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A Material Passport Ontology for a Circular Economy

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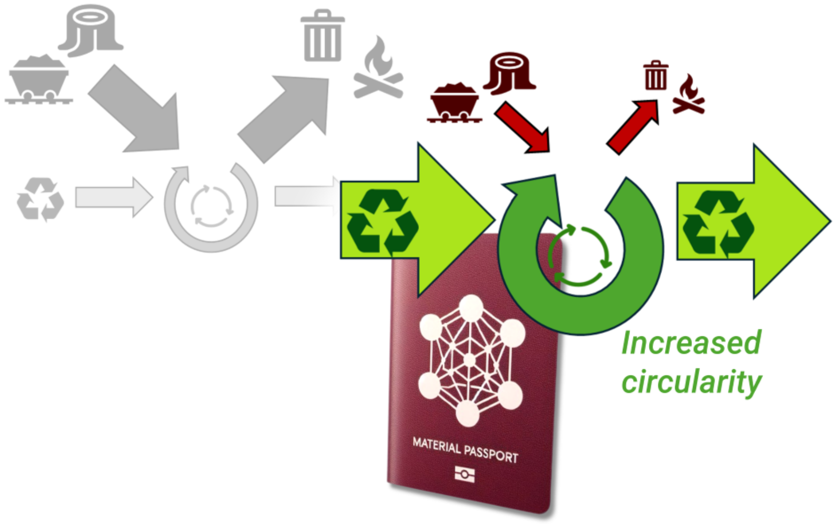
Abstract

This paper introduces a new Material Passport Ontology (MPO) that is designed to support the attainment of a circular economy. The ontology was developed using a formal ontology engineering method. The MPO is organised into facets describing the physical properties, composition and sustainability, biological and other properties of products, components and materials. A set of SHACL constraints was developed to validate data, ensuring the maintenance of an accurate, consistent and reliable knowledge graph. The information provided by the knowledge graph enables the assessment of the circularity of products, components and materials. The MPO was validated using reasoning tools and in collaboration with domain experts from industrial partners representing two use cases – the manufacture of components for motor vehicles and blades for wind turbines – demonstrating its effectiveness and applicability in identifying recyclable materials, maximising resource reuse, and enhancing sustainability practices, thereby facilitating the transition to a circular economy. The MPO, along with the SHACL constraints, enhances transparency and reliability among stakeholders, aiding the identification of recyclable materials and maximising resource reuse.



Highlights

- Material Passport Ontology to represent manufactured product data and metadata
- Material passport knowledge graph to measure metrics of circular economy
- SHACL constraints for accurate, consistent, and reliable knowledge graph

Contents

1 Introduction

The Earth's natural resources are finite. Over 100 billion tonnes of resources are consumed annually, leading to severe environmental and health issues, including approximately 9 million premature deaths from pollution [34]. This includes the annual production of 300 million tonnes of plastic waste, 54 million tonnes of electronic waste, $460 billion worth of garment waste and a contribution of 45% of annual greenhouse gas emissions – a figure that could potentially double by 2050 [39]. This immense consumption and waste production puts tremendous pressure on virgin resources and landfill capacity.

The problem lies in the 'once-through' use of resources, where virgin materials are used to produce things that end up in landfills. This is often described as a linear model. In contrast, a circular model identifies and seeks to maximise restorative material flows that recycle and reuse materials to reduce unrecoverable waste [14]. The Ellen MacArthur Foundation emphasises two metrics for circularity [14]:

- The **Material Circularity Indicator (MCI)** measures the proportion of material forming a restorative flow.
- The **Linear Flow Index (LFI)** measures the proportion of material ending as unrecoverable waste.

Figure 1 illustrates these concepts and shows how the restorative part of the flow creates a closed loop after old products reach the end of their lives.

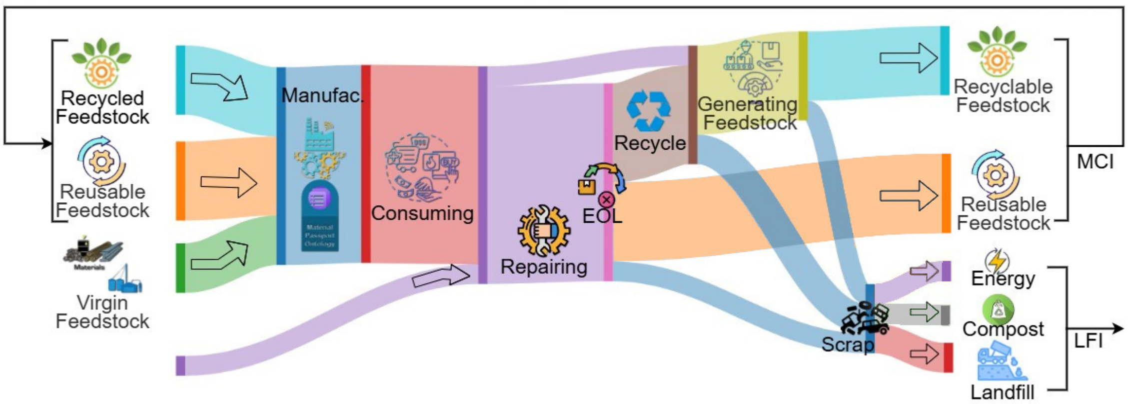


Figure 1: *Circularity of material through the product life cycle.*

The MCI has been shown to create opportunities for value in construction [23]. Central to enabling circularity is the idea of material passports [7, 8] – digital documents that provide detailed information about the composition, origin, and life cycle of materials in products. The use of digital material passports is set to be mandated in the EU in the near future [3, 51]. However, the lack of standardisation and interoperability of current material passports presents a significant challenge to stakeholders. Material passports lack a unified structure across industries and applications, posing data consistency and integration challenges. Furthermore, noisy data present a challenge in accurately calculating the MCI and LFI.

The introduction of an ontology [45] to provide a unifying definition of the concepts and relationships required for material passports to support circular economies has the potential to address these issues by enabling the consistent representation of information in a machine-understandable knowledge graph. Constraints on the ontology, represented using SHACL – the W3C-recommended Shapes Constraint Language [32], can play a pivotal role in ensuring accurate, consistent, and reliable knowledge graphs for a circular economy. This would enable stakeholders to perform advanced queries and derive meaningful insights across different applications – an essential requirement for interoperability and standardisation.

Various ontologies have been developed to support material passports for specific applications. Most have been developed for the building and construction industry [29, 33, 42, 48, 49, 61], a few for railways [54, 55], textiles [52], food and agriculture [24, 25], and aerospace manufacturing [46]. Several ontologies cater for a circular economy in building construction, including BiOnto [4], BUILDMAT [61], BPO [63], and BCAO [42]. The CEO/CAMO ontology [53] focuses on textiles. In manufacturing, AMO [1], MASON [35], MSDL [2], and Collaborative Manufacturing Services Ontology (COMPOSITION) [44] focus on various aspects of data formalisation and supply chain interactions. The MDO [36], MatOnto [10], MPO [38], and BUILDMAT [61] ontologies cover different facets of material properties and usage. PRONTO [62], VERONTO [58], and BPO [63] focus on product information and versioning. MSO-OFM and GPO [59] cover manufacturing and logistics, while IMAMO [27] and ROMAIN [28] target maintenance management. Unfortunately, significant challenges arise from such domain-specific ontologies. None comprehensively form a generic Material Passport Ontology that can combine physical, composition, and sustainability properties. This creates challenges in the assessment of circularity and the calculation of metrics such as the MCI and LFI, creating a barrier to the development of circularity.

The purpose of **this paper** is to define a Material Passport Ontology (MPO) and an overlay of SHACL constraints to represent manufactured products, components, and materials with sufficient detail to enable dynamic calculation of metrics such as MCI and LFI. The ontology is applied to two industrial manufacturing use cases – automotive components and wind turbines – to create material passports and assess the circularity potential of materials. The use cases demonstrate the efficiency and relevance of the MPO in enabling accurate circularity assessments, facilitating the improvement of sustainability practices across industries, and the shift towards a circular economy.

The remainder of this paper is organised as follows. Section 2 describes the methods used to develop the MPO. The different facets of the MPO along with the necessary constraints defined in SHACL are explained in Section 3. Section 4 outlines the procedures used to assess the use of the MPO aginst the needs of the use cases. Conclusions and future directions are discussed in Section 5. Throughout this paper, we use the following typesetting convention: **bold typeface** for emphasis; *italic typeface* for captions and for the concepts, properties and relations defined in the MPO; and `monospace typeface` for codes.

2 Ontology engineering method

The Material Passport Ontology (MPO) was developed using a general-purpose ontology development method rooted in the theory of Teleosemantics [15, 16]. The method develops several ordered representation layers:

(i) **Universal Knowledge Core (UKC)**, a linguistic-level reference ontology [17, 18].

