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Acronyms and Abbreviations

BoM	Bill of Materials
CC	Concept Core
CM	Circular Manufacturing
CQs	Competency Questions
DPP	Digital Product Passport
EMMO	European Materials Modelling Ontology
EOL	End of Life
ER	Entity Relationship
EU	European Union
JAD	Joint-Application Development
LC	Language Core
LFI	Linear Flow Index
MCI	Material Circularity Indicator
OntoMPLC	Ontology for Material and Product lifecycle
OWL	Web Ontology Language
PCB	Printed Circuit Board
RDF	Resource Description Framework
RTM	Resin Transfer Moulding
TVS	Technovative Solutions
UCAM	University of Cambridge
UKC	Universal Knowledge Core
UNITN	University of Trento
VARTM	Vacuum Assisted Resin Transfer Moulding
BoM	Bill of Materials
CC	Concept Core
CM	Circular Manufacturing

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1. Executive Summary

This deliverable has a number of objectives: (i) to survey and analyse data contributing partners' requirements, and to select the state-of-the-art application ontologies that can potentially be reused and extended within JIDEP, (ii) to illustrate the ontological facet development through a series of discussions (iii) to develop application ontologies that enable the representation of concepts and properties required for instantiating different aspects of product, component and material data of all three application use cases, and (iv) to test the application ontology against use-case data to ensure quality and usability. To this end, the current (first) version of the deliverable details: (i) the review of related documentation, including manual and research papers to analyse and extract concepts, relations, and datatype properties; (ii) the Joint-Application Development (JAD) based requirement analysis and illustration of individual facets of our application ontology, (iii) the first version of the application ontology, OntoMPLC, has been developed in JIDEP that has captured the concepts and relationships which are common across all three use case applications, and (iv) the quality assessment phase that includes verification and validation process so that the ontology can provide answers to the competency questions.

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2. Introduction

This deliverable is on application ontologies, which are often formally specified in a way that it fits the need for a specific user community with some computational application to reason automatically within the computationally tractable representational framework [1]. To achieve a circular economy with the existing manufacturing process is a formidable task. However, we aim to solve the challenge by introducing several ontologies, including the common application ontology called OntoMPLC, which stands for Ontology for Material and Product Life Cycle. We have developed this ontology to support the manufacturing ecosystem so that circularity can be increased to achieve a higher circular economy. It provides a comprehensive set of concepts, relations, and datatype properties related to products, components and materials. We will use 'concepts' and 'classes' interchangeably in the rest of the document. The ontology is intended to be used by a variety of stakeholders.

We have reviewed many user manuals, European Union (EU) projects and literature, related documents, research articles, and other related ontologies to extract the relevant concepts and entities. Our application ontology captures the concepts, relations, and datatype properties that are extracted from the stakeholder-provided documents so that it can address the issues appropriately. We have extracted information and developed the application ontology by defining facets incrementally in several Joint Application Development (JAD) meetings. Nevertheless, the entries in the ontology are extended and verified by the experts and stakeholders in a series of discussions.

We have defined the OntoMPLC ontology for describing the data and semantics of material, component, and product lifecycles with the complete integration of Top-Level Ontology and domain ontologies with the common application ontology. We have created classes, relations, and datatype properties that are not available in the selected ontologies to enhance the coverage of OntoMPLC to meet the requirements of applications in capturing both domain and application-specific data and knowledge.

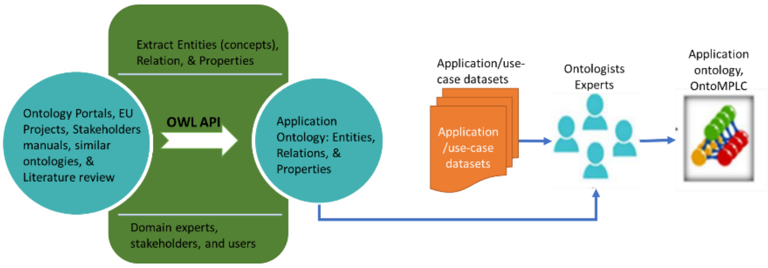

Figure 1. Approach for defining the application ontology for materials and products lifecycle (OntoMPLC) representation.

Our application ontology is organised into several main components: (i) **Material Passport** contains a set of metadata about a product, component, or material describing necessary lifecycle states; (ii) **Physical property** describes the physical properties of a product, component, or material. It can articulate density, mass, dimension, rigidity, and resilience; (iii) **Composition property** can define the microstructure of a product or component to identify quantities and the sources of constituent parts and the materials; (iv) **Temporal properties** can represent the lifespan, durability, and maintenance, whereas the **thermal properties** can explain thermal characteristics to improve thermal design and insulation; (v) **Sustainability property** to reflect the Material Circularity Indicator (MCI) that has the potential to enable circular economy, (vi) **Chemical properties** can express the toxicity and flammability, whereas **biological properties** may reveal the environmental sustainability through

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biodegradability; (vii) **Manufacturing process** is a process that converts raw materials into finished products; (viii) **Quantity** refers to the quantitative properties of products, components or materials; (ix) **Measure** represents numerical values of quantities associated with quantitative properties and units.

The intended audience for this deliverable within the context of JIDEP is as follows:

- Use-Case Domain Experts: subjects involved in the project, having significant competencies in the domain of interest and use-case modelling to represent the JIDEP project use cases.
- Knowledge Engineers: technical subjects involved, as part of the overall knowledge representation and application processes, by acting over the knowledge management activities (knowledge graph instantiation, application modelling, process modelling, traceability analysis, etc.).
- Use-case Stakeholder: Use case subjects interested in computer applications and sharing information across companies of interest.

The rest of the document is organised as follows: Section 3 describes how we have analysed different related documents such as manuals, documentation, datasets, and state-of-the-art research articles to extract concepts, relations, and datatype properties for the common application ontology. Our series of discussions with the data contributing partners and other stakeholders for requirement analysis and evaluation of ontology facets have been articulated in Section 4. The ontology development methodology is illustrated in Section 5. Section 6 explains the different facets of our application ontology. The verification and validation process that ensures the quality of our application ontology is described in Section 7. The concluding remarks and future directives are discussed in Section 8.

3. Related document review

JIDEP aims to achieve a vision of credible pathways to maximise the project results through data-exchange-driven collaboration. We model and exploit ontologies to achieve the goal of data exchange across different stakeholders, targeting the automobile, wind turbine, and industrial electronics use cases. We develop OntoMPLC ontology that includes Material Passport, Sustainability Property, Temporal, Thermal, Physical, Chemical and Biological Properties along with the Units of Measure. In this connection, we analyse the collected data-related documentation, such as manuals, datasets, and research articles, in which relevant application and use case data is published. The goal of our review and analysis is to extract concepts, relations, and properties. Although we have discussed the related documents in this section, the following section also discusses the Joint-Application Development (JAD) with the data-contributing partners to understand the data, capture knowledge, and collect competency questions that helped us to develop application ontology in several facets.

Reviewed documentation:

Our data-providing use-case partners supplied us with several documents to help us develop an understanding of the specific materials needed for a circular economy within their industrial community and procurement network. Resources analysed for the automotive use case were rather diverse. They included descriptions of digital product passports for automotive vehicles, which contained data about manufacturing location, production year, quantity of circular materials, and primary material [25]. There were also battery passports with information to track the entire lifecycle of batteries in compliance with the EU battery regulation [26] and

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digital material passports with detailed information about materials used in manufacturing products [27]. The documentation provided for a wind turbine was immensely specific. It covered the circularity of wind turbine blades after their end of life [28]. Additionally, it included the wind turbine blade specification with properties such as mass, length, root diameter, max chord, and max laminate thickness, as well as the percentage of blade materials [29][30].

