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Demonstrating an Ontological Framework for Sustainable PVC Material Science: A Holistic Study Combining Granta EduPack, Bibliometric Analysis, Thematic Analysis, Content Analysis, and Protégé

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Abstract

Addressing the growing need for sustainable innovation in PVC materials, this study presents an illustrative framework that develops and demonstrates an ontological system that integrates lifecycle simulation using Granta EduPack, systematic literature analysis (including bibliometric, thematic, and content analytics) of peer-reviewed publications, and Protégé-based semantic reasoning, and their combination, in a holistic manner. Material and use-phase data for PVC, HDPE, PP, PET, and FRP cooling-tower components were sourced from ANSYS Granta EduPack Level-3 Polymer Sustainability 2023 R2 Version; 23.2.1, and a systematic analysis of the literature was then encoded as ontology classes, properties, and individuals following the Seven-Step ontology development method. Eco-audit simulations, standardised to a functional unit of 1 kg cooling tower fill material, reveal that the use phase dominates environmental impact (67 MJ primary energy, ~80% of total lifecycle), while material production and end-of-life recycling contribute ~15% and credits of ~900 MJ and 28 kg CO_2 via recycling offsets. Ontology reasoning with corrected SWRL rules and SPARQL queries classifies VirginPVCRef and PVC10ES as strong structural materials (tensile strength $\geq$ 40 MPa), identifies PVCRH40 as high-moisture-risk (water absorption > 0.10 g/g), and ranks hydro-thermal dechlorination (recyclability 0.90) over mechanical recycling (0.55). A systematic analysis of 40 Scopus-indexed publications (2015–2025) highlighted key themes in recycling technologies, LCA emissions, additive toxicity, ontology frameworks, machine learning integration, circular economy policy, and cooling-tower applications. Demonstrated via a simulation-based cooling-tower case study, hybrid PVC-FRP designs yield the highest justified Material Sustainability Performance Index (MSPI), outperforming PVC-only and FRP-only alternatives. This framework provides a conceptual decision-support tool for exploring PVC material optimisation, illustrating pathways to enhancing circularity and environmental responsibility in industrial applications. The proposed framework is, therefore, not intended as a validated decision-support tool, nor does it claim analytical optimisation or predictive performance but rather serves as a method of illustration that shows how domain knowledge can be formally structured using ontology principles linked to simulation representations, and that was examined for internal logical consistency.

Keywords: PVC sustainability; ontology analysis; circular economy; cooling tower; lifecycle assessment; PVC recycling

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1. Introduction

Sustainability in Polyvinyl Chloride (PVC) manufacturing is an emerging focus in modern industry due to its significant benefits. Manufacturers, industry end users, researchers and practitioners, government agencies, and other stakeholders have recognised the adverse impacts that the current conventional, non-sustainable approach has on the environment and our way of life, both now and in the future, if we do not adopt changes in how we produce and manage plastics [1]. This has led to numerous research initiatives aimed at improving sustainability and promoting the circular economy concept in polymer manufacturing and waste management. One approach involves utilising modern information and communications technologies, including Artificial Intelligence (AI) and data-driven analytics, to enhance various aspects of polymer production and utilisation. Consequently, there is also ongoing interest in approaches that can conceptually integrate heterogeneous modelling paradigms to support clearer system representation and structured analysis.

Incinerating PVC waste, for instance, typically emits hazardous substances such as hydrogen chloride and dioxins, whereas mechanical recycling often yields lower-quality, downcycled products. As a result, the sustainability challenges associated with PVC manufacturing and waste management necessitate the development of frameworks that go beyond traditional waste management methods [2]. Additionally, current life cycle assessments (LCAs) indicate that PVC significantly contributes to greenhouse gas (GHG) emissions during both production and disposal stages, with estimated emissions ranging from 2.1 kg to 3.2 kg CO_2-eq per kilogram of PVC produced [3].

Therefore, the adoption of innovative approaches that integrate lifecycle thinking, data-driven analysis, and ontological modelling is essential to advancing material innovation and promoting sustainability and environmental responsibility in polymer manufacturing.

The present study is intentionally positioned as a conceptual and illustrative framework demonstration. Its objective is not to propose a novel analytical method, to optimise manufacturing performance, or to provide a validated decision-support tool. Instead, the study demonstrates how ontology modelling, simulation representations, and systematic analytical structuring may be conceptually combined to support a holistic representation of a PVC manufacturing system. The contribution lies in clarifying how such integration may be structured, rather than in evaluating how well it performs in empirical or decision-making contexts.

To support this demonstrative objective, a representative PVC manufacturing scenario is employed as an illustrative case. This scenario is not intended to reflect a specific industrial facility, nor to serve as a basis for empirical validation or comparative analysis. Rather, it functions as a conceptual vehicle through which the proposed framework can be described, applied, and examined for internal logical consistency.

Accordingly, any references to validation within this study are strictly limited to internal rule coherence and structural consistency within the ontology and its linkage to the illustrative simulation representation. No claims are made regarding predictive accuracy, optimisation capability, comparative superiority, or real-world decision-support effectiveness.

By explicitly adopting this demonstrative scope, the study aims to contribute a transparent and well-bounded example of integrated system representation that may inform future research. Subsequent work may extend this framework through empirical validation, external benchmarking, and application within real industrial decision contexts, which are beyond the scope of the present manuscript.

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1.1. Digital Tools for Sustainable Material Science

Emerging digital platforms have introduced the potential for innovative approaches to enhance the sustainability of PVC manufacturing. Granta EduPack enables researchers to conduct eco-audits and life-cycle assessments, thereby quantifying trade-offs among costs, recyclability, and emissions [4]. Likewise, systematic literature analysis, including bibliometric mapping, thematic clustering, and content analysis, has contributed to the identification of sustainable practices in polymer research [5]. Protégé, a popular ontology editing platform, provides a comprehensive framework for encoding domain knowledge in structured taxonomies. This facilitates automated reasoning using the Semantic Web Rule Language (SWRL) and supports query-based decision-making with SPARQL [6]. Together, these tools enable the integration of scientific evidence, lifecycle models, and knowledge at multiple scales.

1.2. Ontology and Knowledge Representation in Circular Economy Contexts

Ontology in material science provides a systematic approach to modelling the relationships among material properties, environmental impacts, and lifecycle stages. By explicitly defining entities such as PVC monomers, additives, and emissions pathways and elucidating their inter-relationships, ontology-based frameworks facilitate transparent reasoning across various industrial scenarios. In the context of the circular economy, ontologies formalise strategies such as closed-loop recycling, additive substitution, and eco-design.