(ii) **Teleontologies**, knowledge-level reference ontologies aligned to the UKC.

(iii) **Teleologies**, ontologies generated from specific requirements aligned with the Teleontology.

2.1 Universal Knowledge Core (UKC)

The Universal Knowledge Core (UKC) is an expandable, *a priori*, multilingual linguistic reference ontology central to the development method. It is used to name and linguistically classify relevant entities, in an expert-driven top-down manner, employing either natural language or domain-specific terms. The UKC consists of two components, the Language Core (LC) and the Concept Core (CC).

The LC organises the linguistic data. It includes a hierarchical structure similar to WordNet [40], comprising a set of words representing real-world objects (*e.g.*, entities and their properties in the materials domain) in a natural language. This structure consists of sets of synonymous words (synsets) and glossaries in multiple languages, covering a range of common-sense and domain-specific terms.

The CC is a language-independent hierarchy of concepts, each uniquely identified by an identifier and linked to the semantically synonymous synset across different language hierarchies. This linkage allows the CC to provide an abstract, unified hierarchy of concepts and words across different natural languages. For example, while 'Virgin Material Mass' can be expressed differently across multiple natural languages (*e.g.*, in English, Italian, *etc.*), the underlying concept remains the same and is represented by a unique identifier.

The MPO uses a UKC developed by the University of Trento. The linguistic representation of the concepts and corresponding identifiers used by the MPO are published with the research data from this paper.[1]

2.2 Teleontologies

Teleontologies are knowledge-level ontologies aligned with the conceptual hierarchy in the UKC. They provide a standardised framework for defining common concepts across a specific domain of discourse, such as materials science. Teleontologies use three primary representational constructs: classes, object properties, and datatype properties. Hierarchies of classes encode recurring concepts, such as engineered materials, which are appli-

[1] See the Data and code availability statement on page 21.

cable across various use-cases, including automotive and wind turbine applications. Object properties define the relationships between different classes within the teleontology. For instance, the object property *has_property* relates a material entity to its associated physical properties. Finally, datatype properties provide specific attributes to describe the concepts within the class hierarchy.

Two key aspects of reference teleontologies are noteworthy. Firstly, they capture the consensus of a community of practice regarding a specific domain, ensuring domain appropriateness. As a result, classes, object properties, and datatype properties are developed in a top-down manner, ensuring general applicability across multiple use cases. Secondly, the concepts within a reference teleontology are designed for reuse, facilitating the creation and alignment of application-specific ontologies based on particular requirements.

The MPO was aligned using the Elementary Multiperspective Material Ontology (EMMO) (formerly known as European Materials Modelling Ontology) [20], developed through the collaboration efforts of the European Materials Modelling Council (EMMC). EMMO provides a comprehensive framework that models various dimensions such as material properties, physical laws governing material behaviour. Teleontologies like EMMO are typically encoded in the Web Ontology Language (OWL) RDF/XML serialisation format, ensuring formal and standardised representation.

2.3 Teleologies

Teleologies are ontologies, aligned to a reference teleontology, which are generated from a concrete set of requirements in an application context. They are generated using a bottom-up approach, starting with detailed requirements, as outlined below:

(i) The knowledge representation requirements for a teleology are first captured in the form of Competency Questions (CQs) [21]. These help identify the application-specific classes, object properties, and datatype properties that need to be modelled. Examples of CQs include:

- What product, component and material properties are needed to create a material passport for calculating circular economy potential?
- Is constituent material a composition property or sustainability property?
- Is specific heat a property of material, component, or product?

(ii) The classes, object properties, and datatype properties identified by consideration of the CQs are then modelled informally using Entity-Relationship (ER) diagrams [9], where classes are represented as nodes and labelled edges encode the object properties. The datatype properties are represented as attribute blocks or left implicit. The diagrams can also include application-specific datatype properties relevant only to a given use case.

(iii) The ER model in step (ii) is formalised as a teleology in OWL RDF/XML format.

At this stage, we have two types of knowledge representation artefacts:

(i) Top-down artefacts. The UKC and reference teleontology aligned with the UKC.

(ii) Bottom-up artefacts. The teleologies.

The method then prescribes two ordered activities to produce a unified ontology:

(i) Middle-out merging. The classes, object properties and datatype properties of the teleologies (all being application-specific) are semantically aligned to their immediate general domain-concept counterparts in the reference teleontology via the subsumption (IS-A) relationship. The result is an enriched and unified teleontology that combines the top-down and bottom-up knowledge representation.

(ii) Knowledge annotation. Each concept in the enriched teleontology is annotated with global identifiers from the UKC CC. This involves semantic searching of the UKC knowledge base for a matching concept. If a UKC concept exists, the identifier of the UKC concept is assigned; otherwise, a new UKC concept is created and assigned. The result is a conceptually unambiguous and enriched teleontology.

3 Material Passport Ontology (MPO)

The Material Passport Ontology (MPO) has been created to support the representation of digital material passports for manufactured products and components. A set of SHACL constraints has been defined to enforce data accuracy, consistency and reliability. **Figure 2** shows an overview of concepts, relations, and properties of the MPO.

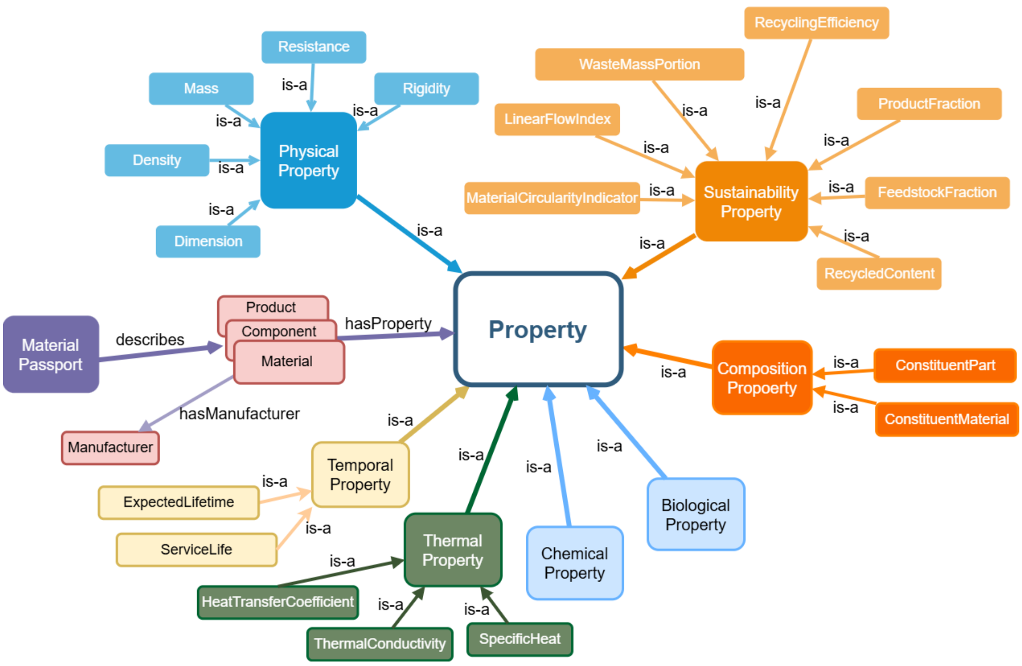


Figure 2: *Overview of the Material Passport Ontology. The colours are used to group concepts belonging to the different facets of the ontology.*

3.1 Ontology facets

The MPO has material passport, physical property, composite material, sustainability property, temporal property, thermal property, and chemical and biological property facets. The role of each facet is described in the sections that follow.

3.1.1 Material passport

Figure 3 shows the material passport facet. This is the core of the MPO. It defines a *Material Passport* that *describes* combinations of *Product*, *Component*, and *Material* to ensure that sufficient information is available to support circularity considerations.

Product, *Component*, and *Material* can have a *Manufacturer* described by various datatype properties. They have a *hasProperty* relation to *Property* that allows the specification of *Physical*, *Composition*, *Temporal*, *Thermal*, *Sustainability*, *Chemical*, and *Biological* properties via the other facets. These enable identification and traversal to further detail.

