long-term investments, such as machines or infrastructure, are typically distributed over several years, as machines have long lifetimes. The carbon footprint of a production environment should therefore be balanced over the manufactured products. Additionally, a PCF calculation scheme must also be able to account for unforeseen events. For example, a machine may fail shortly after maintenance, reach the end of its lifetime earlier than expected, or remain operational significantly longer than initially assumed. Such deviations must be reflected in the carbon footprint of future products without retroactively changing the PCF of products that have already been produced. PCF calculation also must ensure that these events do not yield short-term spikes in calculated carbon footprints, as these may, depending on the carbon pricing, render product batches unsaleable.

To address this challenge, we introduce the concept of a carbon account. The carbon account is inspired by coupled continuous-time (CT) simulations. They often model closed-loop systems that are composed of multiple interacting parts. Input variables of one part depend in this case on the outputs of other parts. In this case, there is often no dependency-free execution order. Simulation models need to predict the values of their input variables at the end of a time step, perform their calculations, and synchronize afterwards. The simulation then checks whether the predicted and calculated values match. If a large deviation occurs, it must be compensated. One common strategy is to apply a correction or compensation factor that gradually moves a variable back towards its correct value while maintaining a continuous trajectory.

The carbon account applies a similar principle to PCF calculation. It records deviations between expected and actual CO_2-related contributions, and, instead of assigning such deviations entirely to a single product or batch, the carbon account distributes them over future products according to a defined allocation rule. This enables an even distribution of CO_2-related contributions over time and avoids disproportionate burdens on individual products or production batches. We propose one account for each relevant source of CO_2 that becomes part of the product PCF. The following equation defines the added value to the PCF V_{AddPCF} from an account type:

$$V_{\mathrm{AddPCF}} = \min\left(\frac{V_{\mathrm{AccTypePCF}}}{C_{\mathrm{ProdInstForAccType}}}, C_{\mathrm{AddPCFForTypeMax}}\right) \tag{2}$$

$C_{\mathrm{ProdInstForAccType}}$ is the predicted number of future product instances over which the current account balance should be distributed. $C_{\mathrm{AddPCFForTypeMax}}$ defines the maximum additional PCF contribution that may be assigned to a single product for this account type. This ensures that larger irregularities are distributed over a longer period of time. If the account balance increases continuously, the value of $C_{\mathrm{ProdInstForAccType}}$ and possibly $C_{\mathrm{AddPCFForTypeMax}}$ should be reduced for the corresponding account type, as a larger amount of carbon emissions need to be allocated to every product.

Leveling collects PCF footprints and distributes them equally among products of a batch. For example, the energy consumption of milling processes gradually increases with tool wear, which would cause continuously increasing PCF footprints for product instances, until the tool is replaced. This is usually not desired, as it adds artificial

quality differences between otherwise equal products. To compensate, a predicted average value for PCF impact factor $\mathrm{Cns_{PCF}}$ is calculated. The actual PCF for a "billing interval" of n products is measured. At the end of the billing interval, the difference between the actually billed CO_2 emissions and the actual measured emissions is calculated, and the positive or negative result is added to the account balance of this factor.

4.2 CO_2 calculation for production steps

Some carbon factor calculations are common for many process steps in discrete manufacturing. We have therefore extracted them to simplify the description of concrete calculations, and to enable their re-use.

Common calculations

Most process steps rely on non-countable consumables, such as lubricants, shielding gas, compressed air, or process fluids. Their PCF factor is calculated as follows:

$$\mathrm{Cns_{PCF}} = \sum_{i=1}^{m} q_i \cdot \mathrm{CnsIn_{PCF},}_i \tag{3}$$

$$\mathrm{CnsIn_{PCF},}_i$$

is the PCF footprint of a unit of consumable, e.g. 1 liter of lubricant. Factor $\mathrm{q_i}$ denotes the quantity of the consumable units assigned to the production step. The allocation of consumables with long replacement intervals, for example one liter of lubricant used for 100 process executions, is supported by the carbon account. Likewise, premature replacement of consumables can be compensated through the carbon account.