1.3. Research Gaps and Aim of the Study

Although numerous studies have examined PVC recycling, additive toxicity, and energy recovery, there is still a notable lack of comprehensive frameworks that integrate simulation, ontology, and systematic literature analysis within decision-support systems [7,8]. Furthermore, industrial case applications, such as PVC-based cooling tower fills and structural components, have not been systematically evaluated through ontological modelling, leaving a gap in addressing practical sustainability challenges through digital innovation. This study aims to bridge this gap by developing and demonstrating an integrated framework with the understanding that its validation in this context is primarily logical and illustrative, providing a foundation for future industrial pilot studies.

Also, this research aims to develop and demonstrate an ontological framework to advance sustainable innovation in PVC materials manufacturing by integrating Granta EduPack simulations, systematic literature analytics, and Protégé-based semantic modelling, using a simulation-based illustrative study of industrial cooling towers as a case study for framework demonstration and evaluation.

To achieve this aim, the study pursues the following objectives: (i) identify and map sustainability challenges in PVC materials across their lifecycle, encompassing production, use, and end-of-life stages, using Granta EduPack datasets, industrial databases, and environmental reports; (ii) develop a domain ontology in Protégé that formalises key entities, properties, and relationships within the PVC lifecycle, including sustainability metrics, recycling pathways, and environmental performance; (iii) incorporate systematic literature analysis and lifecycle datasets to enhance ontology development and generate data-driven insights for sustainable PVC innovation; (iv) implement rule-based reasoning (SWRL) and semantic queries (SPARQL) to evaluate sustainability indicators, circular economy strategies, and decision-support outcomes; (v) evaluate and demonstrate the ontological framework through simulation-based illustrative case studies of industrial cooling towers and demonstrate its applicability to material selection, eco-efficiency assessment, and lifecycle optimisation; and (vi) assess the framework's potential effectiveness in fostering environmental responsibility and circularity within PVC-based industrial systems.

Accordingly, this research addresses the following questions: How can ontology-based modelling boost sustainable innovation and lifecycle insights in PVC material science? How does semantic reasoning with SWRL and SPARQL aid decision-making throughout the PVC manufacturing process and related sectors? In what ways can integrating systematic literature analysis enhance the development and evaluation of ontological frameworks for sustainable polymer systems? Finally, to what degree can the proposed ontology-driven framework demonstrate potential to improve sustainability in industrial practices, particularly in cooling tower design and material reuse?

1.4. Ontology and Lifecycle Thinking for PVC Material Systems

Integrating lifecycle thinking into PVC research enhances the capacity to evaluate trade-offs among material selection, processing pathways, and end-of-life strategies. When ontology is combined with simulation data, it enables reasoning engines to dynamically calculate sustainability metrics. For instance, the lifecycle impact (LCI) of PVC production is expressed as follows:

$$LCI_{\{PVC\}} = \sum_{\{i=1\}}^{\{n\}} (M_i \times EF_i) \quad (1)$$

where M_i indicates material or energy input at stage i and EF_i represents the emission factor related to that input [9]. This formulation lays the foundation for semantic encoding, facilitating automated reasoning about sustainability scenarios.

In summary, this research validates the notion that PVC sustainability efforts are facilitated by a combination of the application of systematic analysis, ontology, and semantic simulations as depicted in Figure 1.

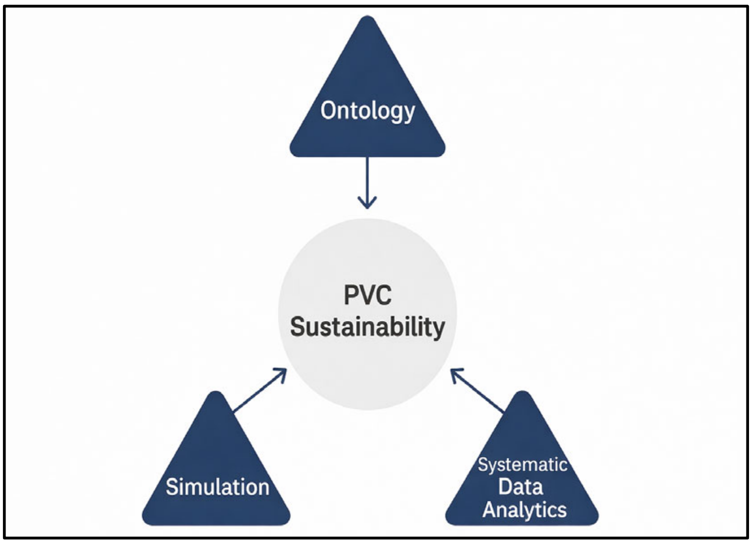

Figure 1. Conceptual positioning of ontology, simulation, and data analytics in sustainable PVC manufacturing [Author's elaboration].

Table 1 presents a concise summary of the major sustainability challenges faced in PVC manufacturing due to the current traditional means of production and how the application of the tripartite framework of ontology, simulations, and systematic analysis may fix these challenges. The literature review in the next section now builds on this foundation by surveying existing tools and frameworks.

Table 1. Sustainability challenges of PVC and the role of ontological/data-driven approaches. [Author's own elaboration].

Sustainability Challenge	Conventional Approach	Ontology/Data-Driven Approach
Additive toxicity (e.g., phthalates)	End-of-pipe treatment, substitution trials	Ontology-based lifecycle mapping of additive flows
Complex recycling pathways	Mechanical downcycling	Semantic reasoning for closed-loop recycling
Emissions during incineration	Flue gas treatment	LCA + ontology reasoning for low-emission alternatives
Material selection in industry	Empirical or heuristic	Integrated decision-support via SWRL/SPARQL

2. Literature Review and Conceptual Basis

2.1. PVC in Sustainable Materials Research

The widespread use of PVC in various aspects of contemporary life has prompted discussions about its environmental sustainability. Its durability and cost-effectiveness contribute to its preference as a material for pipes, flooring, and electrical installations. However, its chlorine content and stabiliser additives complicate recycling efforts [2].

Numerous studies have emphasised concerns about the incineration of PVC, which emits hydrochloric acid and potentially dioxins into the environment [10]. While mechanical recycling offers limited downstream options, chemical recycling and feedstock recovery are increasingly viable alternatives [3]. However, integrating these processes into a circular economy necessitates more than just technical recycling methods. In essence, it requires comprehensive lifecycle models that encompass environmental, economic, and social dimensions.