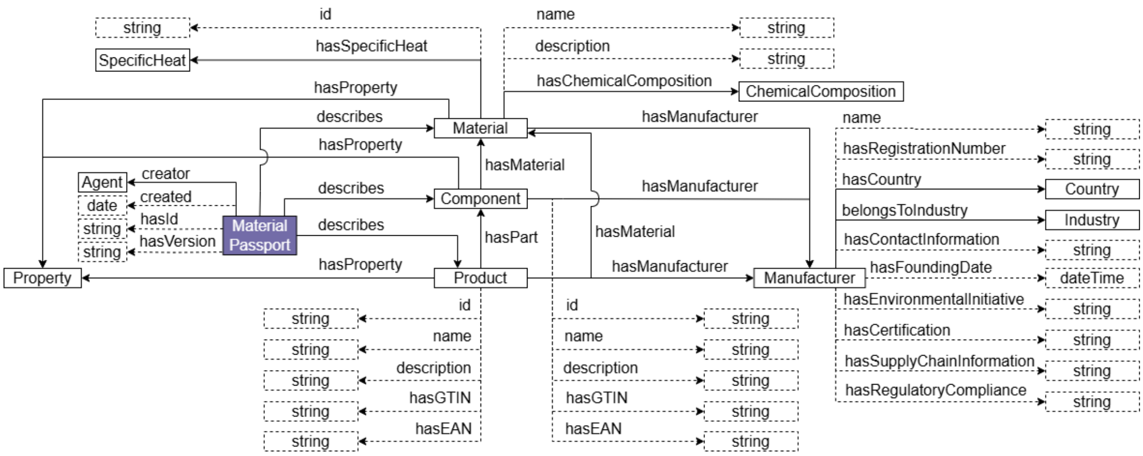


Figure 3: *Material passport facet of the MPO.*

Product and *Component* have datatype properties (*e.g.*, *id*, *name*, *description*, *hasGTIN*, and *hasEAN*) to store additional metadata. For example, a *chassis* is a product used in the manufacture of automotive vehicles. A chassis *hasPart* crossbeam, which has a material passport that includes descriptors like name, description, European Article Number (*EAN*), Global Trade Item Number (*GTIN*), *etc.* alongside details of the manufacturer.

3.1.2 Physical properties

Figure 4 shows the physical property facet. This is used to describe characteristics like density, mass, and rigidity. These are important because they facilitate the calculation of the MCI, enabling the identification of recoverable, reusable and recyclable parts of products, thereby promoting the principles of circularity.

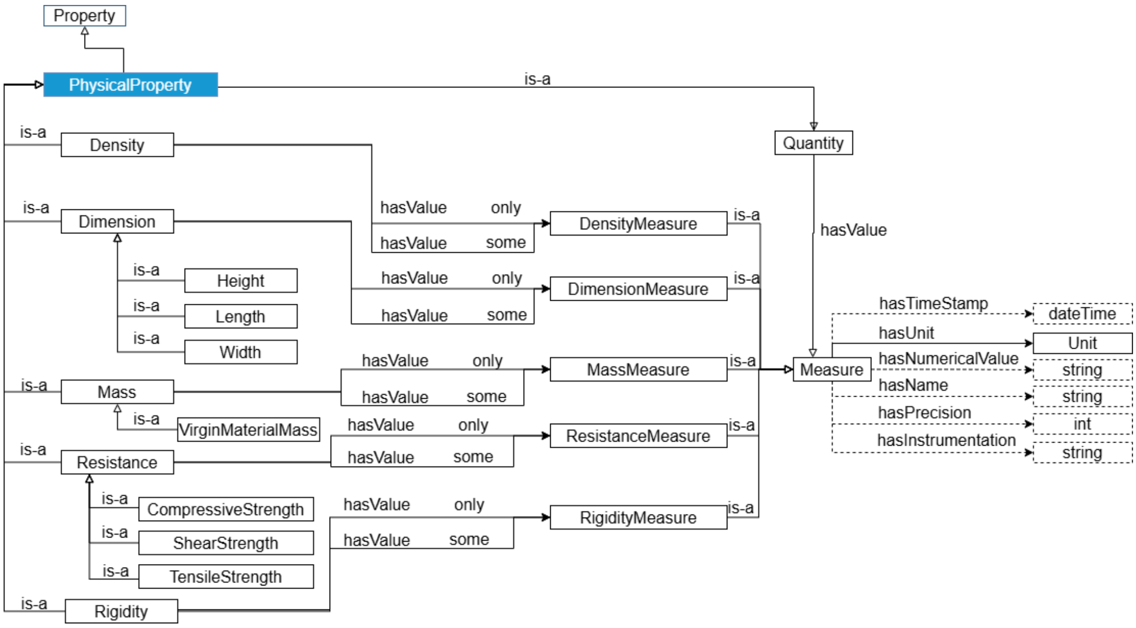


Figure 4: *Physical property facet of the MPO.*

The specification of *PhysicalProperty* includes *Density*, *Dimension*, *Mass*, *Resistance* (to deformation), and *Rigidity*. For instance, crossbeam has *Mass* property, which *hasValue* 1386 and *hasUnit* 'g'.

3.1.3 Composition properties

Figure 5 shows the composition property facet. This block of ontology helps to optimise the selection, processing, and assembly of the constituent parts and materials of a product and facilitates their separation, dismantling, and recycling at the end of life of a product to maximise the circularity.

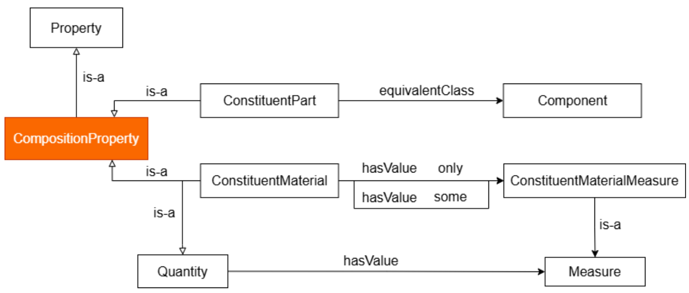


Figure 5: *Composition property facet of the MPO.*

CompositionProperty has two subclasses, *ConstituentPart* and *ConstituentMaterial*. For example, crossbeam has constituent materials carbon fibre, glass fibre, epoxy resin, aluminium, foam, and film adhesive that have mass, and a source and destination in a circular economy.

3.1.4 Sustainability properties

Figure 6 shows the sustainability property facet. The main objective of this facet is to enable the comprehensive and transparent assessment of the sustainability of a material or product. Such assessments are a key aspect of making decisions about the selection, use, and end-of-life management of materials or products to reduce environmental impact.

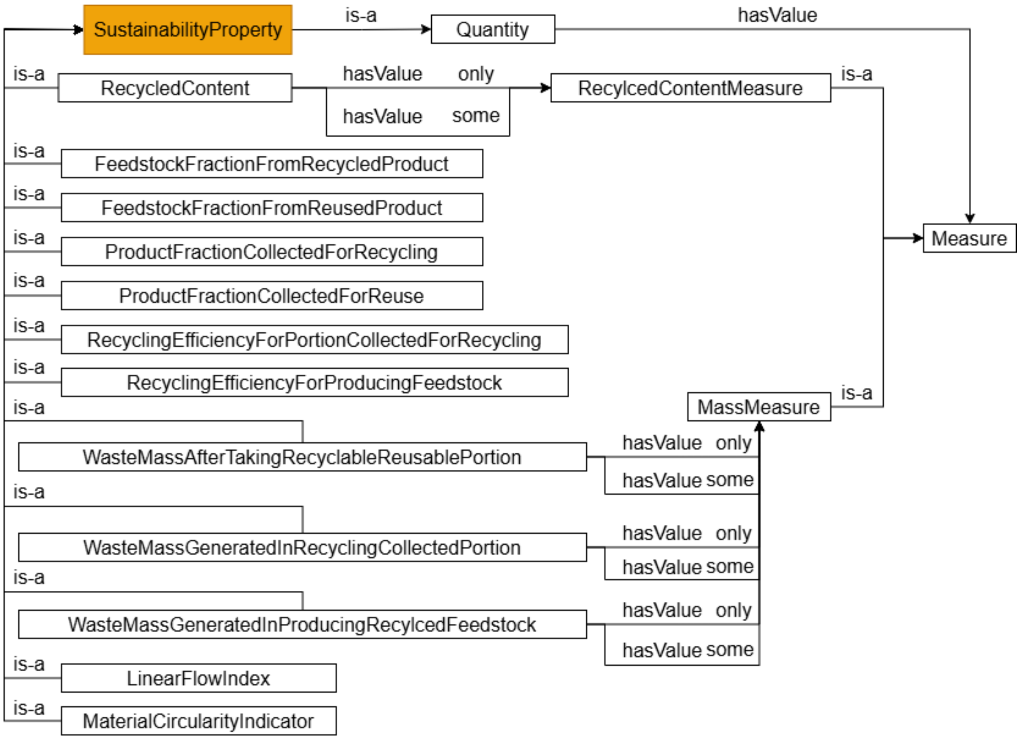


Figure 6: *Sustainability property facet of the MPO.*

The sub-concepts of *SustainabilityProperty* are specified to enable the calculation of the Linear Flow Index (LFI) and Material Circularity Indicator (MCI) [14]. Examples for the constituent carbon fibre, glass fibre, epoxy resin, aluminium, foam, and film adhesive present in the crossbeam described in Section 3.1.3 are illustrated in Figure 11.