The required energy for a process step $\mathrm{E_{step}}$ is either a predicted mean value, or a measured value. The energy source $\mathrm{F_{Energy}}$ represents the amount of carbon dioxide emitted per unit of consumed energy, e.g. per kWh. For a single energy source, the required energy for the process step is multiplied with the energy factor:

$$En_{\mathrm{PCF}} = E_{\mathrm{step}} \cdot F_{\mathrm{Energy}} \tag{4}$$

If multiple energy carriers or energy-consuming functions are involved, the energy-related PCF is calculated as follows:

$$En_{\mathrm{PCF}} = \sum_{i=1}^{n} E_{\mathrm{step},i} \cdot F_{\mathrm{Energy},i} \tag{5}$$

The maintenance factor $\mathrm{Mnt_{PCF}}$ represents direct carbon emissions from maintenance tasks, e.g. energy or material use during maintenance or setup times. Similar to the other factors, the maintenance factor $\mathrm{Mnt_{PCF}}$ is calculated by summarizing maintenance efforts, and by distributing them on a number of products, e.g. the predicted number of products that will be produced during the interval until the next maintenance is performed. The maintenance-related PCF contribution is calculated as follows:

$$Mnt_{\mathrm{PCF}} = \sum_{i=1}^{m} MntIn_{\mathrm{PCF},i} \cdot Sh_{\mathrm{Use},j,i} \tag{6}$$

with

$$Sh_{\mathrm{Use,j}} = \frac{V_{\mathrm{AstPCF}}}{Products_{\mathrm{Lifetime}} \cdot j_{\max}} \tag{7}$$

Here, Mnt_{PCF} denotes the total carbon footprint of the maintenance tasks, and $Products_{\mathrm{Lifetime}}$ denotes the predicted product instances over the maintenance period. Sh_{Use} may be calculated for multiple products if multiple significantly different products are manufactured with the asset during the interval. In this case, product instances $Products_{\mathrm{Lifetime}}$ must be predicted for $j_{\max}$ products, and the product specific value of Sh_{Use} must be used when calculating Mnt_{PCF}. Mismatches between predicted and actual product instances must be tracked, added to the account balance of the factor, and added/removed from future products.

The asset factor Ast_{PCF} that represents the carbon footprint of an asset, e.g. a machine, is calculated in a similar manner, considering the product instances over the predicted lifetime instead of a maintenance period.

Waste treatment factor Wst_{PCF} covers remainders, e.g. unusable consumables, scrap material, but also defective products that permanently failed a quality check. We consider recyclable waste and non-recyclable waste individually: Recyclable waste requires added energy for a recycling process, and then yields a new consumable, material, or a product (part). In this case, the difference between the carbon footprint of a new part, and the energy fraction of the recycled part plus the energy required for recycling should be added to the waste account and distributed to future products. Scrap will be added to the account as well, increasing the added PCF of future products. Good recycling will therefore reduce the carbon footprint of future products.

The factors Cns_{PCF}, En_{PCF}, Mnt_{PCF}, and Ast_{PCF} may use leveling and therefore rely on predicted manufactured product instances or batches. Proper monitoring and possible adjustments of accounting and added PCF factors from account balances is therefore mandatory for maintaining accurate PCF footprints over longer runtimes.

Combining processes

Combining processes (e.g., welding, soldering, adhesive bonding, or mechanical assembly) create a new product by joining multiple input products and adding materials, consumables, energy, maintenance, and asset-related contributions. The PCF of all incoming products is therefore transferred to the combined product:

$$\mathrm{Prd}_{\mathrm{PCF}} = \sum_{i=1}^{m} \mathrm{PrdIn}_{\mathrm{PCF},i} \tag{8}$$

The PCF of the countable materials factor that become part of the product, such as screws, rivets, or inserts, is calculated as follows:

$$\mathrm{Mat}_{\mathrm{PCF}} = \sum_{i=1}^{m} q_i \cdot \mathrm{MatIn}_{\mathrm{PCF},i} \tag{9}$$

If a material is completely incorporated into the product, q_i equals the number of material instances used. For example, ($q_i = 2$) if two screws represented by $\mathrm{MatIn}_{\mathrm{PCF},i}$ are assembled into the product. If only a fraction of a material is incorporated into the product, q_i denotes the incorporated fraction. The remainder fraction of material that is unusable, and will not be anymore incorporated into any product contributes to waste, and may be recycled.

Calculation of the other factors is as described in the Common calculations subsection.

Milling processes

Milling processes permanently change a product, and usually remove parts of it. In contrast to combining processes, milling processes only process one incoming product instance. For milling, waste treatment is important: A good product after milling will be only a fraction q_i of the original product. Therefore, the $Product_{PCF}$ will also only be the fraction of $q_i \cdot Product_{PCF}$. The removed parts $1 - q_i$ are moved to waste, and according to the degree of recycling, added to the waste factor to be distributed among future products.