Reviewed research papers:

Apart from the reviewed documentation, we reviewed various state-of-the-art research articles that focus on the contents of material passport and ontology construction to ensure a circular economy. We got insights about the challenges and opportunities of using a Material Passport (MP), often called a Digital Product Passport (DPP). An article assessed 76 recent diverse DPP initiatives based on 13 criteria [4]. Another review article on circular manufacturing (CM) strategies aimed to identify the relevant information and data required to support the manufacturer's decision process and to identify the necessity of data standardisation to exchange data [5].

The Material passport collected in the Digital thread of safety-critical applications has been overviewed by its structure, material properties, and specification in another article [6]. Adisorn et al. [7] in their comprehensive review of digital product passports, suggested that MP should contain materials inventory, composition, origin, maintenance, quality, recyclability, environmental impact, reusability, and disposal procedure.

In many articles, material passport [8] has been termed differently, such as Product Passport [9], Recycling Passport [10], Resource Passport [11] and so on. A review paper by Debacker and Manshoven [12] also listed other similar terms such as "workwear passport", "circularity passport", "resource identity tag", and "technical passport for equipment" to represent material passport to some extent. However, Material Passport was the most frequently used term [13]. "Bill of Materials (BoM)" also represents a material passport to register all subassemblies, intermediates, parts, raw materials, and their quantities to assemble a product [14].

Langley et al. [15] orchestrated the digital product passport about products' composition, environmental footprint, and opportunities for a circular industrial ecosystem to source production materials to monitor production processes, use of the product, and reclaiming material. It also collects data for curation, processing, and sharing with digital product passports. The research articles have identified various essential elements for creating a material passport by applying different approaches.

4. Requirement Analysis by Joint-Application Development

As part of the Joint Application Development (JAD) process for requirement analysis, we had a face-to-face meeting with the data-contributing partners in Austria, which resulted in a significant outcome. Moreover, we had several online meetings to understand the data, capture knowledge, and collect competency questions. We met with the stakeholders and discussed a range of focused issues, leading us to develop our application ontology by facets. We then verified it in subsequent meetings.

Understanding Data: JAD sessions made the physical system and the target improvement very clear to the ontology experts. During the JAD sessions, in addition to understanding the current state of the existing system, the participants also pinpointed the specific changes or enhancements required to improve the system. We often reached unanimous agreement on information or judgments. The unanimous consensus included a more comprehensive range of information, both in terms of depth and breadth. Moreover, the participation of data-

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contributing partners helped test and integrate the information. We had an opportunity to gain a deep understanding of the data, make suitable extensions, and verify it accurately.

Finding Competency questions: During the JAD sessions, we identified the competency questions that assisted us in eliciting the needs, expectations, and preferences of the stakeholders. We gained clear insights into how they performed a particular task, solved a problem, or achieved a goal in the existing situation. We were able to i) identify the functional and non-functional requirements of the system, ii) validate and verify the requirements by comparing them, iii) prioritise and rank the requirements by assessing their importance and urgency, iv) reduce ambiguity and misunderstanding by using clear and specific language.

Over the JAD sessions, we were able to identify several competency questions, including but not limited to the following:
- Which product, component and material properties should we define to create a material passport to calculate the circular economy potential?
- Is constituent material a composition property or sustainable property?
- Is specific heat a property of material, component, or product?
- Is pultrusion composite a composite based on the manufacturing process or a composite based on reinforcement type?
- Is woven structure a structural composite or composite based on structure?
- Is recycled content a sustainability property or biological property?
- Is joulePerKelvinKilogram a unit of specific heat or thermal conductivity?
- Which units are relevant for describing resistance?

Capturing Knowledge: We succeeded in confirming the necessary concepts, relations, and properties that were identified earlier from different sources, such as scientific papers, datasets, and documentation for the application ontology. We modelled the knowledge formalising in the form of ontology facets, which were verified by SPARQL queries and validated by the stakeholders to address their necessity appropriately.

5. Ontology development methodology

This section discusses the various layers of the general-purpose ontology development methodology relevant to the scope of this deliverable (for a more complete description, see [14]). The scientific basis of the methodology is rooted in the theory of Teleosemantics (see [15,16]). Firstly, we itemise the different ordered representation layers of the proposed methodology as follows:

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

2. *Teleontologies* are reference knowledge-level ontologies aligned to the UKC.

3. *Teleologies* ([15,16]) are ontologies (aligned to a Teleontology) which are generated from a concrete set of requirements in an application context.

We now describe each of the above representation layers in some detail (for full description and exemplification, see [14]).

Universal Knowledge Core (UKC): The Universal Knowledge Core (UKC) is an *a priori*, expandable, multilingual linguistic reference ontology core to the ontology development methodology. It is employed to name and linguistically classify relevant entities, in an expert-driven top-down manner, of the universe of discourse using natural language or domain-

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specific terms. The Language Core (LC) and the Concept Core (CC) are the two component layers that comprise the UKC. We describe each component layer briefly as follows.

The LC is where the UKC's linguistic data is arranged. To that end, it is comprised of a linguistic (WordNet-like) hierarchy [19] of a set of words naming real-world objects (e.g., entities and their properties in the materials domain) in a natural language, a set of synsets grouping synonyms for each word, a set of senses relating words to their relative synsets, and a gloss which examines the intended meaning of each synset. In addition, there are examples associated with glosses that exemplify the meaning of words in a corresponding synset. Notice two things. Firstly, the LC is comprised of linguistic hierarchies (as defined above) in multiple languages covering different depths of common-sense natural language terms and domain-specific terms.

The second component layer of the UKC is the CC. The CC is a language-independent hierarchy of concepts wherein each concept is uniquely identified via an identifier. Each concept in the CC hierarchy is linked to their semantically synonymous synset (if they exist) in different language hierarchies in the LC. In this way, the CC conceptual hierarchy provides an abstract language-independent unified hierarchy linking concepts and words in natural languages of interest. Let us illustrate the above with an example scenario. While the word *Virgin Material Mass* can be lexicalised in different natural languages (e.g., in the English, Italian, etc., LC hierarchies), the concept behind all such language-specific instantiations is the same (e.g., the concept *87890* in the CC hierarchy denoting the class of *Virgin Material Mass*). For a detailed illustration (out of the primary scope of this deliverable) of the above notions, please refer to [14,17,18].

Teleontologies: Teleontologies are knowledge-level ontologies which are aligned to the UKC conceptual hierarchy. They encode definitions of common concepts across a domain of discourse (e.g., in the materials science domain). Such definitions are modelled via three representational constructs of teleontologies: classes, object properties and datatype properties. Hierarchies of classes are employed to encode concepts (e.g., the concept of *engineered materials)* which recur across different application use-cases (e.g., automotive use-case, wind turbine use-case) of a particular reference teleontology. Object properties relate one class to another class(es) in teleontology. For example, the object property: *has_property* relates a material entity to a physical property of that entity. Finally, data properties are used to describe, via attributes, the concepts defined in the class hierarchy. Notice two things. Firstly, a reference teleontology is to model domain appropriateness, which, in other words, means capturing the shared consensus of a community of practice about a (part of a) domain of discourse, e.g., of the materials modelling community. To that end, the classes, object properties and data properties are modelled top-down and are general enough to be valid for multiple application use cases. Secondly, the concepts in a reference teleontology are modelled to be reused over and over while creating and aligning application-specific requirements-based ontologies.