2.2. Ontological Frameworks in Material Science and Engineering

Ontologies, as structured knowledge representations, have gained prominence in materials science due to their ability to formalise concepts such as material properties, lifecycle stages, and sustainability indicators. For instance, domain ontologies have been employed to develop energy-efficient building materials and sustainable composites [4,11]. Recent advances include dynamic ontologies that update based on real-time data streams and the integration of ontologies with digital twins for enhanced decision support [12,13]. In the context of PVC, ontology-based models can explicitly encode relationships, such as PVC-lifecycle stage-emissions impact, thereby enabling automated reasoning to identify hotspots and opportunities for improvement.

2.3. Semantic Web Tools: Protégé, SWRL, and SPARQL Applications

Protégé, an open-source ontology editor, offers an interface for constructing class hierarchies, defining properties, and linking concepts to individual entities. By employing SWRL (Semantic Web Rule Language), reasoning rules are established. For example, if PVC waste contains phthalates, it should be classified as a "hazardous recycling pathway" [6]. SPARQL facilitates querying of ontological datasets, thereby enabling informed decision-making. For instance, a query can retrieve all PVC lifecycle scenarios with carbon footprints exceeding 2.5 kg CO_2-eq/kg [14].

2.4. Simulation and Data Integration in Materials Science

Granta EduPack facilitates lifecycle-based material selection and environmental profiling. It computes embodied energy and carbon emissions throughout the stages of production, utilisation, and disposal. Regarding PVC, eco-audit simulations indicate that replacing it with polyethene (PE) can reduce life-cycle CO_2 emissions by up to 15% in specific applications [15]. Moreover, the utilisation of a systematic literature analysis in polymer research employs bibliometric analysis (via VOSviewer version 1.6.20), thematic clustering (via QDA Miner), and content analysis to synthesise trends in polymer sustainability [5,11,16].

2.5. Decision-Support Frameworks in Sustainable Manufacturing

Decision-support systems that integrate ontology, simulations, and data analytics enable industries to make well-informed decisions regarding material selection. For example, hybrid frameworks have been proposed for composites and bio-based plastics [7,8]. Extending these frameworks to PVC could assist policymakers and manufacturers in selecting additives, formulations, and recycling technologies that align with principles of environmental responsibility.

2.6. Case Context: Cooling Towers as Industrial Applications of PVC

Cooling towers utilise fill materials and structural components that must harmonise durability, cost-efficiency, and environmental considerations. PVC and fibreglass-reinforced plastics (FRP) are favoured owing to their lightweight and corrosion-resistant characteristics [17]. However, challenges such as biofouling, additive leaching, and corrosion impede long-term sustainability objectives [18]. The following examples are evident in the literature:

- Petrochemical cooling tower retrofit: Replacement of wooden fills with PVC reduced maintenance expenditure but increased chlorine-related leachate [19,20].
- PVC-based fill material performance: Thermal efficiency improved by 12%, but recyclability concerns increased [21].
- CFD optimisation and material selection: Simulations indicated that hybrid PVC–FRP structures can lower energy demand [22].
- Lifecycle assessment of cooling towers: End-of-life challenges are well emphasised, with incineration as the primary disposal method [23].
- Corrosion and environmental challenges: Heavy metals are known to leach from PVC stabilisers [24].

Figure 2 illustrates the ontology layers in materials science, from raw data to reasoning-based decision support. It is a conceptual pyramid illustrating the transformation of raw data into actionable insights for sustainable materials research and application through ontology-based approaches.

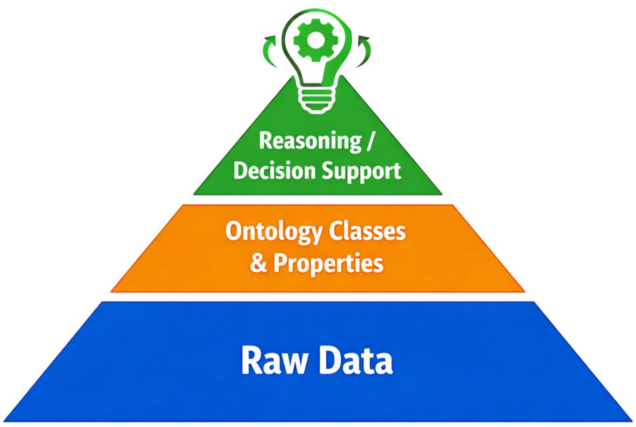

Figure 2. Ontology layers in sustainable materials research [Author's own elaboration].

Figure 3 presents a schematic comparison of PVC-filled and FRP structures, with arrows indicating performance, recyclability, and emissions impacts.

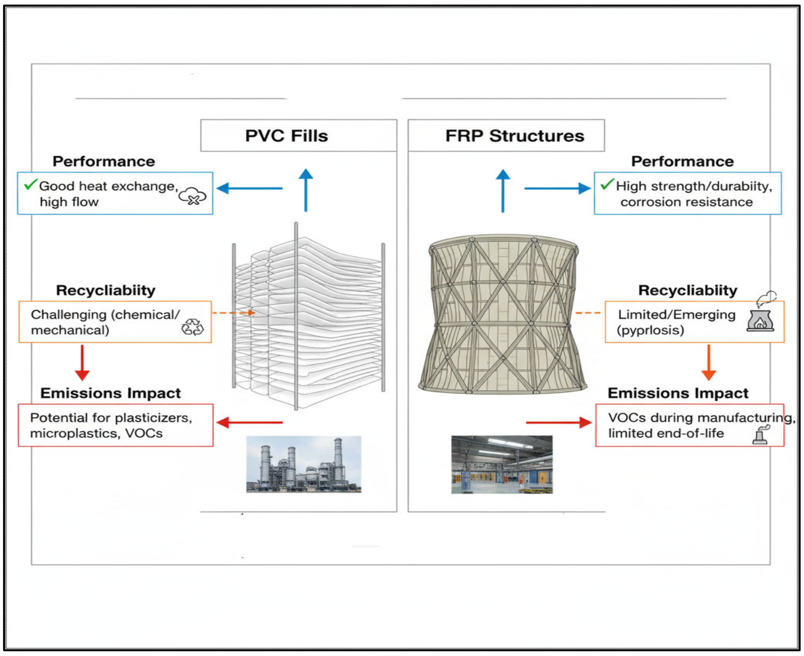

Figure 3. Case application of PVC and FRP in cooling towers (Green tick and blue arrows signify respective pros while red arrows signify cons). [Author's own elaboration].