Transport processes

Transport processes move a product asset without (intentionally) changing its physical structure. The incoming product PCF is therefore unchanged. Transportation can therefore be applied to a single product asset, or to a batch of product assets:

$$\mathrm{ProductPCF}_{\mathrm{out}} = \mathrm{ProductPCF}_{\mathrm{in}} + \mathrm{En}_{\mathrm{PCF}} + \mathrm{Cns}_{\mathrm{PCF}} + \mathrm{Mnt}_{\mathrm{PCF}} + \mathrm{Ast}_{\mathrm{PCF}}$$

The energy-related contribution $\mathrm{En}_{\mathrm{PCF}}$ covers the energy required for the transport operation. It may change according to routes or waiting times. If several energy carriers are used, their contributions are calculated separately and summed as described above.

Transport processes may also require consumables, such as lubricants, hydraulic fluids, tires, belts, or rollers. Since these are usually consumed over many transport operations, their contribution is assigned via $\mathrm{Cns}_{\mathrm{PCF}}$ and, where necessary, handled through the carbon account. The same applies to maintenance-related contributions and to the embodied PCF of transport assets.

The allocation driver should reflect the transport context. Transport-related PCF should be leveled over transported product instances that have the same source/destination positions, e.g. by calculating average carbon footprints for transport steps and adding them to transported asset instances. The carbon account should be used to distribute short-term spikes over longer time intervals.

5 gDEZ-Based Data Foundation for Product-Related CO_2 Allocation

The allocation logic introduced in Section 4 defines how production-related CO_2 contributions are assigned to products, batches, accounting periods, or future production. However, the quality of this allocation depends on the quality and granularity of the underlying activity data and emission factors. This is particularly relevant for energy-related PCF contributions, where the resulting CO_2 value depends not only on the amount of electricity consumed, but also on the source of that electricity and, in the case of grid electricity, on the carbon intensity at the time of consumption.

The purpose of this section is therefore to specify the energy-related data foundation required by the allocation model. This foundation must distinguish between different electricity sources, link energy consumption to production orders and machines, represent production resources with their initial PCF, and preserve the calculation context needed for later reconciliation and auditing. Without such a foundation, the allocation logic could still be applied formally, but the resulting product-level PCF values would not be sufficiently traceable or operationally meaningful.

5.1 Energy Sources, Consumers, and Measurement

The gDEZ provides this foundation by structuring the relevant production and energy data through Asset Administration Shells. For the energy-related part of the allocation model, two types of electrical energy are distinguished:

1. Grid electricity, i.e., energy purchased from the public electricity grid; and
2. Self-generated electricity, such as energy produced from photovoltaic or wind, optionally interim stored in batteries.

Both of these power sources are measured using individual power meters: one for the public grid and one for the electricity produced independently. This is necessary to allocate CO_2e emissions from the electricity mix only to energy consumed from the public grid [19, 20].

The different types of consumers are divided between those that can be directly associated with production and those that cannot. In Figure 1, those consumers that are directly associated with production are generalized as machines. Also, for the sake of completeness it should be mentioned that this also includes other production assets that may not generally be understood as machines, such as conveyor belts.

Machines are further divided into Type A and Type B machines. The energy consumption of Type A machines is not measured directly. Instead, average consumption values for each work step the machine performs are stored in a lookup table. These lookup tables contain consumption values in W for each work step that can be performed with the respective machine. These consumption values must be initially recorded by measurement and periodically verified by random sampling. The consumption of type B machines is directly measured, i.e., each machine of type B has its own meter. It is measuring the total consumption in kWh rather than distinct power values in W, because total consumption allows missing values to be interpolated, whereas with a distinct measurement, missing values would remain undetected.

The justification for Type A machines with lookup tables for capturing consumption is that companies are not required to purchase and install stationary measuring devices for their entire plant in advance. However, to achieve more accurate results, it is recommended that all machines are retrofitted with power meters in the long term.

Overhead consumption refers to all consumers that are not directly involved in production, such as lighting or heating, ventilation, and air conditioning (HVAC).