The deliverable D2.3 (beta version) report in [14] identified several potential reference teleontologies (the relevant fragments) which can be reused while aligning application ontologies in the context of the JIDEP project. For example, a prominent reference to teleontology identified is the European Materials Modelling Ontology (EMMO) [20] which has been developed as a multidisciplinary outcome of the European Materials Modelling Council (EMMC). EMMO models dimensions such as properties of a material, physical laws that govern the behaviour of a material, etc. Finally, note that teleontologies are usually formally encoded in Web Ontology Language (OWL) RDF/XML serialisation format.

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Teleologies: Teleologies are ontologies aligned to a reference teleontology, generated from a concrete set of requirements in an application context. They are developed, bottom-up, from the requirements of an application context as per the following steps:

1. The knowledge representation requirements that are expected of teleology in the context of an application use case are usually first captured and tabulated as Competency Questions (CQs) [21] which the teleology is expected to encode and answer. The CQs indicate the application-specific classes, object and datatype properties, which should be modelled in the teleology. Some examples of CQs can be:
    a. Which product, component and material properties should we define to create a material passport to calculate the circular economy potential?
    b. Is constituent material a composition property or sustainable property?
    c. Is specific heat a property of a material, component, or product?
2. The application-specific classes, object properties and datatype properties which are extracted from the CQs are then informally modelled as an Entity-Relationship (ER) diagram [22], wherein the classes are nodes in the ER model, and the labelled edges encode the object properties. The datatype properties can be expressed in various ways in an ER diagram, e.g., as a set of attribute enumeration blocks, or are often left implicit. Notice that the ER model schema might contain several application-specific datatype properties, valid only for a particular application use case.
3. Next, the ER model in step (II) is formalised as a formal teleology in the OWL, preferably in the OWL RDF/XML serialisation format.

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

a. the top-down modelled artefacts, including the UKC and the reference teleontology aligned to the UKC, and,
b. the bottom-up modelled artefact, which is the teleology modelled as per the application use-case requirements.

Next, the methodology prescribes two ordered activities to produce the final ontology combining the top-down and bottom-up knowledge:

A. Middle-Out Merging: In this step, each class, object property and datatype property of a teleology (all being application-specific) is semantically aligned to their immediate general domain concept in the reference teleontology via the subsumption (is-a) relationship. The result of this step is an enriched and unified teleontology which combines the top-down and bottom-up knowledge representation.
B. Knowledge (Teleontology) Annotation: In this step, each concept (class, object property and datatype property) of the enriched and unified teleontology, one at a time, is annotated with global identifiers from the UKC CC to make them conceptually unambiguous. To that end, the teleontology concept is semantically searched in the UKC knowledge base. If a UKC concept (or a synonymous counterpart) exists in the UKC CC, its identifier is assigned to the teleontology concept. If there is no synonymous UKC concept, then a new UKC concept is created corresponding to the teleontology concept. The identifier of this new UKC concept is assigned to the teleontology concept. The final output of this step is a UKC CC identifier annotated conceptually unambiguous enriched and unified teleontology.

To summarise, the high-level sequence of the proposed general-purpose ontology development methodology is as follows:

<u>Top-Down Modelling:</u>

i. UKC (given *a priori*), which gives the linguistic hierarchy of words (and concepts) to name things

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ii. Reference Teleontology, aligned to the UKC conceptual hierarchy, provides reusable community-consensus-driven classes, object properties and datatype properties, which can be reused across several application use cases in a domain.

Bottom-Up Modelling:

i. Modelling the knowledge representation requirements as CQs, which indicate the relevant application use-case-driven classes, object properties and datatype properties to model.
ii. Model an ER diagram out of (i) above.
iii. Formal representation of (ii) as a teleology, preferably using OWL RDF/XML.

Middle-Out Merging:

The teleology is semantically aligned to the reference teleontology (and, therefore, ultimately, to the UKC conceptual hierarchy) to form an enriched and unified teleontology.

Knowledge (Teleontology) Annotation:

The enriched and unified teleontology is rendered conceptually unambiguous by annotating it with identifiers from the UKC concept core. The final output is a conceptually unambiguous enriched teleontology.

A fuller illustrated description of the ordered representation layers of the methodology can be found in [14]. The next section provides highlights of the application-specific ontology modelling activities for the JIDEP project following suitable implementation of (parts of) the afore-described general-purpose ontology development methodology.

6. Application-specific ontology modelling

The vision of a circular economy can be achieved with application-specific ontology modelling. The ontology can ease the circulatory process in manufacturing by finding materials underlying a product:

- to reduce virgin feedstock utilisation by prioritising the use of renewable, reusable, and non-toxic resources.
- to reuse the valuable parts/components of a product after the end of life (EOL).
- to recycle the discarded materials as a source of secondary resources.
- to repair/refurbish to maximise the life of a product through a take-back strategy.
- to re-manufacture through cooperation and collaboration among multi-sector industry actors.

Our main goal is to reduce the utilisation of the virgin feedstock. In this connection, every product should contain enough material passport information so that we can repair/refurbish it to give it a second life, or it can be collected and dismounted after the end-of-life to split into readily reusable and recyclable parts. The recyclable parts come back as a secondary resource after necessary modification. However, the collectors often need to understand the material circulatory indicator or the linear flow index to ensure sustainability. The minimal residual material will go to the landfill or energy recovery field. This fact is depicted in Figure 2.

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Figure 1. Diagrammatic representation of material flows [31].

Therefore, we need to know the feasibility of including recycled materials in the product beforehand so that the industry can maximise its profit, even reducing the utilisation of virgin feedstock. The feasibility depends on the components and constituent material; often, a material passport tells us about the physical properties, composition properties, temporal and thermal properties, sustainability properties, manufacturing processes, and chemical and biological properties. Some properties need to be measured with an instance of the unit of measure. The bigger comprehensive picture has been portrayed in Figure 3 to represent concepts, relations, and properties as a common application-specific ontology.

6.1 Material passport

The main objective of the material passport is to enable the tracking and tracing of materials and products throughout their lifecycle to optimise the use of resources. It is an important resource that supports the transition from a linear to a circular economy in the manufacturing industry by providing transparent and reliable information to different stakeholders, such as manufacturers, consumers, collectors/recyclers, and regulators. The material passport can also eliminate the barriers and challenges that hinder the circularity of materials, such as information asymmetry, lack of trust, technical complexity, and regulatory uncertainty.

In the ontology, Material Passport describes the concepts such as Product, Component, and Material in the form that states that Product hasPart Component, Component hasMaterial Material, and Product hasMaterial Material, where describes, hasPart, and hasMaterial are the object properties. Product, Component, and Material have Manufacturer. The relationship between Product, Component, or Material and Manufacturer has been established with an object property named hasManufacturer. Moreover, the common properties of Product, Component, and Material can be represented by instantiating the concept Property. This concept has subclasses: PhysicalProperty, CompositionProperty, TemporalProperty, ThermalProperty, SustainabilityProperty, ChemicalProperty, and BiologicalProperty. The properties of Material include ChemicalComposition and SpecificHeat as well. The ChemicalComposition specifies the elements and compounds that make up the Material.