The digital tools identified above, which were taken forward in the study, are summarised in Table 2.

Table 2. Comparison of digital tools for sustainable material science [Author's own elaboration].

Tool	Application in PVC Research	Strengths	Limitations
Granta EduPack	Lifecycle eco-audits, material substitution scenarios	Quantitative LCA metrics, user-friendly	Limited domain specificity
Systematic Literature Analysis	Literature mapping, recyclability prediction	Trend discovery, predictive capabilities	Dependent on the literature database quality
Protégé (Ontology)	Lifecycle knowledge representation, SWRL reasoning	Formal reasoning, interoperability	Requires expert input for accuracy

Finally, the following composite index (Formula (2)) is identified and represents a formula that enables the comparison of PVC with alternative materials that may be deemed equally suitable for manufacturing.

$$SI_{\{PVC\}} = \frac{\sum (W_i \times S_i)}{\sum W_i} \quad (2)$$

where W_i = weight of indicator i (e.g., emissions, recyclability, toxicity) and S_i = normalised sustainability score for indicator i.

The preceding review of the literature confirms PVC challenges, like additive leaching and incineration emissions, while highlighting ontology's potential. With this in mind, and with reference to the case application and observations in Table 2, the next section details how this study operationalizes these tools through Protégé development and Granta simulations.

3. Materials and Methods

3.1. Research Design

This study employs a mixed research design and methods that utilise ontology-based domain knowledge of PVC materials, incorporating an ontological framework to advance sustainable materials science. It directly derives from the research objectives and questions, integrating modelling and simulation using the Granta EduPack, systematic literature analysis, and datasets to examine trends in PVC with respect to sustainability and the circular economy.

The research design adopted in this study is conceptual and demonstrative in nature. Rather than aiming to test hypotheses, optimise system performance, or evaluate decision outcomes, the design is intended to illustrate how multiple modelling components may be structurally integrated within a single analytical framework.

The study employs thematic clustering algorithms to generate data-driven categories that inform ontology class hierarchies and property structures. It utilises Protégé-based semantic modelling to advance environmental responsibility and circularity through an illustrative simulation-based case study evaluation of industrial cooling tower systems.

The integration of these approaches facilitates the assessment of PVC material science indicators and the qualitative organisation of domain knowledge, which are quantified through ontology-based rule reasoning, SPARQL analysis, and decision support queries. Figure 4 illustrates the methodological framework employed in this research, encompassing knowledge representation, computational modelling, and framework evaluation.

Figure 4. Research framework for PVC materials science sustainability [Author's own elaboration].

At this stage of development, a demonstrative design allows the internal logic, consistency, and transparency of the framework to be examined without introducing confounding assumptions related to data calibration, optimisation criteria, or real-world operational variability. Empirical validation and decision-oriented evaluation are, therefore, intentionally deferred to future research.

3.2. Data Collection and Sources

Material science metrics, including environmental benefits, cost, recyclability, and embodied energy data, were extracted from scientific journals on PVC materials science, encompassing a systematically selected set of 10 peer-reviewed papers on mechanical performance, tensile strength, thermal stability, degradation pathways, recycling technologies, and cooling tower lifecycle impacts.

Additional datasets were obtained from the ANSYS Granta EduPack material science property libraries, which encompass more than 2000 materials pertinent to bioengineering, sustainability, materials science and engineering, eco-design, and polymer catalogues. This enabled the development of material selection charts and evaluations of PVC material sustainability.

Material grades were compared with polypropylene (PP), high-density polyethene (HDPE), polyethene terephthalate (PET), and fibre-reinforced plastics (FRP). Eco-design cradle-to-grave life cycle assessment (LCA) models were developed for PVC cooling tower fill materials, encompassing polymer production, compounding processes, operational water and fan energy consumption, and end-of-life options such as mechanical recycling, chemical recycling, and landfilling. A consistent functional unit of 1 kg of fill material, providing equivalent cooling performance, was established for all LCA calculations.

Ontology modelling was also employed to formalise knowledge on PVC materials science with respect to environmental sustainability indicators, including ontology classes, object properties that connect lifecycle stages, and data-type properties. Furthermore, SWRL rules were implemented to facilitate automated reasoning within sustainability analysis. SPARQL queries were utilised to identify the most suitable material candidates and recycling pathways based on environmental impact indicators, thereby enhancing decision-making processes.

Systematic Bibliometric Analysis Protocol

A systematic bibliometric analysis was conducted to identify the relevant literature and research trends. The search was performed in Scopus and Web of Science databases using the query string: ((“polyvinyl chloride” OR PVC) AND (sustainability OR “circular economy” OR recycling OR “life cycle assessment”) AND (ontology OR “semantic web” OR “decision support”)). The search was limited to English-language peer-reviewed articles published between 2010 and 2025. The initial search yielded 382 records. After removing duplicates, 294 records were screened by title and abstract based on the following exclusion criteria:

- Not focused on PVC or polymer sustainability.
- Not related to digital methods or decision support.
- Not conference proceedings or non-peer-reviewed sources.

This resulted in 52 articles for full-text review. After full-text assessment, 40 articles were selected for final analysis based on relevance to the study’s objectives. The selection process is summarised in Figure 5 (PRISMA flowchart).

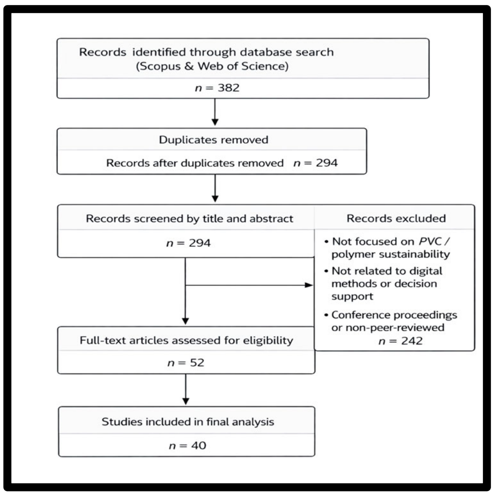

Figure 5. PRISMA flowchart of the literature selection process [Author’s own elaboration].

3.3. Ontology Development Using Protégé

The ontology was developed following the widely recognised Seven-Step Methodology for ontology development [25]. This structured approach ensured methodological rigour and semantic coherence. The steps include the following:

- Defining the domain and scope (PVC lifecycle sustainability),
- Considering existing ontologies for reuse (none were directly applicable),
- Enumerating important terms (material properties, lifecycle stages, environmental impacts),
- Defining classes and the class hierarchy,
- Defining properties of classes,
- Defining constraints and rules, and
- Creating instances.