The Material Circularity Indicator (MCI) of a product

$$MCI = 1 - LFI \cdot F(X), \tag{1}$$

where $F(X) = \frac{0.9}{X}$ and X is the product utility, which encapsulates the idea of maximising the usefulness and lifespan of a product to reduce waste and resource consumption [14]. The Linear Flow Index (LFI)

$$LFI = \frac{(V+W)}{2M}, \tag{2}$$

where V is the total mass of virgin feedstock, M is the mass of the product and W is the mass of unrecoverable waste

$$W = W_0 + W_\mathrm{F} + W_\mathrm{C}, \tag{3}$$

where W_0 is the mass of waste that goes to landfill at the end of life, W_F is the mass of waste from recycled feedstock, and W_C is the mass of unrecoverable waste generated when recycling parts of a product. The LFI takes values in the interval $[0,1]$. The lower the value of LFI, the higher the circularity. For example, a product that uses no virgin feedstock ($V = 0$) and that produces no waste ($W = 0$) would have $LFI = 0$. Conversely, a product that uses only virgin feedstock and that sends everything to landfill ($M = V = W$) would have $LFI = 1$.

3.1.5 Temporal properties

Figure 7 shows the temporal property facet. The temporal properties play an essential role in the life cycle management of products and materials.

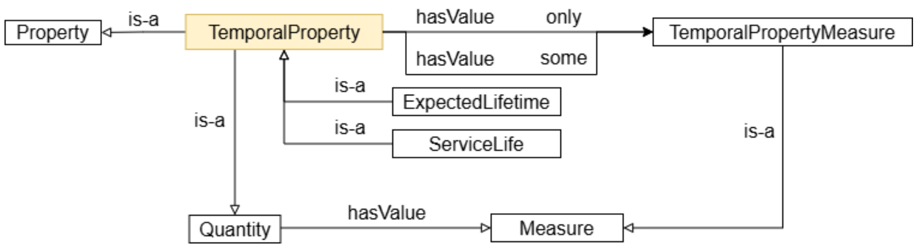


Figure 7: *Temporal properties facet of the MPO.*

The *TemporalProperty* is used to describe time-related properties such as the *ExpectedLifetime* and *ServiceLife*. The inclusion of these data helps to support estimates the durability of products, and decisions about the timing, frequency, and method of maintenance, repair, and replacement of materials, warranties, and replacement cycles.

3.1.6 Thermal properties

Figure 8 shows the thermal property facet. The *ThermalProperty* describes the thermal characteristics of materials and products, including the *HeatTransferCoefficient*, *ThermalConductivity*, and *SpecificHeat*. These are critical in optimising product designs for effective thermal management, insulation, and to meet regulations.

3.1.7 Chemical and biological properties

Figure 9 shows the chemical and biological property facet. These properties are essential for determining the appropriate end-of-life management of materials, including their potential for energy recovery, composting, and disposal in landfills.

The *ChemicalProperty* is used to describe the *Toxicity* and *Flammability* of a of a product, component, or material. The *BiologicalProperty* is used to represent *Biodegradability*. Understanding toxicity and flammability is important for preventing environmental contamination, while knowledge of biodegradability informs composting practices, thereby reducing long-term environmental impact. For example, film adhesive and epoxy resin in the crossbeam can be used for energy recovery, while PU foam may be directed to landfill.

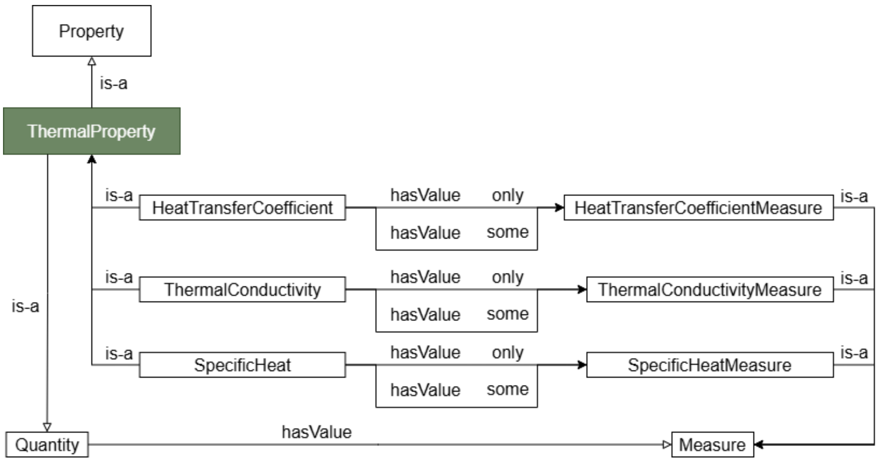


Figure 8: *Thermal properties facet of the MPO.*

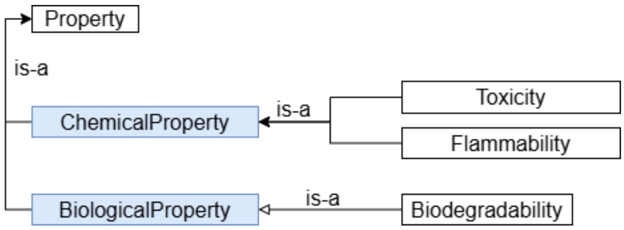


Figure 9: *Chemical and biological properties facet of the MPO.*

3.2 Reuse of ontologies

The Material Passport Ontology reuses existing ontological constructs wherever possible to avoid 'reinventing the wheel'. **Table 1** summarises the reused entities.

The *Agent* concept is reused from the Friend of a Friend (FOAF) ontology [6], *Country* from DBPedia [11], *Image* and *URI* from Dublin Core [12], and *Name* from GoodRelations [22]. The *Property* and *ThermalConductivity* concepts are reused from OntoCAPE, the Ontology for Chemical Process Engineering [41], *Material* from the Elementary Multiperspective Material Ontology (EMMO) (formerly known as the European Materials Modelling Ontology) [13], and *PhysicalProperty* from the Manufacturing Deliverable Ontology (MDO) [37]. *Measure, HeatTransferCoefficient, ThermalConductivity, Quantity, Unit* and *hasNumericValue* are reused from the Ontology of Materials (OM) [50]. This reuse broadens the scope to apply the MPO across different use cases.

3.3 SHACL constraints

We defined the concepts and relationships between entities of MPO using Web Ontology Language (OWL). While OWL can define basic constraints modelled by the XML schema [5], it provides no portable means of restricting datatypes [43]. Such a capability is important, particularly in manufacturing where accurately measuring material circularity depends on precise constraint modelling [26]. This is addressed in the MPO by

Table 1: *Concepts and properties that are reused in the Material Passport Ontology.*

Ontology Part	Element Name	Ontology
Concepts	*Agent*	FOAF
	Country	DBPedia
	Image	Dublin Core
	Material	EMMO, MDO
	Measure, HeatTransferCoefficient,	OM
	ThermalConductivity, Quantity, Unit	OM
	Property	OntoCAPE
	ThermalConductivity	OM, OntoCAPE
	PhysicalProperty	MDO
Object Property	*hasUnit, hasValue*	OM
Datatype Property	*name*	GoodRelations
	hasNumericValue	OM
	URI	Dublin Core

defining a set of constraints using SHACL, the Shape Constraints Language [32], that provide a context sensitive, dynamic overlay to the ontology.

Table 2 summarises the constraints. These constraints are essential for validation to produce accurate, consistent, and reliable knowledge graphs. A validated knowledge graph is crucial for accurately measuring the Material Circularity Indicator (MCI). In contrast, a non-validated knowledge graph may produce incorrect MCI values, leading stakeholders in the wrong direction and ultimately hindering the achievement of a circular economy. An example of how to define a constraint is given in **Listing 1**.

```
:ProductMciShape #This is the user-defined name or identifier
    a sh:NodeShape ; #This defines ProductMciShape as a SHACL shape
    sh:targetClass :MaterialCircularityIndicator ;
    #This shape targets the MaterialCircularityIndicator class as domain

     sh:property [
        sh:path :hasMaterialCircularityIndicator ; #value is a property
        sh:datatype xsd:decimal ; #datatype of value is a decimal
        sh:minInclusive 0 ; #value must be >= 0
        sh:maxInclusive 1 ; #value must be <= 1
    ] .
```

Listing 1: *SHACL Constraint: Material Circularity Indicator (MCI) value should be a decimal between 0 and 1.*