In contrast, the SpecificHeat defines the heat required to increase the temperature of one gram of a material or substance by one °C. Furthermore, MaterialPassport, Product, Component, and Manufacturer can be described with different types of datatype properties represented by the dashed lines to boxes. The core part of the material passport has been portrayed in Figure 4.

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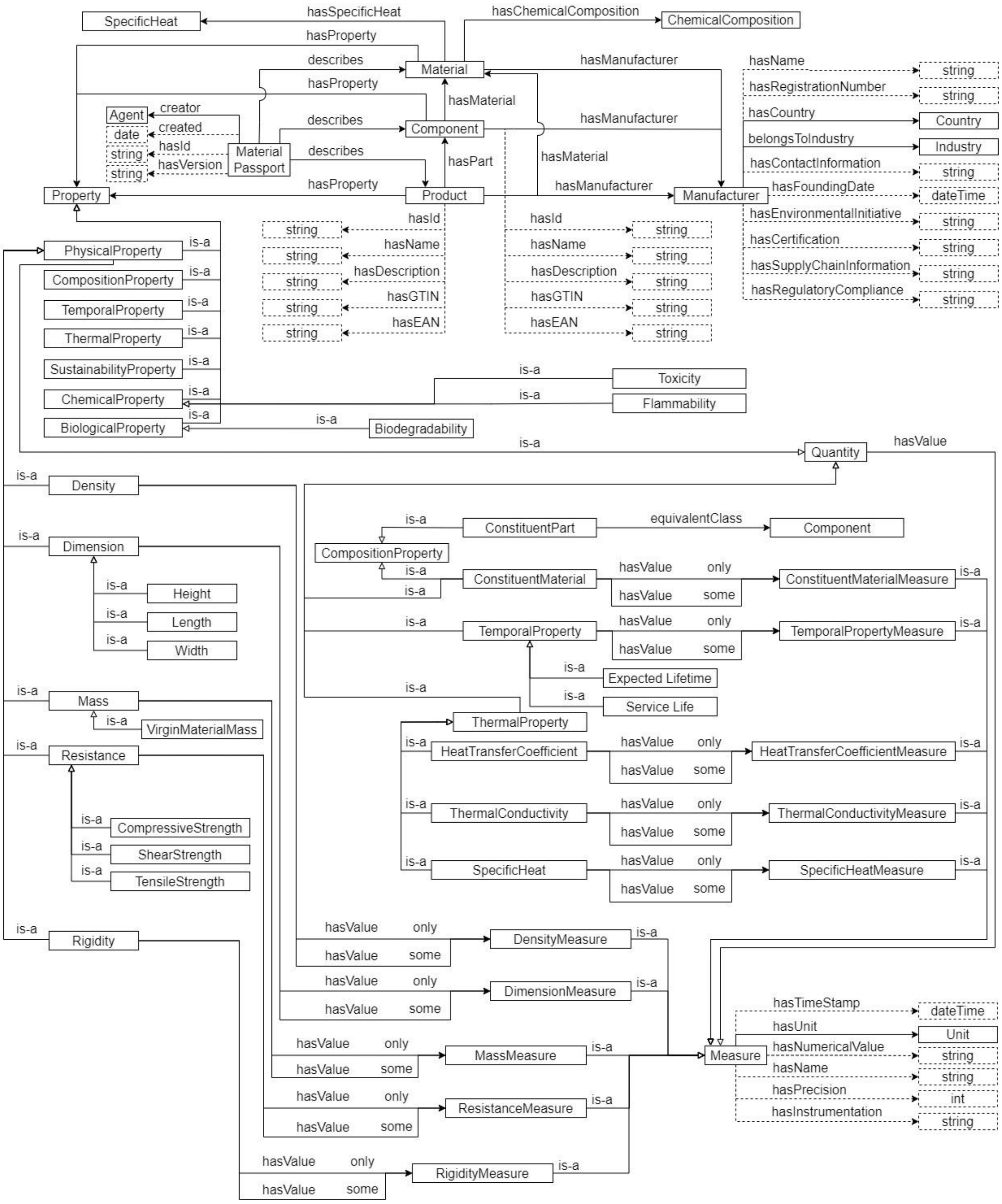

Figure 2. Common application ontology represents concepts, relations and datatype properties to describe material and product lifecycle, physical properties, chemical properties, composition (microstructural) properties, biological properties and so on.

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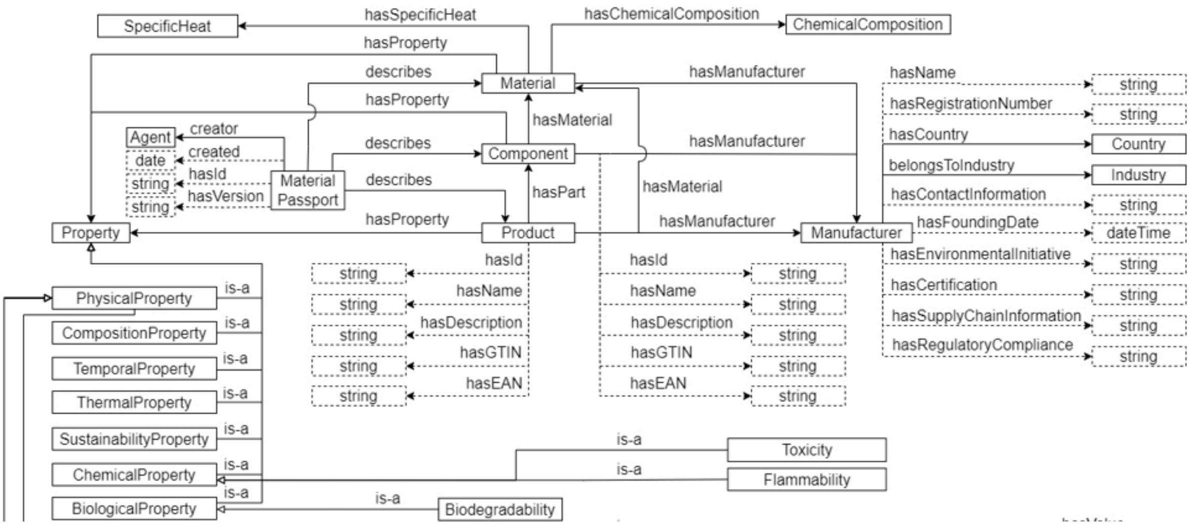

Figure 3. The Material Passport facet of the common application-specific ontology, OntoMPLC.

Nevertheless, the more specific properties of the class Property have been illustrated in the following subsections.

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6.2 Physical property

Physical property is essential, especially to measure the quantity of a material in terms of density, dimension, mass, resistance, and rigidity. This property can provide accurate and reliable data about the characteristics of Products, Components, and Materials to enable their circularity and, as a result, to achieve sustainability. It can potentially identify the value of interest for recovery, reuse, or recycling to calculate material circulatory indicators in a circular economy. Manufacturers can optimise the design to comply with regulations and standards, and the recycler can estimate the value to promote circular economy principles.

The PhysicalProperty facet of OntoMPLC is depicted in Figure 5. In the ontology structure, PhysicalProperty is a subclass of Property and a subclass of Quantity. Mass is a subclass of PhysicalProperty that has at least an instance of MassMeasure as its value. MassMeasure is a child class of Measure. The Measure is a generic concept defined with various datatype properties such as hasTimeStamp, hasNumericValue, hasUnit, hasName, hasPrecision and hasInstrumentation. That is, a particular measuring quantity can be defined by its value, unit, precision, measuring time, and instrumentation.