- Based on the systematically selected literature, an ontology representation in Protégé was developed as a conceptual framework within the top-level class hierarchy (OWL2). The class hierarchy (classes, individuals, objects, and data-type properties) was structured around core domain concepts, including the following: 'Material', 'LifecycleStage', 'EnvironmentalImpact', 'Property', 'RecyclingPathway', and 'Application'. Class hierarchy:
- Lifecycle classes
- Cooling tower domain classes
- Object properties
- Data-type properties
- Rules and constraints (SWRL)
- Query structure (SPARQL)

Figure 6 presents the taxonomies and hierarchies generated from Protégé.

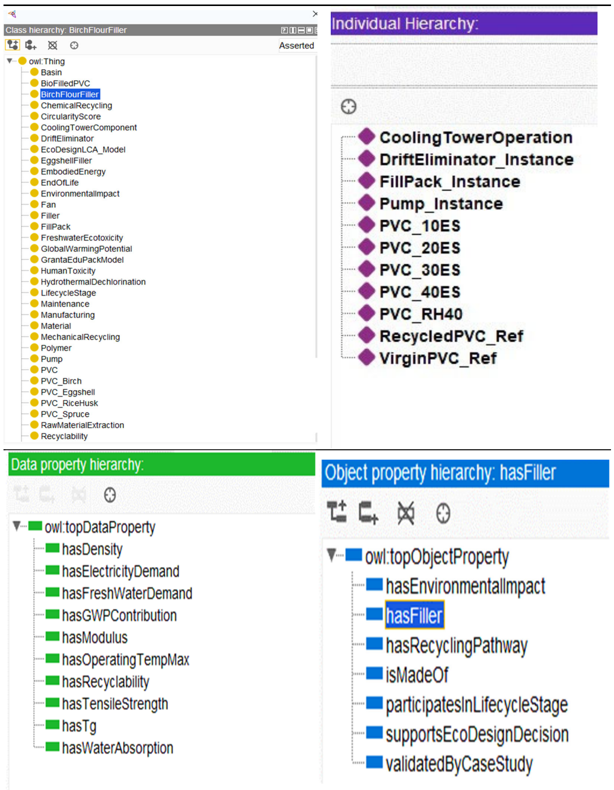

Figure 6. Screenshots of class hierarchy, object properties, data properties, and individual hierarchy generated from Ontology Protégé [26].

3.4. Data Extracted for Ontology Domain

Table 3 below presents data that were entered into SPARQL queries to generate results. Figure 7 above also illustrates these data outputs.

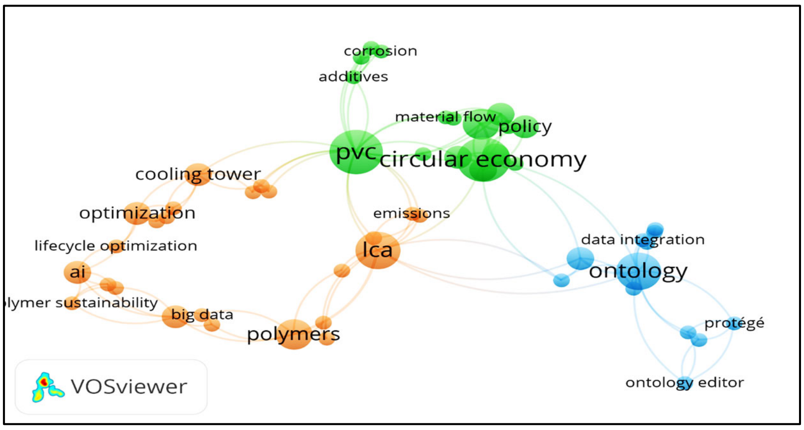

Figure 7. Bibliometric map of PVC sustainability research clusters [27].

Table 3. Ontology Protégé data used for SPARQL [26].

Datatype Property	Domain	Extracted Values from 10 Papers	Source
hasTensileStrength	Material	5.5 → 46.5 MPa	Polymers 14-04372 and 16-01551
hasModulus	Material	1235 → 1787 Mpa	Polymers
hasWaterAbsorption	Material	0.1 → 0.16 g/g	Polymers
hasOperatingTempMax	Material	135 → 150 °C	Polymers and Materials
hasElectricityDemand	UsePhase	169.53 MJ	Cooling Tower LCA
hasFreshWaterDemand	UsePhase	23.10 m^3	Cooling Tower LCA
hasRecyclability	RecyclingProcess	0.55 → 0.90	PVC Risk

3.5. SWRL Rule-Based Reasoning, SPARQL Query and Validation, and Reasoning Accuracy

We now present the SWRL reasoning logic used in this research. Table 4 shows the SWRL rules applied in the ontology, Table 5 shows the data properties and SPARQL queries used, and Table 6 shows the data validation and reasoning used, expected results, and supporting sources, all in Protégé.

Table 4. Ontology Protégé SWRL rule-based [26].

Rule Name	SWRL Logic	Purpose
Cooling Tower Suitability	Material (? m) ˆhasOperatingTempMax (? m, t) ˆswrlb: Then (? t, 120) → SuitableForCoolingTowerMaterial (? m)	Classifies materials suitable for fill packs
High Strength Detection	Material (? m) ˆhasTensileStrength (? mms) ˆswrlb: Then (? s, 30) → HighStrengthMaterial (? m)	Supports material choice
Moisture Risk	Material (? m) ˆhasWaterAbsorption (? m, w)ˆswrlb:greaterThan (? w, 0.10) → HighMoistureRisk (? m)	Finds degradation risks
CE Priority	Material (? m) ˆhasRecyclability (? m, ? r) ˆswrlb:greaterThan (? r, 0.80) → PreferredCircularMaterial (? m)	Supports CE optimisation

Table 5. Ontology Protégé data property [26].

Purpose	SPARQL Query
Find the best CT materials.	SELECT? m WHERE {? m ex: hasOperatingTempMax? t. FILTER (? t > 120)}
Find high-strength PVC	SELECT? m WHERE {? m ex: hasTensileStrength? s. FILTER (? s > 30)}
Detect moisture risk composites.	SELECT? m WHERE {? m ex: hasWaterAbsorption? wa. FILTER (? was > 0.10)}
Rank recycling options	SELECT? p WHERE {? p ex: hasRecyclability? r } ORDER BY DESC (? r)

Table 6. Ontology Protégé data validation and reasoning [26].