Table 2: *Target classes that require value constraints on properties.*

Target class[†]	**On property**	**Value constraint**	**Description**
Product $\bigcup$ *Component* $\bigcup$ *Constituent*	*id*	required, unique	Each product, component or constituent must have a unique id.
Product $\bigcup$ *Component*	*hasManufacturer*	required, $\lvert Manufacturer \rvert \geq 1$	Each product or component must have at least one associated manufacturer.
Product $\bigcup$ *Component* $\bigcup$ *Constituent*	*isHazardous* *hasHazardSummaryDocument*	optional, boolean optional, url	If a product, component, or constituent is hazardous, it must have a hazard summary document url.
Product $\bigcup$ *Component*	*hasGTIN*, or	optional, 13/14 digits	Each product or component must have at least one of GTIN or EAN. GTIN is optional 13 or 14-digit number.
	hasEAN	optional, 13 digits	EAN is also optional with 13-digit number.
Product $\bigcup$ *Component* $\bigcup$ *Constituent*	*hasMCI*	$0 \leq MCI \leq 1$	Each product, component or constituent may have *hasMCI* value such that $0 \leq MCI \leq 1$.
Product $\bigcup$ *Component* $\bigcup$ *Constituent*	*hasMassInKg*[‡]	required	Each product, component or constituent must specify value to hasMassInKg.
Product $\bigcup$ *Component* $\bigcup$ *Constituent*	*isBiodegradable*	required, boolean	Each Product, Component or Constituent must specify whether they are biodegradable.
RecycledContent $\bigcup$ *WasteMass* $\bigcup$ *WasteMassAfterTakingRecyclableAndReusablePortion* $\bigcup$ *WasteMassGeneratedInRecyclingCollectionPortion* $\bigcup$ *WasteMassGeneratedInProducingRecycledFeedstock*	*hasValue*	required, *Measure*	Specify the mass of recycled content *etc.*
Measure	*hasNumericValue*	required, ≥ 0	*Measure* must be defined with a specific value $\geq$0 along with a unit.

[†] $\bigcup$ represents the union operator. [‡] The choice was limited by the application, which used kg as the default unit for mass.

3.4 Ontology documentation

The Material Passport Ontology (MPO) has been documented to provide a resource for stakeholders, researchers, and industry professionals to facilitate collaborative knowledge exchange and development. It ensures that manufacturers have a clear, standardised framework for tracking and managing product, component, and material data. The documentation describes all the classes, properties and instances in the MPO, with references to the respective source documentation. The documentation was produced as described in the following steps.

(i) Navigable HTML-based documentation describing the structure, classes, properties and relationships in the MPO was produced from the version of the ontology serialised to OWL using the Live OWL Documentation Environment (LODE) [47]. This provides a streamlined and efficient process to create the basic documentation.

(ii) Additional information, explanations and contextual detail were added manually, including references to ensure proper attribution of things that have been reused from elsewhere. This additional context enhancement process elevates the understanding and utility of ontology within the research community and beyond.

(iii) We assigned an International Resource Identifier (IRI) to ensure a standardised and globally accessible reference.

A living version of the ontology and documentation is available online.[2]

4 Ontology evaluation

The quality and capabilities of the MPO were critically assessed via ontology verification and knowledge graph validation processes, and via its application to two industrial use cases. This evaluation is critical. The availability of a generic MPO will play a key enabling role in promoting circular economy principles through efficient and autonomous calculation of sustainability metrics such as the MCI.

4.1 Ontology verification

The HermiT [19] reasoner was used to verify that all classes in the MPO ontology could be instantiated without any conflicting assertions. This verifies that the MPO is free of contradictory axioms and assures the satisfiability of restrictions imposed in the ontology. We used a set of test data to verify that the information in the MPO was sufficient to calculate the MCI and LFI.

A similar verification could have been performed using the Pellet [56] reasoner.

[2] See the Data and code availability statement on page 21.

4.2 Knowledge graph validation

The MPO was applied to generate knowledge graphs to describe data for two use cases – automotive manufacturing and wind turbine production. The verification tested the ability of the knowledge graph to represent properties accurately, and therefore to ensure the ability to calculate the MCI via queries of the appropriate properties.

The MPO knowledge graphs were validated using the corresponding SHACL shapes and the online TopQuadrant SHACL validator [31] which uses the TopBraid SHACL API [30]. **Algorithm 1** summarises the validation process. The validation reports any violations of the defined constraints, providing a mechanism to detect and require the correction of any problems. This process ensures the correctness, consistency, and reliability of MPO-based knowledge graphs. Similar validation could have been performed using a variety of other tools including the Apache Jena-based SHACL [60] and PySHACL[57] command line tools. **Listing A.1** and **Listing A.2** in the Appendix show example SPARQL queries to retrieve the physical and sustainability properties needed to calculate the MCI.

Algorithm 1 SHACL validation process.

```
1: Load defined SHACL shapes
2: Load data/knowledge graph
3: Validate the knowledge graph against the SHACL shapes
4: if there are constraint violations then
5:     Report violations and provide details to the user
6:     Goto Step-2
7: else
8:     Store the knowledge graph in the material passport repository (e.g., triple store)
9: end if
```

4.3 Industrial user testing

A web-based user interface was developed to allow users to work with MPO-based material passports. The interface was used to test the ability of industrial partners to create material passports for automotive and wind turbine products.

Figure 10 shows an example material passport for the crossbeam used as part of an automotive chassis. The crossbeam has constituent materials including carbon fibre, glass fibre, epoxy resin, aluminum [sic], PU foam and film adhesive. The material passport contains details of the physical, energy and thermal performance properties of the crossbeam, and information about each component including dimension and mass, information about the source (*e.g.*, virgin and recycled) material, the proportion of mass that is collected as waste and the destination (*e.g.*, recycle, reuse, or landfill) at end-of-life. **Figure 11** shows further details of the composition properties. The MPO-based material passport allows the calculation of the MCI, which underlies the circularity indicator seen in the bottom right of Figure 11.

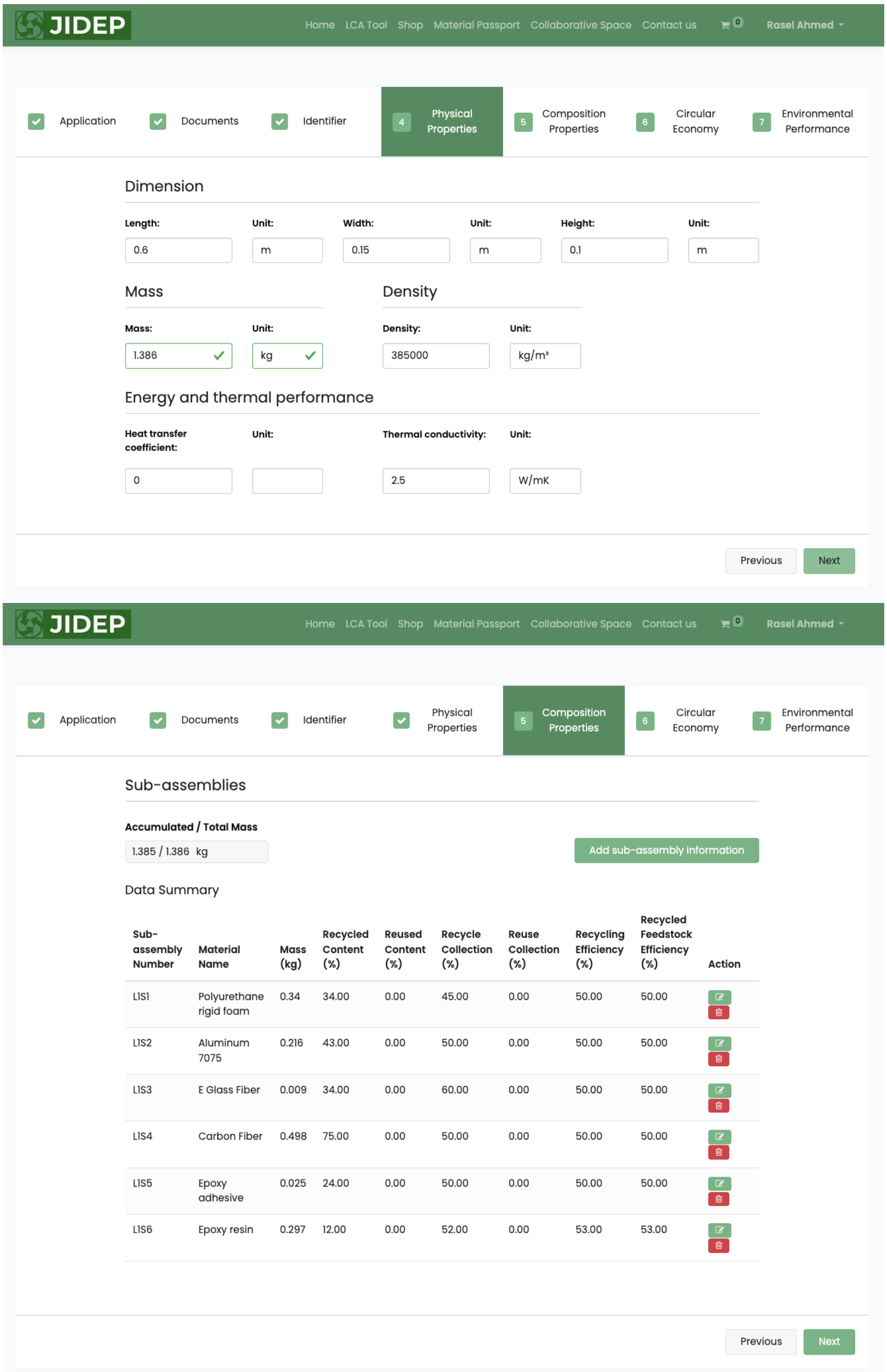


Figure 10: *User interface to provide data about properties of products or components: (a) Physical properties, (b) Composition properties.*