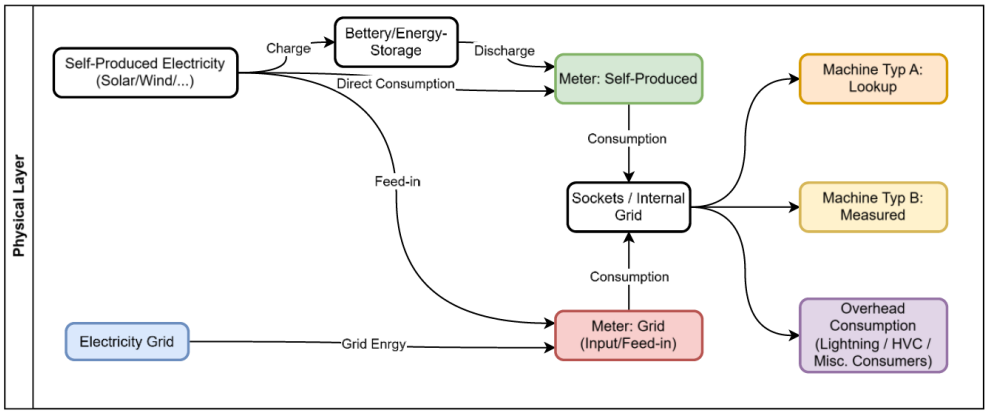


Fig. 1 Physical energy and production layer with corresponding AAS-based data representation

To capture the carbon impact of grid electricity, the system dynamically incorporates the carbon intensity of the grid at the time of energy consumption. Forecasts (e.g., ENTSO-E mix and intensity) guide operational planning and simulation; external disclosures remain aggregated to annual values per GHG Protocol Scope 2.

The forecasting and prediction logic itself is not redefined in this paper but builds on our previous work on digital twin–based energy-aware production scheduling. In that work, Asset Administration Shell–based digital twins are used to integrate time-varying grid CO_2 intensity forecasts, machine energy profiles, and production constraints into a simulation-driven scheduling process. A Monte Carlo–based approach evaluates alternative production schedules against predicted energy consumption and CO_2 emissions, enabling the selection of schedules that align energy-intensive operations with periods of lower grid carbon intensity [1].

5.2 Data Management with Asset Administration Shells

All data are managed within a structured set of Asset Administration Shells, which serve as digital representations of system entities. Figure 2 shows the Asset Administration Shells that were defined within the proposed gDEZ-based data architecture. A production order can be simulated against alternative start times using forecasted hourly grid intensities. The gDEZ combines machine-specific energy profiles with predicted renewable availability, enabling the system to select the start time with minimal expected CO_2e intensity.