For example, Chassis is a Product or Component having Mass as its PhysicalProperty that has at least one value from the class MassMeasure defined by a generic class Measure with hasNumericValue=200, hasUnit= ‘kg’, hasName=‘Kilogram’, hasPrecision=‘’, hasInstrumentation=‘scale’, and it is measured at hasTimeStamp=‘2023/10/23 10:33:25 AM’.

Similarly, Density is a subclass of PhysicalProperty that hasValue of at least one as DensityMeasure, a child class of Measure. Dimension is a subclass of PhysicalProperty with at least an instance of DimensionMeasure as its value. Likewise, Resistance has a value of at least one instance of ResistanceMeasure, and Rigidity has a value of at least one instance of RigidityMeasure.

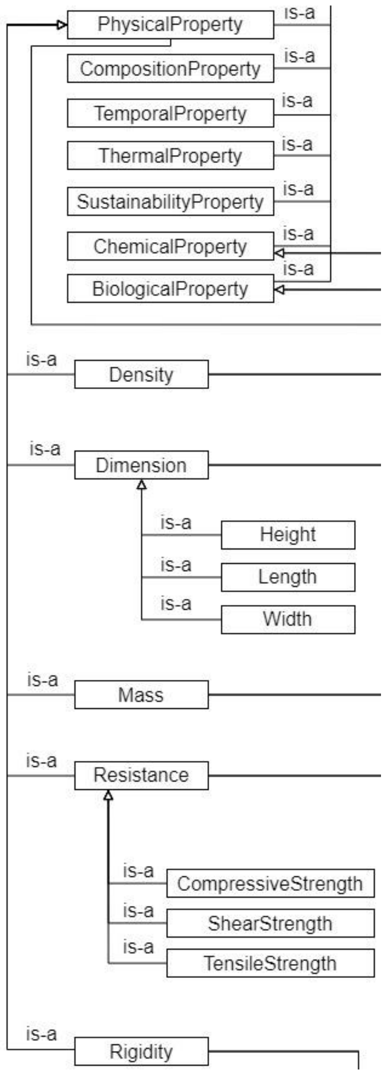

Figure 4. The PhysicalProperty facet of OntoMPLC.

6.3 Composition Property

CompositionProperty provides the necessary information on the composition of materials of products that are made of multiple or complex components. It can identify quantities and the source of constituent parts and the materials. This part of application ontology has the potential to help optimise the selection, processing, and assembly of the constituent parts and materials, as well as to enable their separation, disassembly, and recycling at the end of life.

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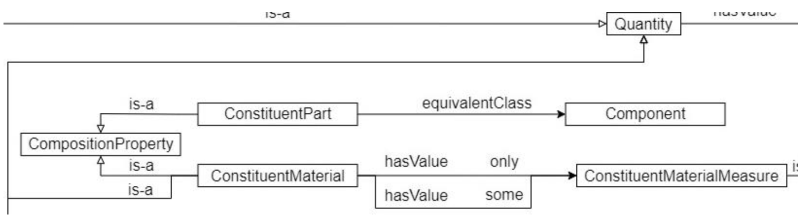

Figure 5. The CompositionProperty facet of OntoMPLC

As shown in Figure 6, in the ontology, ConstituentPart and ConstituentMaterial are two subclasses of CompositionProperty, a subclass of Property that can define a Product, Component or Material (e.g., Composite Material). The ConstituentPart class is an equivalent class of the Component class so that it can describe different functional components of a product. Moreover, ConstituentMaterial is defined as a quantitative property that hasValue of at least one as ConstituentMaterialMeasure that is defined as a subclass of Measure.

6.4 Temporal and Thermal Properties

The temporal and thermal properties are two essential properties of material and product defined in our common application-specific ontology. The temporal property denotes the time-related properties to identify the lifespan and durability and, as a result, degradation of materials, components or products. It can be used to optimise the timing, frequency, and method of maintenance, repair, and replacement of materials, components or products. On the other hand, the thermal property reflects the thermal characteristics, including thermal conductivity and heat transfer coefficient, that can be taken into consideration to improve the thermal design and insulation of products or components. Both properties may affect the circularity and sustainability of a product, component or material.

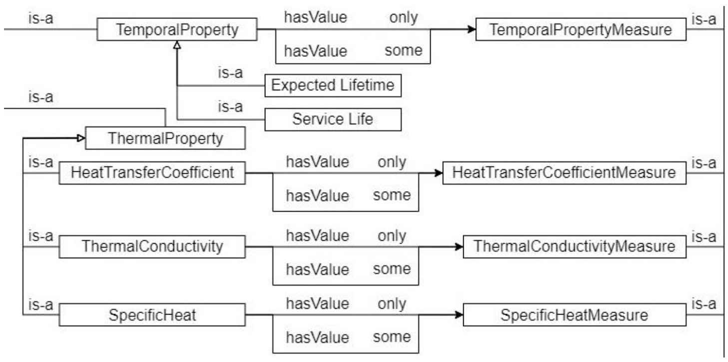

Figure 6. Temporal and Thermal Property facets of OntoMPLC

The temporal and thermal property facets of OntoMPLC are articulated in Figure 7. In our application-specific ontology, ExpectedLifetime and SeviceLifetime are two subclasses of TemporalProperty that can be defined as a quantitative property that hasValue of at least one as TemporalPropertyMeasure. ThermalProperty is a subclass of Property having three subclasses such as HeatTransferCoefficient, ThermalConductivity, and SpecificHeat. HeatTransferCoefficient is defined as a quantitative value that hasValue of at least one as HeatTransferCoefficientMeasure. ThermalConductivity of a product, component, or material can be characterised as a quantitative property with a value of at least one instance of ThermalConductivityMeasure. Moreover, SpecificHeat is defined as a quantitative property that hasValue of at least one as SpecificHeatMeasure. HeatTransferCoefficientMeasure, ThermalConductivityMeasure, and SpecificHeatMeasure are all subclasses of Measure.

6.5 Sustainability property

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The main objective of the sustainability property of a material passport is to provide a comprehensive and transparent assessment of the sustainability of a material, component or product. We can utilise this information to decide the selection, use, and end-of-life management of materials to reduce environmental impact and promote a circular economy. In this regard, we have included several terminologies in the SustainabilityProperty facet of our application-specific ontology depicted in Figure 9. We can define the following terms to understand the sustainability property classes used in our ontology easily:

- **Recycled content**: The total mass collected from a product after end-of-life for recycling.
- **Feedstock fraction from recycled product** (F_R): At the time of recycling, the ratio of the feedstock derived from a recycled product to feed into the manufacturing process.
- **Feedstock fraction from the reused product** (F_U): At the time of component reusing, the ratio of the feedstock derived from a reused product that can be fed into the manufacturing process.
- **Product fraction collected for recycling** (C_R): After the end of life, a fraction of the product can be collected for recycling. The ratio of recycling part to the product is called the product fraction collected for recycling, i.e., Product fraction collected for recycling = (Mass of product collected for recycling) / (Mass of product).
- **Product fraction collected for reuse** (C_U): After the end of life, a fraction of the product can be collected for reuse. The ratio of reusing part to the product is called the product fraction collected for reuse, i.e., Product fraction collected for reuse = (Mass of product collected for reuse) / (Mass of product).
- **Recycling efficiency for the portion collected for recycling** is the percentage of recyclable materials that are recycled. It is calculated by dividing the mass of recycled material by the mass of recyclable material collected for recycling. For example, if 100 tons of recyclable material are collected, and 80 tons of that material are recycled, the recycling efficiency is 80%.
- **Recycling efficiency for producing feedstock** is the percentage of recyclable materials converted into feedstock for a new product. It is calculated by dividing the mass of feedstock produced from recyclable materials by the mass of recyclable materials leaving the recycling process. This is an important metric for measuring the success of recycling programs for identifying opportunities to improve the circular economy.
- **Waste mass after taking recyclable and reusable portions** (W_0) is the mass of waste that remains after all recyclable and reusable materials have been removed. It is calculated by subtracting the mass of recyclable and reusable materials from the product after end-of-life.
- **Waste mass generated in the collected portion for recycling** (W_C) is the mass of waste that is generated during the collection, sorting, processing, and transportation of recyclable materials, where the waste is generated due to mistaken mixture, damage, contamination, and residue.
- **Waste mass generated in producing recycled feedstock** (W_F) is the mass of waste that is generated during the process of converting recyclable materials into recycled feedstock. For example,
    - Recyclable materials processed = 100 tons
    - Recycled feedstock produced = 80 tons
    - Waste mass generated in producing recycled feedstock = 20 tons
- **Linear Flow Index** (*LFI*) is a metric that measures the linearity of a material's flow through the economy.

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- **The Material Circularity Indicator** (*MCI*) [26] of a product indicates how the restorative flow can be maximised to keep minimising the linear flow. It is derived from the following properties depicted in Figure 8 and in equations below:
    - The mass of a product, M
    - The mass of virgin raw material, V
    - The mass of unrecoverable waste, W
    - Utility factor, F(X)

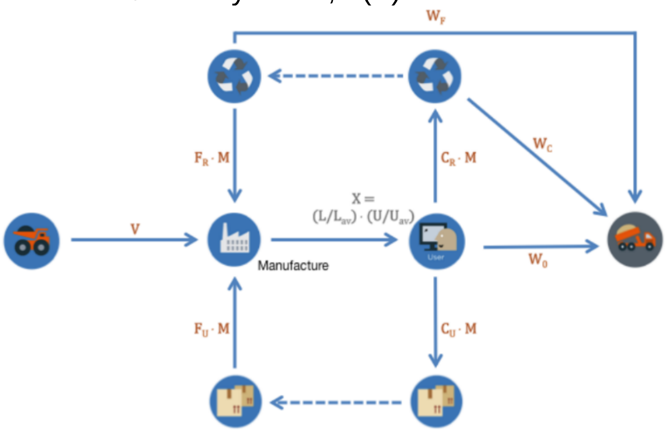

Figure 8. Diagrammatic representation of material flows that articulates different measures by the label of arrows [31].

Where,

$V = M(1 - F_R - F_U - F_S)$, where F_S is the biologically sustainable production.

$W = W_0 + \frac{W_F + W_C}{2}$

Then, $LFI = \frac{V+W}{2M}$

$MCI = 1 - LFI \cdot F(X)$ such that $F(X) = \frac{0.9}{X}$, $where\ X = 1$ and $F(X)$ is the utility factor defined as a function of the utility X of a product.

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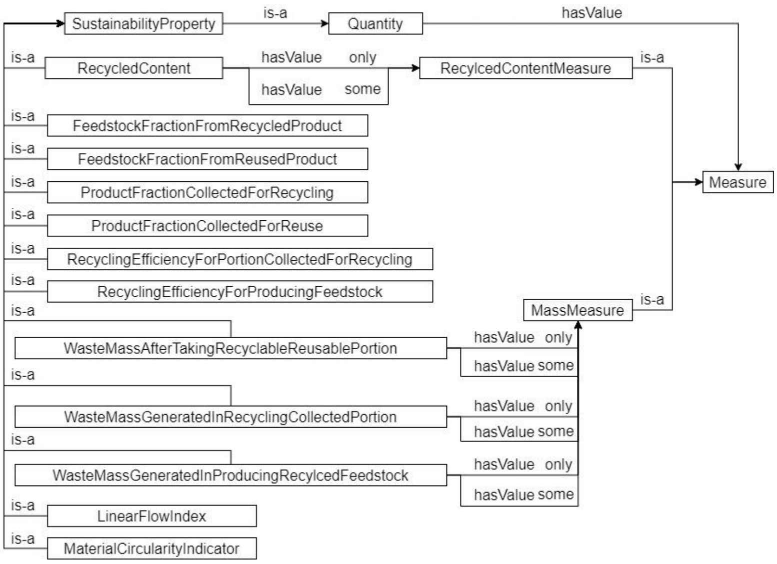

Figure 7. The SustainabilityProperty facet of OntoMPLC.

As depicted in Figure 9, within our application-specific ontology, SustainabilityProperty has been defined to identify various parameters for calculating the Linear Flow Index (*LFI*) and the Material Circularity Indicator (*MCI*). This allows us to predict circularity before a product undergoes recycling, ensuring the feasibility of the business process and enabling a circular economy in manufacturing.

6.6 Chemical and Biological Properties

Chemical properties are the properties of a product, component, or material that are determined by its toxicity, flammability and so on. In addition to the toxicity and flammability, the property also includes pH, corrosiveness, reactivity, volatility and so on. However, they are not of interest to our project. The toxicity shows the ability to harm living organisms. Moreover, the capability of catching fire is addressed by its flammability. On the other hand, biological properties determine the characteristics of, for example, biodegradability, which refers to the ability to be broken down by microorganisms.

Figure 10 shows that in our ontology, Toxicity and Flammability are subclasses of ChemicalProperty, which is again a subclass of Property defining different characteristics of a product, component or material. Furthermore, we are interested in Biodegradability, a subclass of BiologicalProperty. Biodegradability helps reduce the environmental impact.

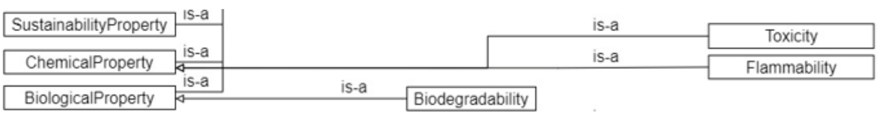

Figure 8. The Chemical and biological property facets of OntoMPLC.

6.7 Manufacturing process

In our application-specific ontology, we defined the manufacturing process used for the composite material in such a way that the process is further divided into subclasses: wet layup process, resin transfer moulding process, pultrusion process, filament winding process,

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compression moulding process, injection moulding process, vacuum infusion process, and autoclave process. The manufacturing process facet of OntoMPLC is portrayed in Figure 11.

WetLayUpProcess is a labour-intensive composite manufacturing process that involves manually placing layers of reinforcing fibres in a mould and saturating them with a liquid resin. This process is further classified into HandLayUpProcess and SprayUpProcess.

ResinTransferMouldingProcess represents the process that injects resin under pressure to ensure full impregnation of the fibres. This process is further classified into ClosedMouldRTM and OpenMouldRTM.

PultrusionProcess refers to the continuous process that involves pulling reinforcing fibres through a resin bath to produce long and slender composites.

FilamentWindingProcess renders the winding process reinforcing the already coated filaments around a rotating mandrel. Axial, Helical and RedialFilamentWinding are subclasses of this process.