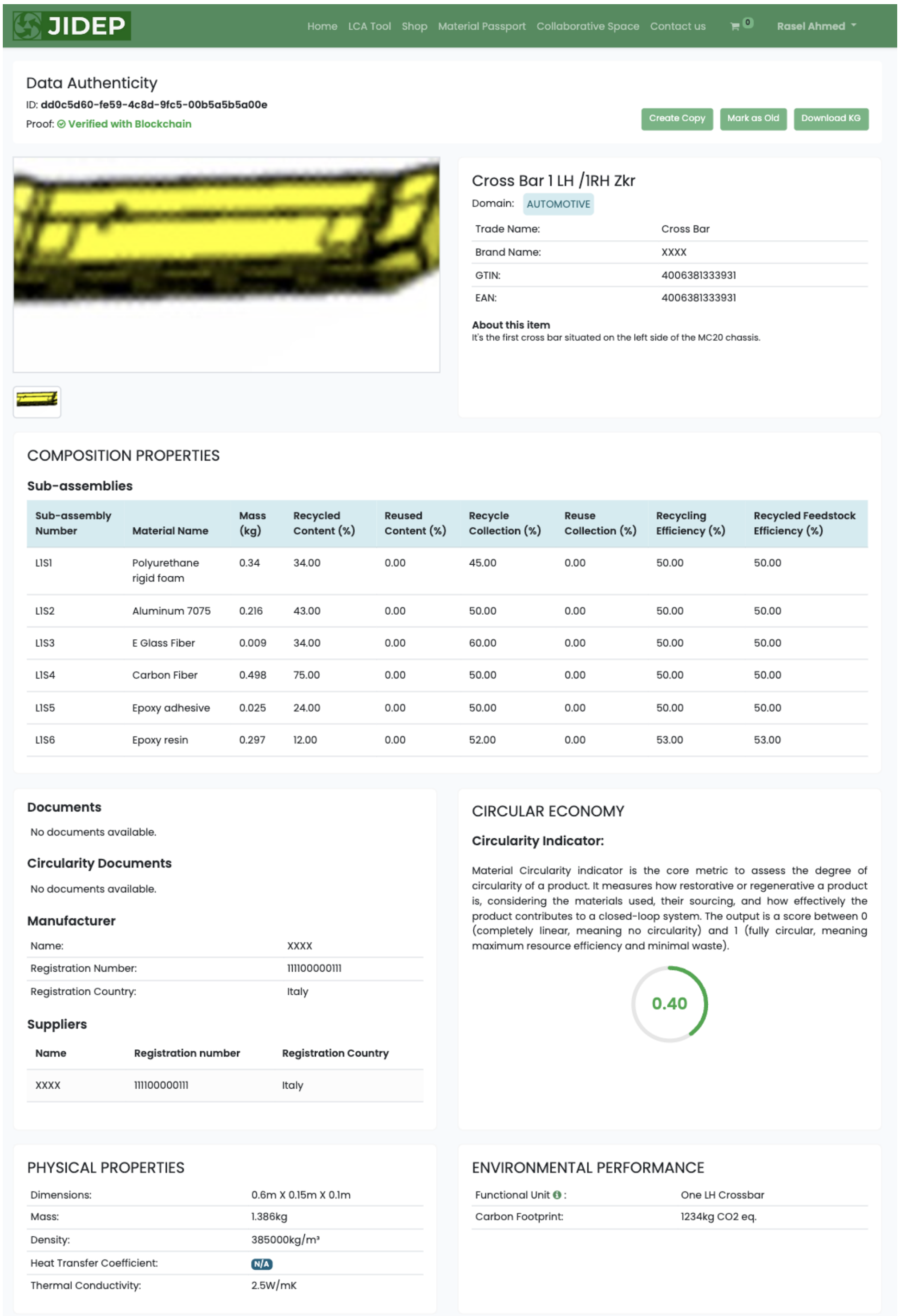


Figure 11: *The framework presents a material passport that includes detailed information about product, including manufacturer, composition properties, physical properties, environmental performance and a circularity indicator.*

The user interface allowed the development of analogous material passports and the calculation of circularity indicators for wind turbine blades. The two use cases demonstrate the practical application of the MPO and SHACL constraints. They were shown to fulfil the data representation requirements of different stakeholders, including manufacturers, collectors, and recyclers, and enable the calculation of sustainability metrics across the automotive manufacturing and wind turbine production sectors.

The use of MPO-based materials passports ensures transparency and accountability throughout the entire product life cycle, helping stakeholders make well-informed decisions related to recycling and reuse of products, components and materials. It is hoped that the adoption of the MPO in automotive manufacturing and wind turbine production can lead to significant improvements in material efficiency, waste reduction, and regulatory compliance, ultimately fostering a more circular economy.

5 Conclusions

We propose a Material Passport Ontology (MPO) along with an overlay of SHACL constraints to represent manufactured products, components, and materials. The ontology includes sustainability and composition properties, as well as the physical and temporal properties necessary for the dynamic calculation of the Material Circularity Indicator (MCI) and Linear Flow Index (LFI).

The composition properties define a product by detailing its components and materials, enabling the calculation of a cumulative MCI. These properties include information about constituent parts, repair, and refurbishment, which help increase product lifespan and reduce waste generation.

The SHACL constraints ensure knowledge validation, providing accurate, consistent, and reliable data. This validation is essential for supporting the dynamic calculations offered by the MPO and helps build trust in manufactured products through transparency and the ability to offer warranties on circularity credentials. These steps are critical for quantitatively evaluating the circularity of different manufacturing options and supporting decisions that promote circularity.

The ability of the MPO and SHACL constraints to enable interoperability between information from different industrial sectors has been evaluated through their application in representing accurate, consistent information from industrial partners involved in the manufacture of automotive components and wind turbines. A graphical portal was developed and made available to these partners, allowing them to upload and share data describing the circularity properties of their products. This process verified that the portal, along with the MPO and SHACL constraints, was sufficient to support the use of digital material passports, which are likely to be mandated in the EU in the near future [3, 51].

Future work should aim to test and generalise this approach across a broader range of manufacturing domains and diversified international supply chains. This will enhance data standardisation and harmonisation while ensuring data privacy and security. These improvements will be implemented through ontology versioning to maintain consistency and traceability of changes.

Nomenclature

$F(X)$ Utility factor

F_R Fraction of mass of a product from recycled sources

F_S Fraction of mass from sustainable production

F_U Fraction of mass of a product from reused sources

M Mass of product

V Mass of virgin feedstock

W Mass of unrecoverable waste

W_0 Mass that goes to landfill at end of life

W_C Mass of waste collected after a product has been used

W_F Mass of waste from recycled feedstock

X Product utility

CC Concept Core

EMMO Elementary Multiperspective Material Ontology (formerly known as the European Materials Modelling Ontology)

FOAF Friend of a Friend

KG Knowledge Graph

LC Language Core

LFI Linear Flow Index

MCI Material Circularity Indicator

MDO Materials Design Ontology

MPO Material Passport Ontology

MP Material Passport

OM Ontology of Materials

OWL Web Ontology Language

RDF Resource Description Framework

SHACL Shapes Constraint Language

SPARQL SPARQL Protocol and RDF Query Language

UKC Universal Knowledge Core

URI Uniform Resource Identifier

XML eXtensive Markup Language

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Declaration of Generative AI and AI-assisted technologies in the writing process

The authors used ChatGPT version 3.5 during the preparation of this work to enhance the readability and language of the manuscript. After using this tool, the authors reviewed and edited the content as needed and take full responsibility for the content of the publication.

Data and code availability

Archival machine-readable versions of the ontology, SHACL constraints, and specification document are available via the University of Cambridge data repository. See doi:10.17863/CAM.111136. A living version of the ontology is available via https://github.com/cambridge-cares/TheWorldAvatar. The data used to populate the material passport framework contains confidential information, protected by a non-disclosure agreement covering Horizon Europe grant 101058732 and UKRI grant 10038588. This data cannot be made available.

Conflicts of interest

There are no conflicts to declare.