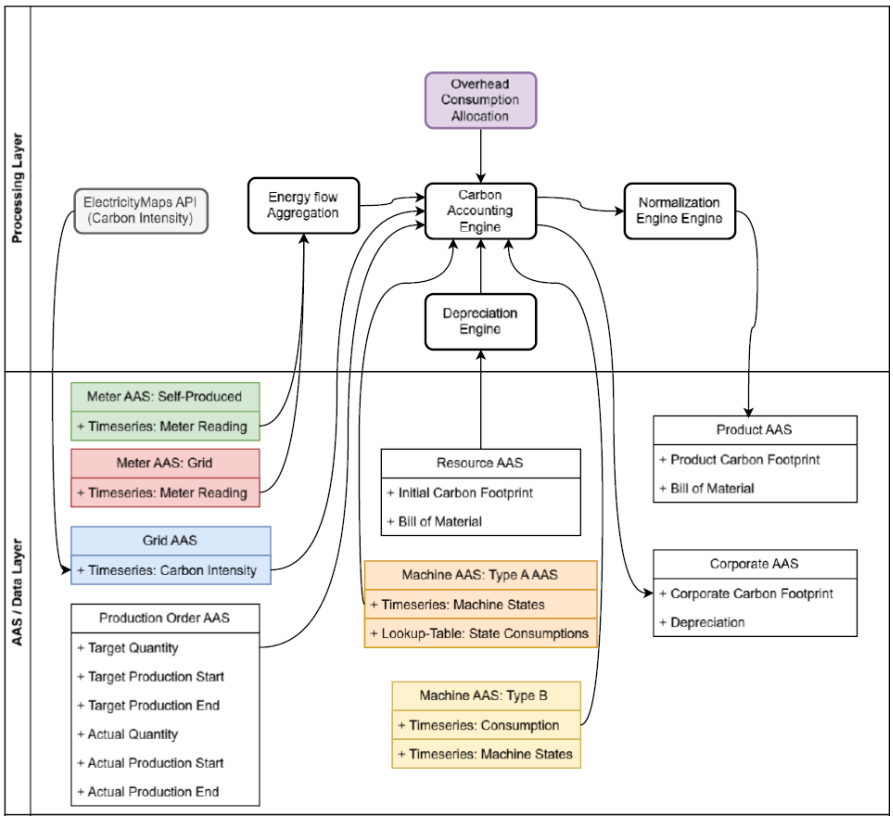


Fig. 2 Physical and AAS Data Layer connection

Energy consumption is recorded in the corresponding meter shells for self-generated energy, and for purchased energy from the public grid. A separate administration shell for the power grid aggregates current, historical, and forecast values for carbon intensity and the composition of the electricity mix. If an energy storage system (e.g., battery) is present, it is measured as part of the self-generated energy circuit. The meter does not differentiate whether the energy originates directly from the renewable source or from the storage system. All meter readings are stored as time series for carbon-footprint calculation, subsequent analysis, and documentation. All production resources come with an initial carbon footprint, which is the embodied carbon footprint they have collected during their production and transport. This includes assets used to produce self-generated energy. The Production Order AAS is the linchpin for carbon calculations. It contains information about the target quantity of units, the planned start of production, the planned completion date, and the corresponding actual values, which are dynamically updated during production. Apart from the name for the carbon footprint, Product AAS and Resource AAS hardly differ.

Ultimately, they contain the same data; the difference lies solely in their use. Products are units that are created during the manufacturing process, while resources are all assets used for the manufacturing process.

In discrete manufacturing, complex products are typically manufactured in many production steps. This results in products becoming parts of other products. In this case the intermediate product is considered as resource for further production. Consequently, when such a part is further processed, its accumulated PCF is considered as initial carbon footprint.

5.3 Indirect Energy Consumers and Overhead Allocation

The CO_2e emissions from energy consumed by non-production-related systems (e.g., lighting, heating, ventilation, and air conditioning – HVAC) are treated as overhead costs. These are determined as the difference between total measured consumption and the sum of all known or measured production-related consumptions. The resulting overhead emissions are proportionally distributed across production processes that occur within the same time window as the corresponding production orders. In the Product AAS, overhead costs, are modeled as a residual variable by adjusting the total consumption (grid consumption plus internally used PV energy) by the sum of the explicitly recorded machine consumption during the period under consideration.

This residual is allocated to parallel production processes in proportion to the active processing time, measured energy consumption, or another physically justified driver. ISO 14044/14067 requires a causal and transparently justified choice; where available, PEF category rules (PEFCRs) or EPD PCRs take precedence. The same principle applies to non-production assets, like equipment used for on-site energy generation.

Thus, the gDEZ-based energy accounting foundation provides the temporally resolved and source-specific emission data required by the allocation methodology introduced in this paper. The following implementation section shows how this foundation and the proposed allocation model can be operationalized in an AAS/BaSyx-based environment.

6 Operationalization Example

This section describes an exemplary operationalization of the CNC milling process in an AAS-based environment using Eclipse BaSyx. The purpose of the deployment is to show how the data foundation and the component-wise PCF calculation introduced in the previous sections can be represented technically. The deployment is not intended as a mandatory or production-ready industrial architecture. It provides one possible reference configuration for representing the relevant product, process, resource, energy, and PCF data in a traceable form.

6.1 Use-Case: CNC Milling

The CNC milling scenario serves as the example of this paper and illustrates how the component-specific calculation rules interact within one production step. An

aluminium blank with an incoming PCF is processed into a housing component. The central methodological question regarding Section 4 is not whether the resulting CO_2 contributions are considered, but at which allocation level they enter the product-related PCF.

For the milling operation, directly quantifiable contributions can be assigned at a fine level of granularity. This applies, for example, to the incoming PCF of the aluminium blank and to measured or reliably estimated energy consumption during the milling operation. Material removed during machining is assigned to the waste or recycling stream according to the selected waste allocation rule and offset against the product PCF.

Other contributions require leveling. Tool wear, coolant use, machine shares, and maintenance-related contributions are typically not caused by a single product instance in a meaningful way. They are therefore distributed over a suitable reference quantity, such as a batch, a predicted number of product instances, an accounting period, or subsequent production. If actual values deviate from the expected values, for example due to premature tool failure or unexpected scrap, the difference is recorded in the corresponding carbon account and considered in future product-level PCF updates.

The example shows that the proposed model does not require one uniform allocation rule for all PCF components. Instead, each contribution is assigned according to its causal relation to the production step, the available data, and the risk of creating distorted product-level PCF values. To operationalize this logic, the entities involved in the milling step must be represented together with their PCF-relevant data and calculation context. The following section therefore introduces an exemplary BaSyx deployment that maps the physical product, workstation, milling machine, tool, and meter to AASs and submodels that can be used as the basis for the component-wise PCF calculation.