CompressionMouldingProcess involves placing pre-impregnated reinforcing fibres and then applying pressure to compact the fibres and resin. There are three types: HotPress, VacuumAssisted, and PrepregCompressionMoulding.

InjectionMouldingProcess injects molten resin into a heated mould. The process is classified into Reaction, StructuralReaction and ResinTransferInjectionMoulding.

VacuumInfusionProcess pictures the process of placing pre-impregnated reinforcing fibres into a vacuum bag. There are two subclasses: VacuumBaggingInfusion and VacuumAssistedResinTransferMoulding (VARTM).

AutoclaveProcess involves expensive curing in a pressurised chamber. There are two types: HighPressureAutoclaveMoulding and HighTemperatureAutoclaveMoulding.

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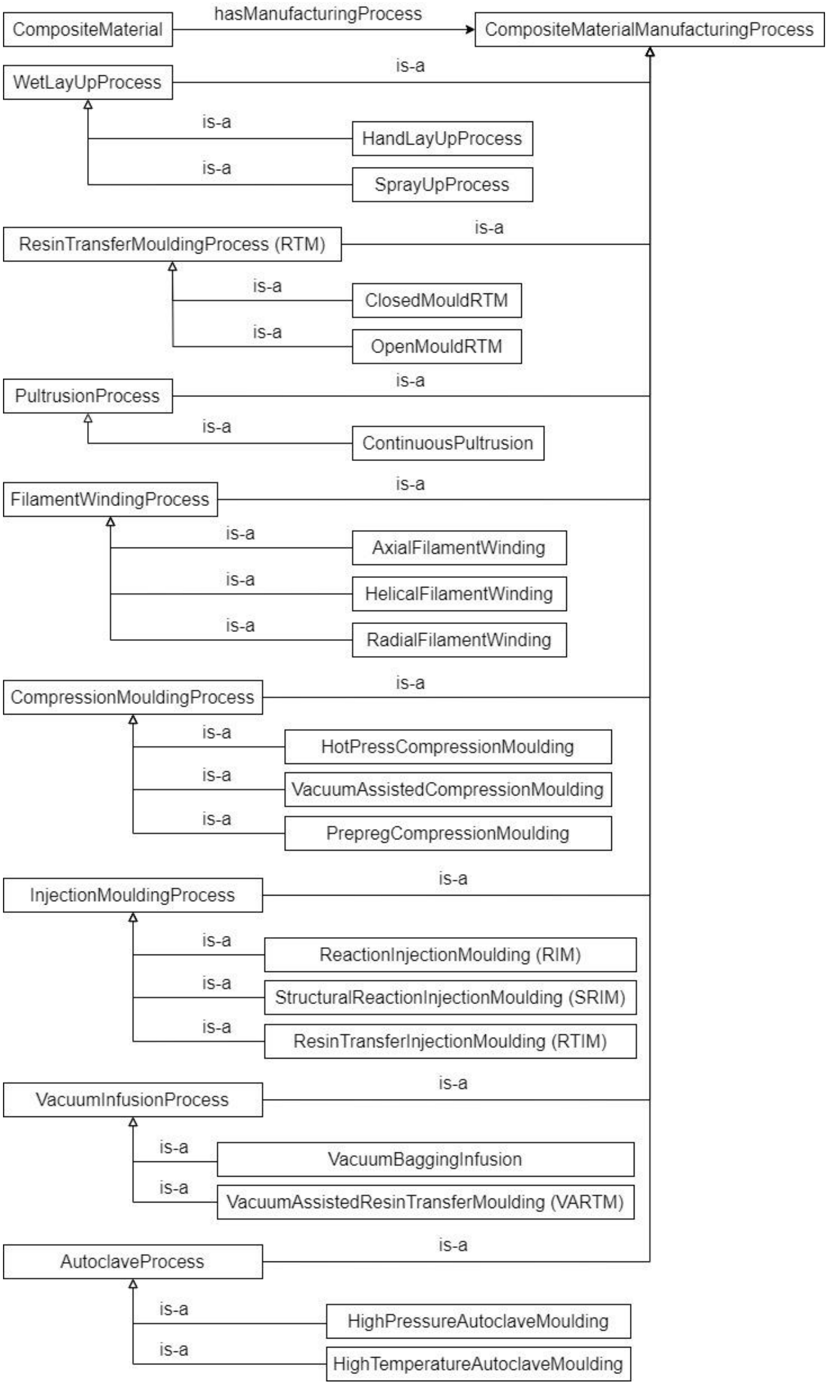

Figure 91. A facet representing manufacturing processes for composite materials.

6.8 Units of measure

The units of measure are necessary to provide specific and accurate information about the quantity of product, component or material in a material passport. For instance, instead of simply stating that a product contains glass fibre, we can state that it has “1000 grams of glass fibre”. This information becomes inevitable as it allows manufacturers to make decisions about the selection and use of materials. For example, a manufacturer may need to know the mass and type of raw materials required to manufacture a new product that meets certain functional requirements.

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As depicted in Figure 12, in our application-specific ontology, we have several subclasses of the Measure class associated with specific unit types, enabling users to select the intended unit easily while creating material passports on the user interface. The subclasses are DensityMeasure, DimensionMeasure, MassMeasure, ResistanceMeasure, RigidityMeasure, ConstituentMaterialMeasure, TemporalPropertyMeasuire, HeatTransferCoefficientMeasjure, ThermalConductivityMeasure, SpecificHeatMeasure, and RecycledContentMeasure.

In some cases, we have reused a similar set of measurement units for different measure classes with a formal definition. For example, MassMeasure has unit values milligram, gram, or kilogram. On the other hand, ConstituentMaterialMeasure has similar unit values. The reason for this choice of ontological modelling is to enable the assignment of different subsets of units for each measure if and when required based on the use cases.