A Appendix

```
#the namespaces for the KG, mpo (material passport ontology), mdo (materials
↪  design ontology), and om (ontology of units of measure) respectively
PREFIX :<http://localhost:8080/source/>
PREFIX mpo:<http://www.theworldavatar.com/kg/ontomatpassport#>
PREFIX mdo:<https://w3id.org/mdo/core/>
PREFIX om:<http://www.ontology-of-units-of-measure.org/resource/om-2/>
#It retrieves values of all PhysicalProperty for crossbeam_component1
SELECT ?component ?measure ?property ?value
WHERE{
  ?measure ?property ?value .
  ?subsubprops om:hasValue ?measure .
  ?subsubprops rdfs:subClassOf ?subprops .
  ?subprops rdf:type mdo:PhysicalProperty .
  ?subprops rdfs:subClassOf ?props .
  ?component mpo:hasProperty ?props .
  FILTER(?component=:crossbeam_component1)
}
```

Listing A.1: *Example SPARQL query to retrieve physical property (e.g., mass) values for a component.*

```
#the namespaces for the KG, mpo (material passport ontology), mdo (materials
↪  design ontology), and om (ontology of units of measure) respectively
PREFIX :<http://localhost:8080/source/>
PREFIX mpo:<http://www.theworldavatar.com/kg/ontomatpassport#>
PREFIX mdo:<https://w3id.org/mdo/core/>
PREFIX om:<http://www.ontology-of-units-of-measure.org/resource/om-2/>
#It retrieves values of all SustainabilityProperty for crossbeam_component1
SELECT ?component ?measure ?property ?value
WHERE{
  ?measure ?property ?value .
  ?subsubprops om:hasValue ?measure .
  ?subsubprops rdfs:subClassOf ?subprops .
  ?subprops rdf:type mdo:SustainabilityProperty .
  ?subprops rdfs:subClassOf ?props .
  ?component mpo:hasProperty ?props .
  FILTER(?component=:crossbeam_component1)
}
```

Listing A.2: *Example SPARQL query to retrieve sustainability properties (e.g., waste mass after taking recyclable and reusable portion) values for a component.*

References

[1] M. M. Ali, R. Rai, J. N. Otte, and B. Smith. A product life cycle ontology for additive manufacturing. *Computers in Industry*, 105:191–203, 2019. doi:10.1016/j.compind.2018.12.007.

[2] F. Ameri, C. Urbanovsky, and C. McArthur. A systematic approach to developing ontologies for manufacturing service modeling. In *Proceedings of the 2nd International Workshop on Ontology and Semantic Web for Manufacturing*, volume 14, Graz, Austria, 2012.

[3] A. Beanland. The EU Digital Product Passport shapes the future of value chains: What it is and how to prepare. WBCSD: World Business Council for Sustainable Development, 2023. URL https://www.wbcsd.org/wp-content/uploads/2023/09/The-EU-DPP-shapes-the-future-of-value-chains_What-it-is-and-how-to-prepare-now.pdf. Accessed: 8 October 2024.

[4] C. Bicchielli, N. Biancone, F. Ferri, and P. Grifoni. BiOnto: An ontology for sustainable bioeconomy and bioproducts. *Sustainability*, 13(8):4265, 2021. doi:10.3390/su13084265.

[5] P. V. Biron and A. Malhotra. XML schema part 2: Datatypes. World Wide Web Consortium (W3C) Recommendation (Second Edition), 2004. URL http://www.w3.org/TR/xmlschema-2/. Accessed: 8 October 2024.

[6] D. Brickley and L. Miller. FOAF vocabulary specification, version 0.99. Online, 2014. URL http://xmlns.com/foaf/spec/. Accessed: 8 October 2024.

[7] S. Çetin, C. De Wolf, and N. Bocken. Circular digital built environment: An emerging framework. *Sustainability*, 13(11):6348, 2021. doi:10.3390/su13116348.

[8] S. Çetin, D. Raghu, M. Honic, A. Straub, and V. Gruis. Data requirements and availabilities for material passports: A digitally enabled framework for improving the circularity of existing buildings. *Sustainable Production and Consumption*, 40: 422–437, 2023. doi:10.1016/j.spc.2023.07.011.

[9] P. P.-S. Chen. The entity-relationship model—toward a unified view of data. *ACM Transactions on Database Systems (TODS)*, 1(1):9–36, 1976. doi:10.1145/320434.320440.

[10] K. Cheung, J. Drennan, and J. Hunter. Towards an ontology for data-driven discovery of new materials. In *Proceedings of the AAAI Spring Symposium: Semantic Scientific Knowledge Integration*, pages 9–14, Stanford University, California, 2008.

[11] DBpedia Contributors. DBpedia: A large-scale, multilingual knowledge base extracted from Wikipedia. Online, 2023. URL https://www.dbpedia.org/. Accessed: 8 October 2024.

[12] DCMI Contributors. Dublin Core Metadata Initiative (DCMI). Online, 2024. URL https://www.dublincore.org/. Accessed: 05 September 2024.

[13] T. De Baerdemaeker, G. M. Kontogeorgis, et al. Elementary multiperspective material ontology (EMMO), version 1.0. Online; GitHub, 2020. URL https://github.com/emmo-repo. Accessed: 8 October 2024.

[14] Ellen Macarthur Foundation. Methodology: An approach to measuring circularity, 2019. URL https://emf.thirdlight.com/link/3jtevhlkbukz-9of4s4/@/preview/1?o. Accessed: 8 October 2024.

[15] F. Giunchiglia and M. Fumagalli. Teleologies: Objects, actions and functions. In *Proceedings of the 36th International Conference on Conceptual Modeling (ICCM)*, pages 520–534, Valencia, Spain, 2017. Springer.

[16] F. Giunchiglia, M. Fumagalli, et al. Concepts as (recognition) abilities. In *Proceedings of the 9th International Conference on Formal Ontology in Information Systems (FOIS)*, pages 153–166, Annecy, France, 2016.

[17] F. Giunchiglia, K. Batsuren, G. Bella, et al. Understanding and exploiting language diversity. In *Proceedings of the International Joint Conference on Artificial Intelligence (IJCAI)*, pages 4009–4017, Melbourne, Australia, 2017.

[18] F. Giunchiglia, K. Batsuren, and A. Alhakim Freihat. One world-seven thousand languages. In *Proceedings of the International Conference on Computational Linguistics and Intelligent Text Processing (CICLing)*, pages 220–235, Hanoi, Vietnam, 2018. Springer.

[19] B. Glimm, I. Horrocks, B. Motik, G. Stoilos, and Z. Wang. HermiT: An OWL 2 reasoner. *Journal of Automated Reasoning*, 53(3):245–269, 2014. doi:10.1007/s10817-014-9305-1.

[20] G. Goldbeck, E. Ghedini, A. Hashibon, G. Schmitz, and J. Friis. A reference language and ontology for materials modelling and interoperability. In *Proceedings of the NAFEMS World Congress*, page NWC_19_86, Quebec City, Canada, 2019.

[21] M. Grüninger and M. S. Fox. The role of competency questions in enterprise engineering. In *Benchmarking—Theory and practice*, pages 22–31. Springer, 1995.

[22] M. Hepp. GoodRelations ontology. Online, 2011. URL https://www.heppnetz.de/ontologies/goodrelations/v1. Accessed: 8 October 2024.

[23] M. S. Hoosain, B. S. Paul, S. M. Raza, and S. Ramakrishna. Material passports and circular economy. In L. Liu and S. Ramakrishna, editors, *An Introduction to Circular Economy*, pages 131–158. Springer, 2021. doi:10.1007/978-981-15-8510-4.

[24] C. Jonquet, A. Toulet, E. Arnaud, S. Aubin, E. D. Yeumo, V. Emonet, J. Graybeal, M.-A. Laporte, M. A. Musen, V. Pesce, et al. AgroPortal: A vocabulary and ontology repository for agronomy. *Computers and Electronics in Agriculture*, 144:126–143, 2018. doi:10.1016/j.compag.2017.10.012.

[25] C. Jonquet, A. Toulet, E. Arnaud, S. Aubin, E. D. Yeumo, V. Emonet, J. Graybeal, M.-A. Laporte, M. A. Musen, V. Pesce, et al. Multi-crop passport ontology. AgroPortal, 2019. URL https://agroportal.lirmm.fr/ontologies/CO_020. Accessed: 8 October 2024.

[26] R. K Soman. Modelling construction scheduling constraints using shapes constraint language (SHACL). In *Proceedings of the European Conference on Computing in Construction (EC3)*, volume 1, pages 351–358, Chania, Crete, Greece, 2019.

[27] M. H. Karray, B. Chebel-Morello, and N. Zerhouni. A formal ontology for industrial maintenance. *Applied Ontology*, 7(3):269–310, 2012. doi:10.3233/AO-2012-0112.