6.2 Exemplary BaSyx Deployment

Figure 3 shows an exemplary BaSyx deployment for the CNC milling example. The physical layer contains the product instance, a workstation, the milling machine, a mounted tool, and a meter that provides energy readings. The product arrives at the workstation, the milling machine performs the process step, and the tool is used during the operation. The deployment layer shown in Figure 3 represents these physical entities through AASs which have central but non-exhaustive submodels for the use case.

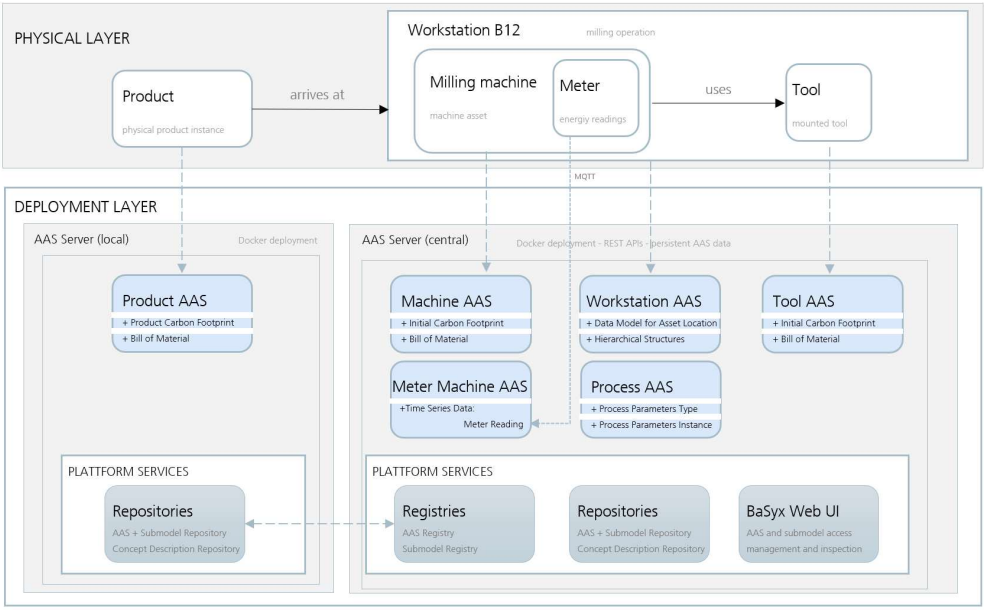


Fig. 3 Exemplary AAS-based deployment mapping for the component-wise PCF calculation

The deployment distinguishes between a local AAS server and a central AAS server. This separation is used only as an exemplary deployment option to show possible operationalization. The local server hosts product-related AAS data, while the central server hosts shared production resources such as the Machine AAS, Tool AAS, Workstation AAS, Meter AAS, and Process AAS. This illustrates a possible distribution in which product-related data remain close to the local production context, whereas shared asset and process descriptions are maintained centrally. The PCF calculation method itself does not depend on this distribution. Both BaSyx deployments provide repository services to persist and expose AAS-related data via standardized interfaces. In this example, these services comprise an AAS Repository, a Submodel Repository, and a Concept Description Repository. In the simplified local deployment, this repository setup is sufficient because only the Product AAS and its associated submodels have to be made available, and the calculation workflow can be configured with their known endpoints directly. Consequently, no local AAS Registry or Submodel Registry is required in this minimal setup. The central deployment includes additional registry services. The AAS Registry provides AAS descriptors that allow clients to locate AAS endpoints based on AAS identifiers. The Submodel Registry provides submodel descriptors that allow clients to locate specific submodel endpoints, for example bill-of-material or product carbon footprint.

The BaSyx Web UI is an optional client component for accessing, managing, and inspecting AASs and submodels. It supports development, validation, and operational inspection, but it is not part of the calculation logic itself.

MQTT is used as an exemplary interface for streaming measurement data from the meter into the AAS-based deployment. Historical measurement values may be stored directly in a Meter AAS submodel and acts as the semantic access point to the data.

6.3 From AAS-Based Input Data to Component-Wise PCF Calculation

After the exemplary BaSyx deployment has introduced the relevant AAS instances, the next step is to show how these AASs can be used to apply the PCF calculation from Section 4 to the CNC milling example. Table 1 summarizes which input data are required for the individual PCF components and from which AASs or submodels they can be retrieved in the simplified deployment. Figure 4 illustrates the same mapping as a calculation-oriented data flow.