Validation Task	Expected Output	Supporting Sources
DL Consistency	All classes satisfiable	OWL 2 DL constraints
SWRL Rule Execution	PVC_40ES → SuitableForCoolingTowerMaterial	Polymers 14-04372
Range Restriction Check	PVC_RH40 fits TS < 10 Mpa range	Polymers 16-01551
LCA Consistency	CT Operation → correctly classified	Schulze et al. [23]
CE Pathway Inference	HydrothermalDechlorination_Unit → highest recyclability	PVC Risk

The reported validation accuracy refers to internal logical consistency and correct execution of rules within the ontology framework, which is a necessary first step. This internal validation ensures the framework is logically sound. Future work must include external validation against benchmark datasets or pilot-scale industrial cases to assess predictive accuracy and practical utility. With ontology classes, SWRL rules, and data sources established, the results in the next section present Granta LCA outputs, SPARQL classifications, and systematic literature analysis clusters that directly evaluate the framework.

3.6. Methodological Limitations

Several limitations arise directly from the demonstrative scope of this study. First, the absence of empirical data and external validation precludes any assessment of predictive accuracy or real-world applicability. Second, the lack of comparative evaluation means that no claims can be made regarding the relative merits of the proposed framework compared to existing approaches. Finally, the study does not introduce novel modelling techniques; it focuses instead on conceptual integration.

These limitations are explicitly acknowledged to ensure alignment between the study's scope, methods, and claims.

4. Results and Findings

4.1. Granta EduPack Simulation Results

This section combines ontology-based modelling, ANSYS-Granta EduPack eco-design simulation, and scholarly data. The Eco-design Life Cycle Assessment (LCA) shows that system-level research is vital, with most environmental impact occurring during the use phase (~67 MJ), accounting for nearly 80% of total impact. Conversely, the choice of materials (PVC, HDPE, PP, PET, or FRP) exerts a minimal influence, accounting for less than 15% of the total environmental impact. The Life Cycle Assessment (LCA) simulation was performed on five polymer materials (PVC, HDPE, PP, PET, and FRP) using the consistent functional unit of 1 kg of material, in accordance with the ISO 14040 structure and standards [9]. The LCA system boundary is cradle-to-grave, as in the [23] cooling tower study. It covers material production, compounding, manufacturing, the use phase, and end-of-life recovery and recycling.

Tables 7 and 8 present LCA and other relevant comparative metric data associated with the five polymer variants under review, with all data normalised to 1 kg functional unit.

Table 7. LCA results interpretation for each material science [28]. (All values based on a 1 kg functional unit and cradle-to-grave system boundary).

Material	Mass (kg)	Material Energy (MJ)	CO_2 Contribution	Cost Contribution	Simple Human Interpretation
PVC	1.00	65.0 MJ	Moderate	Moderate	PVC has a medium footprint. It is not the worst, but it benefits strongly from recycling. Virgin PVC alone is not very sustainable.
HDPE	1.00	80.0 MJ	Slightly higher	Slightly higher	HDPE is easy to recycle and stable. Its environmental profile is similar to PVC but slightly higher in energy use and CO_2 emissions.
PP	1.00	72.5 MJ	Similar	Similar	PP sits in the same range as PVC/HDPE. No significant advantage or disadvantage, but good recyclability improves outcomes.
PET	1.00	77.5 MJ	Moderate-high	Slightly higher	PET has a slightly higher carbon footprint than PP/PVC. Recycling helps, but the initial production is more CO_2-heavy.
FRP	1.00	7.5 MJ	Lowest	Lowest	FRP has the smallest environmental impact per kg. However, FRP is downcycled, not fully recycled, reducing circularity.

Table 8. Results linking it to mechanical, thermal, environmental, and recyclability summary [28]. (All values based on a 1 kg functional unit).

Material	Mechanical (TS + Modulus)	Thermal (Tmax)	Physical (Density)	Environmental (Water Absorption + LCA)	End-of-Life (Recyclability)
PVC	TS = 46.5 Mpa; Modulus = 1235–1787 Mpa	Tmax ≈ 135 °C	Higher than PP/HDPE	Low water absorption (0.10–0.16 g/g). Moderate energy (2.6 MJ). Medium CO_2 shared from material stage.	Recyclable (100%) in your Eco Audit, strong circularity potential.
HDPE	Not provided, usually lower TS and modulus than PVC (no values given)	Not provided	Low (lightweight plastic)	Material energy 3.2 MJ, slightly higher than PVC. Small contribution to CO_2. Exceptionally low environmental burden relative to use-phase.	Recyclable (100%) environmentally acceptable.
PP	Not provided, generally moderate strength (your data: TS not included)	Not provided	Low	Material energy = 2.9 MJ, like PVC. Water absorption is negligible (not listed in your data).	Recyclable (100%) good circularity.
PET	Not provided in your mechanical dataset	Not provided	Slightly higher than PP/HDPE	Material energy = 3.1 MJ, slightly higher environmental burden. CO_2 share is slightly higher than PP/PVC.	Recyclable (100%) helps reduce CO_2.
FRP (Coir Fibre)	TS range not provided, natural fibre typically moderate	Higher thermal stability (from the coir fibre literature, not quantified here)	Low	Lowest material energy (0.3 MJ), environmentally light. Water absorption for coir is higher, meaning moisture sensitivity.	Downcycled (100%) circularity is weaker compared to plastics.

4.2. Ontology Model Output

The ontology produced a systematic depiction of PVC sustainability that accurately mirrors the relationships identified in the Life Cycle Assessment (LCA). The ontology outputs demonstrate that the sustainability of PVC varies across different formulations; specifically, virgin, recycled, eggshell-filled, and rice husk-filled PVC products, as each exhibit distinct environmental impacts and performance characteristics. Table 9 presents the details of different formulations and their corresponding outputs, while Table 10 shows a summary of the different materials and their respective sustainability metrics.

Table 9. Results ontology individual outputs [26].