[28] M. H. Karray, F. Ameri, M. Hodkiewicz, and T. Louge. ROMAIN: Towards a BFO compliant reference ontology for industrial maintenance. *Applied Ontology*, 14(2): 155–177, 2019. doi:10.3233/AO-190208.

[29] F. Kedir, D. F. Bucher, and D. M. Hall. A proposed material passport ontology to enable circularity for industrialized construction. In *Proceedings of the European Conference on Computing in Construction (EC3)*, volume 2, pages 91–98, Rhodes, Greece, 2021. doi:10.35490/EC3.2021.159.

[30] H. Knublauch. TopBraid SHACL API, version 1.4.3, 2024. URL https://github.com/TopQuadrant/shacl. Accessed: 8 October 2024.

[31] H. Knublauch. SHACL playground. Online, 2024. URL https://shacl.org/playground/. Accessed: 8 October 2024.

[32] H. Knublauch and D. Kontokostas. Shapes Constraint Language (SHACL), W3C Recommendation. W3C Recommendation, 2017. URL https://www.w3.org/TR/shacl. Accessed: 8 October 2024.

[33] R. Kuttantharappel Soman, F. N. Kedir, and D. Hall. Towards circular cities: Directions for a material passport ontology. In *Proceedings of the European Conference on Computing in Construction*, pages 229–236, Rhodes, Greece, 2022.

[34] P. J. Landrigan, R. Fuller, N. J. Acosta, O. Adeyi, R. Arnold, A. B. Baldé, R. Bertollini, S. Bose-O'Reilly, J. I. Boufford, P. N. Breysse, et al. The lancet commission on pollution and health. *The Lancet*, 391(10119):462–512, 2018. doi:10.1016/s0140-6736(17)32345-0.

[35] S. Lemaignan, A. Siadat, J.-Y. Dantan, and A. Semenenko. Mason: A proposal for an ontology of manufacturing domain. In *Proceedings of the IEEE Workshop on Distributed Intelligent Systems: Collective Intelligence and Its Applications (DIS'06)*, pages 195–200, Prague, Czech Republic, 2006.

[36] H. Li, R. Armiento, and P. Lambrix. An ontology for the materials design domain. In *Proceedings of the 19th International Semantic Web Conference (ISWC)*, pages 212–227, Athens, Greece, 2020. Springer.

[37] W. Li and W. Hao. Materials Design Ontology (MDO): A formal ontology for materials design. *Journal of Materials Research*, 35(14):1864–1873, 2020. doi:10.1557/jmr.2020.127.

[38] P. V. María and C. F. Serge. Material properties ontology. Ontology Specification Draft, 2020. URL https://bimerr.iot.linkeddata.es/def/material-properties/. Accessed: 8 October 2024.

[39] D. McGinty. 5 opportunities of a circular economy. World Resources Institute, 2021. URL https://www.wri.org/insights/5-opportunities-circular-economy. Accessed: 8 October 2024.

[40] G. A. Miller. WordNet: a lexical database for english. *Communications of the ACM*, 38(11):39–41, 1995. doi:10.1145/219717.219748.

[41] J. Morbach, A. Wiesner, and W. Marquardt. Ontocape—a (re) usable ontology for computer-aided process engineering. *Computers & Chemical Engineering*, 33(10): 1546–1556, 2009. doi:10.1016/j.compchemeng.2009.01.019.

[42] L. Morkunaite, F. H. Al-Naber, E. Petrova, and K. Svidt. An open data platform for early-stage building circularity assessment. In *Proceedings of the 38th International Council for Research and Innovation in Building and Construction (CIB) W78*, pages 813–822, Luxembourg, 2021.

[43] B. Motik and I. Horrocks. OWL datatypes: Design and implementation. In *Proceedings of the 7th International Semantic Web Conference (ISWC)*, volume 5318, pages 307–322, Karlshruhe, Germany, 2008. Springer.

[44] A. Nizamis. Composition collaborative manufacturing services ontology, version 2. Zenodo, 2019. URL https://zenodo.org/records/3374505. Accessed: 8 October 2024.

[45] OWL Working Group. Web Ontology Language (OWL). W3C Semantic Web Standards, 2023. URL https://www.w3.org/OWL. Accessed: 8 October 2024.

[46] C. Paramatmuni and D. Cogswell. Extending the capability of component digital threads using material passports. *Journal of Manufacturing Processes*, 87:245–259, 2023. doi:10.1016/j.jmapro.2023.01.032.

[47] S. Peroni, D. Shotton, and F. Vitali. The live OWL documentation environment: a tool for the automatic generation of ontology documentation. In *Proceedings of the 18th International Conference on Knowledge Engineering and Knowledge Management (EKAW)*, pages 398–412, Galway City, Ireland, 2012. Springer.

[48] M. H. Rasmussen, P. Pauwels, M. Lefrançois, G. F. Schneider, C. A. Hviid, and J. Karlshøj. Recent changes in the building topology ontology. In *Proceedings of the 5th Linked Data in Architecture and Construction Workshop (LDAC)*, pages 1–7, Dijon, France, 2017.

[49] M. H. Rasmussen, M. Lefrançois, M. Bonduel, C. Anker Hviid, and J. Karlshøj. OPM: An ontology for describing properties that evolve over time. In *Proceedings of the 6th Linked Data in Architecture and Construction Workshop*, volume 2159, pages 24–33, Matera, Italy, 2018.

[50] H. Rijgersberg, M. van Assem, and J. Top. Ontology of units of measure and related concepts. *Semantic Web*, 4(1):3–13, 2013. doi:10.3233/sw-2012-0069.

[51] C. A. Rufino Júnior, E. Riva Sanseverino, P. Gallo, D. Koch, S. Diel, G. Walter, L. Trilla, V. J. Ferreira, G. B. Pérez, Y. Kotak, et al. Towards to battery digital passport: Reviewing regulations and standards for second-life batteries. *Batteries*, 10(4):115, 2024. doi:10.3390/batteries10040115.

[52] E. Sauter and M. Witjes. Linked spatial data for a circular economy: Exploring its potential through a textile use case. In *Proceedings of the Posters and Demos Track of SEMANTiCS*, volume 2044, Amsterdam, Netherlands, 2017.

[53] E. Sauter, R. Lemmens, and P. Pauwels. CEO and CAMO ontologies: a circulation medium for materials in the construction industry. In *Proceedings of the 6th International Symposium on Life-Cycle Civil Engineering (IALCCE)*, pages 1645–1652, Rotterdam, The Netherlands, 2019.

[54] V. Shynkarenko and L. Zhuchyi. Ontological harmonization of railway transport information systems. In *Proceedings of the 5th International Conference on Computational Linguistics and Intelligent Systems (COLINS)*, pages 541–554, Lviv, Ukraine, 2021.

[55] V. Shynkarenko, L. Zhuchyi, and O. Ivanov. Ontology-based semantic checking of data in railway infrastructure information systems. *Foundations of Computing and Decision Sciences*, 47(3):291–319, 2022. doi:10.2478/fcds-2022-0016.

[56] E. Sirin, B. Parsia, B. C. Grau, A. Kalyanpur, and Y. Katz. Pellet: A practical OWL-DL reasoner. *Journal of Web Semantics*, 5(2):51–53, 2007. doi:10.1016/j.websem.2007.03.004.

[57] A. Sommer and N. Car. pySHACL, version 0.26.0, 2024.

[58] M. S. Sonzini, M. Vegetti, and H. Leone. Towards an ontology for product version management. *International Journal of Product Lifecycle Management*, 8(1):80–97, 2015. doi:10.1504/IJPLM.2015.068008.

[59] S. Stier. General Process Ontology (GPO), version 0.2.0. Online; GitHub, 2023. URL https://github.com/General-Process-Ontology/ontology. Accessed: 8 October 2024.

[60] The Apache Software Foundation. Apache Jena SHACL Documentation. Online, 2023. URL https://jena.apache.org/documentation/shacl/. Accessed: 8 October 2024.

[61] P. Valluru, J. Karlapudi, K. Menzel, T. Mätäsniemi, and J. Shemeikka. A semantic data model to represent building material data in aec collaborative workflows. In *Proceedings of the Boosting Collaborative Networks 4.0: 21st IFIP WG 5.5 Working Conference on Virtual Enterprises*, volume 592, pages 133–142, Valencia, Spain, 2020. Springer.

[62] M. Vegetti, H. Leone, and G. Henning. PRONTO: An ontology for comprehensive and consistent representation of product information. *Engineering Applications of Artificial Intelligence*, 24(8):1305–1327, 2011. doi:10.1016/j.engappai.2011.02.014.

[63] A. Wagner and U. Rüppel. BPO: The building product ontology for assembled products. In *Proceedings of the 7th Linked Data in Architecture and Construction Workshop (LDAC 2019)*, volume 2389, pages 106–119, Lisbon, Portugal, 2019. CEUR-WS.org.