Table 1 AAS-based input data for the PCF components in the CNC milling example.

PCF component	**Data relation**	**AAS source**	**Submodel**
$PrdInPCF, i$	Incoming PCF of the aluminium blank.	Product AAS	Product Carbon Footprint
MatPCF	Zero since no material is added.	Process AAS or Material AAS	Process Parameter Type Bill of Material
CnsPCF	Coolant, lubricant, and allocated tool wear.	Tool AAS and Machine AAS	Bill of Material
EnPCF	Energy consumption during the milling interval and corresponding emission factor.	Meter Machine AAS and Grid AAS	Time Series Data; Emission factor
MntPCF	Tool change or maintenance effort assigned to the process.	Process AAS	Process Parameter Type
AstPCF	Allocated share of machine, tool, workstation, or metering infrastructure.	Workstation AAS	Hierarchical structures
WstPCF	Removed chips, defective parts, discarded tool material, recycling or disposal.	Process AAS or Waste AAS	Product Carbon Footprint

The mapping is intentionally exemplary. It does not define a mandatory AAS information model and does not claim to cover all possible industrial implementations. Depending on the concrete system architecture, some data may be located in different AASs or represented by more specialized submodels. For example, waste data may be modeled as part of the Process AAS or as a separate Waste submodel, and energy-related emission factors may be stored directly in an energy-related submodel or referenced from a Grid AAS. The purpose of the mapping is to show one consistent way in which the AASs introduced in Section 6.2 can be used for the component-wise PCF calculation of the CNC milling example. The gDEZ-related energy and data-management concepts described in Section 5 are treated as given boundary conditions for this mapping. This section therefore does not detail these concepts again, but focuses on the additional assignment of AAS-based input data to the corresponding PCF components.

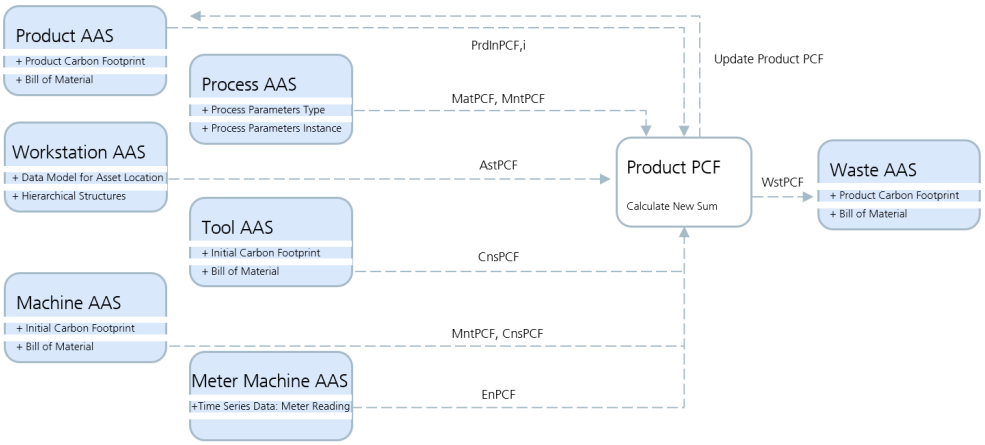


Fig. 4 Mapping of central AAS-based input data to PCF calculation components for the CNC milling example.

In the example, the Product AAS provides the incoming PCF of the aluminium blank. This value corresponds to PrdInPCF and is carried forward into the PCF of the milled housing component. Since the considered milling operation does not add material to the product, MatPCF is zero in this simplified case. The Process AAS documents this process-specific assumption and provides the process context needed to interpret the calculation.

Consumable-related contributions are derived from the Tool AAS and Machine AAS. They include, for example, coolant, lubricant, and the allocated share of tool wear, and are mapped to CnsPCF. Energy-related contributions are derived from the energy consumption assigned to the milling interval and the corresponding emission factor. The Meter Machine AAS provides the measured, while the Grid AAS provides the time-dependent carbon intensity or source-specific emission factor as described in Section 5. Together, these data are used to determine EnPCF for the considered process interval. Maintenance-related contributions, such as a tool change or maintenance effort assigned to the process, are represented through the Process AAS and its process parameterization and contribute to MntPCF.

The allocation of asset-related contributions is represented through the Workstation AAS and its hierarchical structures. These structures define which resources belong to the considered workstation context and therefore which asset shares may be relevant for the milling step. The corresponding contribution is mapped to AstPCF. Finally, the Process AAS or a dedicated waste submodel provides information on removed chips, defective parts, discarded tool material, recycling, or disposal. These data are used to determine WstPCF.