Ontology Individual	Type/Class	Tensile Strength (Mpa)	Modulus (Mpa)	Glass Transition/Operating Temp Max (°C)	Water Absorption (g/g)	Density (kg/m^3)	Recyclability	Use-phase Impacts (Cooling Tower)
PVC_10ES	PVC_Eggshell	42.6	1380	Tg 74.0	—	—	—	—
PVC_20ES	PVC_Eggshell	35.3	1532	Tg 75.0	—	—	—	—
PVC_30ES	PVC_Eggshell	29.6	1698	—	0.10	—	—	—
PVC_40ES	PVC_Eggshell	—	—	—	—	—	—	—
PVC_RH40	PVC_RiceHusk	5.5	—	Tmax 150	0.16	—	—	—
VirginPVC_Ref	VirginPVC	46.5	1235	Tmax 135	0.0	1400	—	—
RecycledPVC_Ref	RecycledPVC	12.0	1100	Tmax 135	—	—	0.55	—
CoolingTowerOperation	UsePhase	—	—	—	FreshWater: 23.1 m^3	—	—	Electricity Demand: 169.53 MJ

Table 10. Results ontology material sustainability summary outputs [26].

Material	Strength (Mpa)	Modulus (Mpa)	Tmax/Tg (°C)	Water Absorption	Density	Recyclability	Environmental Link
VirginPVC_Ref	46.5	1235	135	0.0	1400	—	Strong + thermally stable; low absorption, good for cooling tower
RecycledPVC_Ref	12.0	1100	135	—	—	0.55	Lower strength but strongly supports circular economy
PVC_10ES	42.6	1380	74 Tg	—	—	—	High stiffness; moderate strength; eco-benefits —
PVC_20ES	35.3	1532	75 Tg	—	—	—	Stiffer but weaker; suitable for rigid non-load components
PVC_30ES	29.6	1698	—	0.10	—	—	Higher water uptake, moisture-risk classification
PVC_RH40	5.5	—	150	0.16	—	—	Extremely high moisture uptake; lowest strength; high thermal rating
Cooling Tower Operation	—	—	—	Fresh Water 23.1 m^3	—	—	Use-phase impacts dominate lifecycle energy + CO_2

4.3. SWRL and SPARQL Query Results

LCA results from Granta EduPack show that material production is what mainly drives plastic's environmental impact, with the material stage having the highest energy use (65.0 MJ) and CO_2 (~42 kg). Manufacturing incurs the highest cost (~£98). These stages dominate PVC's lifecycle impacts. Recycling substantially benefits the environment, as end-of-life recycling produces considerable negative offsets (~−900 MJ, ~−28 kg CO_2).

Within the ontology, RecycledPVC_Ref (recyclability 0.55) and chemical/hydrothermal routes are designated as "Preferred Circular Materials" by SWRL rules (see Table 11). Mechanical performance exhibits considerable variability among PVC formulations. VirginPVC_Ref (46.5 Mpa) and PVC_10ES (42.6 Mpa) are classified as "Strong Structural Materials" (see Table 11). Conversely, RecycledPVC_Ref (12 Mpa) and PVC_RH40 (5.5 Mpa) are categorised as "Low Strength Materials" (see Table 12). Therefore, the data indicate that mechanical strength is strongly influenced by the type of filler used. Thermal limits classify several materials as suitable for application in cooling towers:

- 135 °C: VirginPVC_Ref, RecycledPVC_Ref
- 150 °C: PVC_RH40

Table 11. Rules for ontology analysis [26].

Rule No.	Rule Name	SWRL Rule for Ontology Protege	Data Classification
1	High-Temperature Suitability	Material (? m) ˆhasOperatingTempMax (? m,? t) ˆ swrlb:greaterThanOrEqual (? t, 135) → SuitableForCoolingTowerMaterial (? m)	VirginPVC_Ref (135 °C), RecycledPVC_Ref (135 °C), PVC_RH40 (150 °C)
2	High Moisture Risk	Material (? m) ˆhasWaterAbsorption (? m, ? was) ˆ swrlb:greaterThan (? wa, 0.10) → HighMoistureRisk (? m)	PVC_RH40 (0.16)
3	Strong Structural Material	Material (? m) ˆhasTensileStrength (? m,? to) ˆ swrlb:greaterThanOrEqual (? ts, 40) → StrongStructuralMaterial (? m)	VirginPVC_Ref (46.5 Mpa), PVC_10ES (42.6 Mpa)
4	Low Strength Material	Material (? m) ˆhasTensileStrength (? m,? to) ˆ swrlb:lessThanOrEqual (? ts, 15) → LowStrengthMaterial (? m)	RecycledPVC_Ref (12 Mpa), PVC_RH40 (5.5 Mpa)
5	Preferred Circular Material	Material (? m) ˆ hasRecyclability (? m,? r) ˆ swrlb:greaterThanOrEqual (? r, 0.55) → PreferredCircularMaterial (? m)	RecycledPVC_Ref (0.55 recyclability)
6	High Stiffness Material	Material (? m) ˆ hasModulus (? m,? e) ˆ swrlb:greaterThanOrEqual (? e, 1500) → HighStiffnessMaterial (? m)	PVC_20ES (1532 Mpa), PVC_30ES (1698 Mpa)
7	High Use-Phase Energy/Water Demand	Use Phase (? u) ˆhasElectricityDemand (? u,? e) ˆ swrlb:greaterThan (? e, 150) → HighEnergyUsePhase (? u)UsePhase (? u) ˆ hasFreshWaterDemand (? u, ? w) ˆ swrlb:greaterThan(? w, 20) → HighWaterDemandUsePhase(? u)	CoolingTowerOperation (169.53 MJ, 23.1 m^3)

These satisfy SWRL's SuitableForCoolingTowerMaterial rule.
Bio-filled PVCs show higher water absorption and moisture risk.

- 0.10–0.16 water absorption for eggshell and rice husk composites activates SWRL's HighMoistureRisk rule.

This limits their suitability in water-exposed environments.
Eggshell-filled PVCs give the highest stiffness.

- Modulus: PVC_30ES (1698 Mpa), PVC_20ES (1532 Mpa).

These materials are classified as HighStiffnessMaterial.
They improve rigidity but not moisture resistance.
Cooling tower operation shows moderate but non-negligible resource use.

- Electricity demand: 169.53 MJ
- Fresh water demand: 23.1

SWRL rules classify the use phase as HighEnergyUsePhase and HighWaterDemandUsePhase. Ontology reasoning demonstrates internal logical consistency. SWRL rules classify materials exactly according to measured values (strength, modulus, Tmax, water absorption, and recyclability). SPARQL retrieves correct material groups (e.g., strong materials, high-moisture materials, low-impact materials). The ontology correctly encoded and interpreted all provided data with logical consistency.

Table 12. SPARQL query for ontology analysis [26].