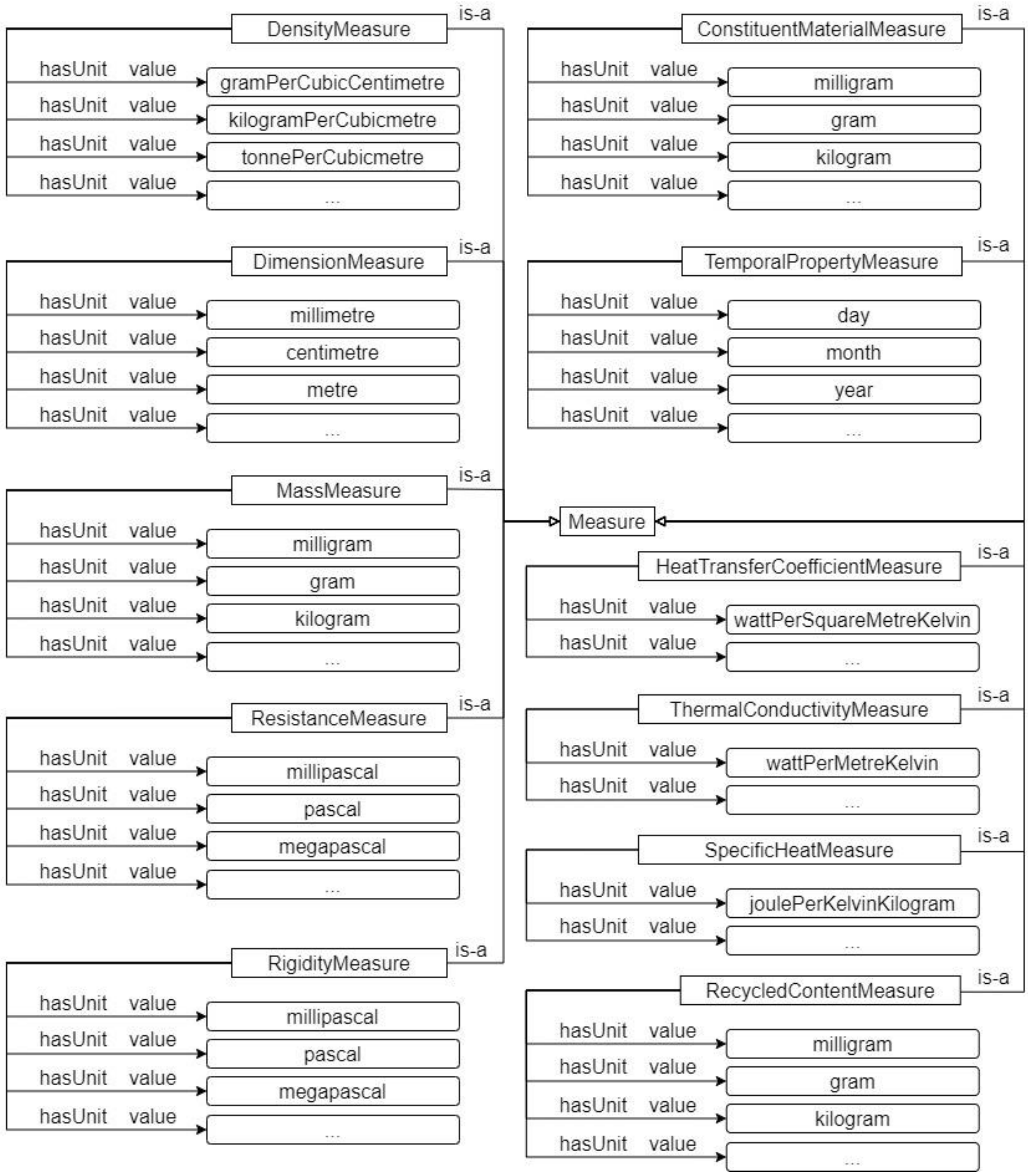

Figure 10. The units of measure facet of OntoMPLC.

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7. Quality assessment

Our quality assessment of application ontology ensures the project meets the requirements of interoperability, machine understandability, and automation. The assessment stages improve the efficiency and productivity of the application ontology by identifying and correcting problems. Moreover, in the context of automobiles, wind turbines, and industrial electronics, we need to ensure the circular economy through a high-quality ontology, which can capture the specificity of Material Circularity Indicator (MCI) and sustainability along with other properties so that the stakeholders can have a clear understanding of the product, component, and material at any stage of product's lifespan. Quality assessment of the application-specific ontology of this project involves two steps: verification and validation.

In the verification process, we ensure that the ontology meets its specified requirements. In this connection, we use SPARQL queries to verify the completeness, consistency, and accuracy of the material passports. This is important because material passports contain essential information about the materials used in products, components, and materials. By verifying the quality of material passports in application-specific ontology, we can ensure high-quality characteristics of our ontology in the context of automobile, wind turbine, and industrial electronics manufacturing.

In the validation process, we utilise the use cases to validate the quality of our application-specific ontology. For example, an automobile manufacturer developed a use case for using recycled carbon fibre to produce a new model of car. The use case would specify the requirements for the recycled carbon fibre, such as its recycled content, mechanical properties, and composition properties. The following subsections elaborate on our verification and validation processes.

7.1 Verification with SPARQL query

Our application ontology, OntoMPLC, contains a material passport that is an essential and powerful tool to assess the circularity in the context of automobiles, wind turbines, and industrial electronics. We check the usability of our ontology through several SPARQL queries. Here are a few examples.

Check for completeness: We can ensure that all of the required properties are included in the material passport of our application ontology. For example, we can use a SPARQL query to retrieve necessary information from the ontological knowledge graph so that the critical parameter MCI for a circular economy can be calculated automatically. We can find all values for a particular product against the sustainability properties such as RecycledContent, FeedstockFractionFromRecycledProduct, FeedstockFractionFromReusedProduct, ProductFractionCollectedForRecycling, ProductFractionCollectedForReuse, RecyclingEfficiencyForPortionCollectedForRecycling, RecyclingEfficiencyForProducingFeedstock, LinearFlowIndex, MaterialCircularityIndicator, WasteMassAfterTakingRecyclabaleReusablePortion, and so on that are essential for circular economy in the automobile, wind turbine blade, and microcontroller board manufacturing.

Check for consistency: We use Protégé, a popular ontology editor, to check the consistency by ontology and domain experts. Moreover, we use HermiT and ELK reasoner to identify inconsistencies in our ontology automatically. It confirms the consistency of our application ontology. It could infer new knowledge from it. Apart from this, we applied a set of SPARQL to verify the consistency of our application ontology.

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Check for accuracy: We have tested a set of SPARQL queries against the knowledge graph to verify the accuracy of retrieved data. We have verified our application ontology with domain experts and tested it with real-world data collected for the use cases.

7.2 Validation with use-cases

We have applied our application ontology to generate a knowledge graph with the automotive and wind turbine use case. Furthermore, we have validated the use-case instances using SPARQL to retrieve all necessary data so that our system can calculate the Material Circularity Indicator (MCI) accurately. To understand the validation, we have included two sample SPARQL described below to retrieve the necessary instances.

Query 1. A SPARQL query to retrieve all physical property (e.g. mass) values for a component.

```
PREFIX mp:<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/>

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 mp:hasProperty ?props .
  ?component rdf:type mp:Component .
}
```

Query 2. A SPARQL query to retrieve all sustainability properties (e.g. waste mass after taking recyclable and reusable portion) values for a component.

```
PREFIX mp:<http://www.theworldavatar.com/kg/ontomatpassport#>
PREFIX om:<http://www.ontology-of-units-of-measure.org/resource/om-2/>

SELECT ?component ?measure ?property ?value
WHERE{
  ?measure ?property ?value .
  ?subsubprops om:hasValue ?measure .
  ?subsubprops rdfs:subClassOf ?subprops .
  ?subprops rdf:type mp:SustainabilityProperty .
  ?subprops rdfs:subClassOf ?props .
  ?component mp:hasProperty ?props .
  ?component rdf:type mp:Component .
}
```

From Queries 1 and 2, we can calculate the Linear Flow Index (LFI) as well as the Material Circulatory Indicator (MCI) successfully with the retrieved data.

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8. Conclusions

The current version of the deliverable formulated various aspects of application ontology that focus on the material passport, physical property, composite property, temporal and thermal properties, sustainability property, chemical and biological properties, manufacturing process, and units of measure. Material passport contains the essential characteristics and change logs with the products so that the stakeholders such as manufacturers, consumers, collectors, and recyclers can read the content dynamically, make business decisions, and calculate Material Circularity Indicator (MCI) along with Linear Flow Index (LFI). Thus, the stakeholders can take appropriate initiative to maximise the circularity of products, reducing the linearity index to enable a circular economy. Moreover, different stakeholders can share their knowledge to maximise their business capacity. The next version of the deliverable will take the current version as the basis and enrich it with more use-case examples of the JIDEP project.

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