The Product PCF node in Figure 4 represents the aggregation step defined in Section 4. The component values PrdInPCF, MatPCF, CnsPCF, EnPCF, MntPCF, AstPCF, and WstPCF are not simply read from the AASs as fixed values. Instead, the AASs provide the required activity data, PCF factors, process context, time intervals,

and allocation drivers from which the product-specific component contributions are calculated. Depending on the component, these contributions are assigned directly to the milling operation or allocated using the appropriate basis, such as product quantity, process time, tool lifetime, or a carbon-account correction.

The resulting component values are then combined to calculate the updated PCF of the housing component after milling. This value can be written back to the Product AAS as the new Product Carbon Footprint. In addition, the calculation context should be preserved, for example by referencing the process instance, meter data, allocation choices, applied drivers, and the AASs or submodels from which the required input data were obtained.

6.4 Exemplary Correction and Reconciliation Flow

The correction flow is illustrated by the tool used in the CNC milling example. Assume that the tool-related contribution is initially allocated based on an expected lifetime of $C_{\text{ProdInstForAccType}} = 10{,}000$ product instances. Each produced housing component therefore receives only the planned share of the corresponding account type, for example as part of CnsPCF, MntPCF, or AstPCF, depending on the selected modelling decision.

If the tool breaks after only 100 products, the original allocation basis is no longer valid. Assigning the remaining tool-related burden to these 100 products would create unrealistic PCF outliers, while ignoring the event would omit an actual CO_2 contribution. Following the carbon-account logic from Section 4, the PCFs of already completed products are not changed retroactively. Instead, the mismatch between the expected and actual tool use is added to $V_{\text{AccTypePCF}}$ of the affected account type.

For subsequent products, the account balance is considered through V_{AddPCF}. The additional contribution is added to the respective PCF component of future products until the residual in $V_{\text{AccTypePCF}}$ has been reduced according to the selected correction rule. If the maximum value $C_{\text{AddPCFForTypeMax}}$ is reached, the remaining balance is carried forward to later products. Thus, the premature tool failure is reflected in the product-related PCF accounting without assigning the entire burden to the first 100 products.

7 Conclusion and Outlook

This paper presented an allocation-oriented approach for product-related CO_2 calculation in manufacturing. The approach addresses the problem that directly assigning production-related emissions to the products currently being manufactured can create distorted Product Carbon Footprint (PCF) values under real operating conditions, for example in the case of tool failure, scrap, maintenance events, fluctuating production quantities, or changing energy conditions.

The proposed model decomposes the PCF contribution of a manufacturing step into component-specific factors, including incoming product PCFs, materials, consumables, energy use, maintenance, asset and infrastructure shares, waste treatment and transport. These components do not have to follow one uniform allocation rule.

Instead, each contribution is assigned according to its causal relation to the production step, the available data, and the risk of creating misleading product-level outliers. To handle deviations between expected and actual production conditions, the paper introduced a carbon-account-based correction mechanism.

The paper further showed how the required data and calculation context can be represented using a gDEZ-based foundation with Asset Administration Shells. The exemplary BaSyx deployment demonstrated how PCF-related data can be structured and linked for the component-wise calculation. This deployment is not intended as a mandatory industrial architecture, but as one possible operationalization of the proposed approach.

The presented work is limited by its conceptual and exemplary character. It does not yet include a full ERP or MES integration, and it relies on simplified assumptions for overhead consumption, tool lifetime, maintenance intervals, future production quantities, and data availability. Future work should therefore focus on industrial validation, a more explicit allocation decision logic, integration with production and enterprise systems, and a systematic treatment of uncertainty and data quality. In addition, distributed AAS deployment patterns and the extension to more complex multi-step or continuous production processes should be investigated.

Statements and Declarations

Author Contributions

Thomas Kuhn and Jana Heinrich contributed to conceptualization, methodology, and writing of the original draft. Pablo Antonino contributed to supervision, methodological discussion, and review of the manuscript. All authors read and approved the final manuscript.

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Competing Interests

The authors have no relevant financial or non-financial interests to disclose.

Data Availability

No datasets were generated during the current study.

Use of Generative AI

ChatGPT was used to support language editing, grammar correction, and readability improvements of author-generated text. The authors reviewed and revised all

AI-assisted edits and take full responsibility for the final content. All content and conclusions are original authors' work.

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