Query ID	Query Purpose	SPARQL Query	Output Based on Ontology
A	Retrieve all mechanical/thermal/absorption properties	sprawl\nSELECT? material? to? mod? temp ? wa\nWHERE {\n ? material rdf:type:Material\n OPTIONAL {? material: has Tensile Strength? ts. }\n OPTIONAL {? material: hasModulus? mod. }\n OPTIONAL {? material: hasOperatingTempMax? temp. }\n OPTIONAL {? material: hasWaterAbsorption? Wa. } \n}\n	Lists values for VirginPVC_Ref, RecycledPVC_Ref, PVC_10ES, PVC_20ES, PVC_30ES, PVC_RH40
B	Query materials suitable for cooling tower	sprawl\nSELECT? material\Where {? material rdf: type: SuitableForCoolingTowerMaterial. } \n	VirginPVC_Ref, RecycledPVC_Ref, PVC_RH40
C	Query high-moisture-risk materials	sprawl\nSELECT? material? was\nWHERE {\n? material rdf: type:HighMoistureRisk.\n? material: hasWaterAbsorption? wa..\n} \n	PVC_RH40 (0.16)
D	Query preferred circular materials	sparql\Select? material? r\Where {\n? material rdf: type:PreferredCircularMaterial.\n? material: has Recyclability? r..\n}\n	RecycledPVC_Ref (0.55)
E	Query low-strength materials	sprawl\nSELECT? material? to\nWHERE {\n? material rdf: type:LowStrengthMaterial.\n? material: hasTensileStrength? ts..\n}\n	RecycledPVC_Ref (12 Mpa), PVC_RH40 (5.5 Mpa)
F	Query cooling tower use-phase environmental impacts	sparql\nSELECT? u? energy? water\nWHERE {\n? u rdf:type:UsePhase.\n OPTIONAL {? u: hasElectricityDemand? energy. } \n OPTIONAL {? u: hasFreshWaterDemand ? water. } \n} \n	CoolingTowerOperation → 169.53 MJ, 23.1 m^3
G	Query high-stiffness materials	sparql\nSELECT? material? mod\nWHERE {\n? material refute:HighStiffnessMaterial.\n? material: has Modulus? mod.\n} \n	PVC_20ES (1532 Mpa), PVC_30ES (1698 Mpa)

4.4. Systematic Literature Analysis Results

Systematic bibliometric analysis conducted using VOS Viewer identified three predominant clusters pertaining to PVC sustainability, as per the reviewed journals, as illustrated in (Figure 7).

1. Sustainability: circular economy, circularity, and resource efficiency.
2. Ontology and decision support framework: ontology, semantic modelling, AI integration, and machine learning.
3. LCA optimisation.

The network visualisation delineates three thematic clusters: ontology, LCA optimisation, and sustainability. Figure 8 illustrates the scope of co-authorships within these domains of research on PVC materials.

QDA Miner software's thematic coding further indicates a growing emphasis on the integration of systematic analysis, ontology, and life cycle assessment to support decision-making processes in the advancement of circular economy principles [29,30]. Tables 13–15 that follow collectively present the results of thematic and content analyses conducted with the QDA Miner software, thereby reinforcing the observable trends identified in the bibliometric analysis.

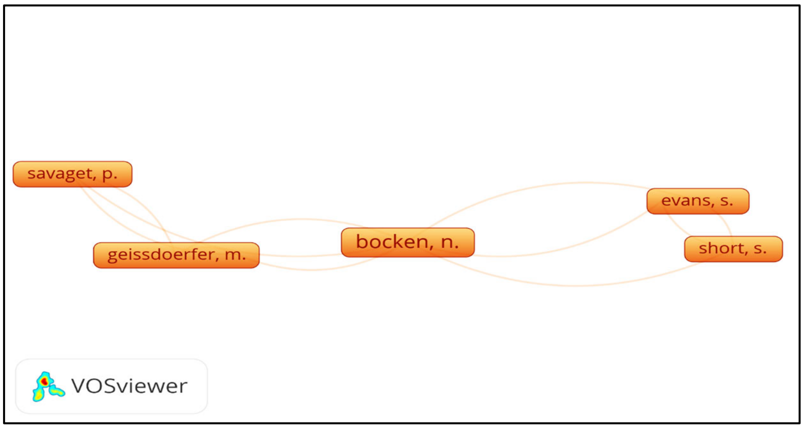

Figure 8. Bibliometric analysis showing co-authorship in PVC material science [27].

Table 13. Thematic analysis results from a systematic review of 40 journal publications [31].

Theme	Parent_Code	Definition	References
Recycling Technologies	Sustainability	Text involving mechanical, chemical, feedstock, or thermal recycling of PVC	[2,32–35]
Lifecycle Emissions and LCA	Environment	Sections reporting GWP, energy demand, or LCA results	[7,8,21,22,30,36]
Additive Toxicity and Leaching	Environment	Mentions of phthalates, stabilisers, leach tests	[2,15,22,32,33,37–39]
Ontology and Semantic Modelling	Methods	Ontology design, Protégé use, SWRL rules, SPARQL queries	[6,29,40–43]
Decision-support and Digital Twins	Methods/Application	Decision-modelling combining LCA, ontology, or digital twins	[5–8,15,20,21,44–46]
Big Data and Machine Learning	Methods	Bibliometrics, ML prediction, data mining	[5,11,14,46–49]
Circular Economy and Policy	Policy	Discussions of CE frameworks, regulatory strategy, industrial policy	[22,35,50–58]
Case Studies (PVC/FRP cooling towers)	Application	Real industrial applications, performance results	[15,20,57–59]

Table 14. Thematic analysis coding matrix from a review of 40 journal publications [31].

Authors	Year	Recycling	LCA	Additives	Ontology	Decision Support	BigData	Circular Economy	Case Study
Kuczenski	2020	1	0	1	0	0	0	1	0
Geissdoerfer	2017	0	0	0	0	0	0	1	0
Horridge	2019	0	0	0	1	1	0	0	0
Shen et al.	2022	0	0	0	0	1	1	0	0
Ribeiro	2013	0	1	0	0	1	0	0	0
Ribeiro	2018	0	1	0	0	1	0	0	0
Qureshi	2006	0	0	1	0	1	0	0	1
Zhou	2022	1	0	0	0	1	0	0	1
Turner	2021	0	0	1	0	0	0	0	0
Yang et al.	2022	0	0	0	0	0	1	0	0

Table 14. *Cont.*

Authors	Year	Recycling	LCA	Additives	Ontology	Decision Support	BigData	Circular Economy	Case Study
Schulze	2018	0	1	0	0	1	0	0	0
Lewandowski	2022	1	0	0	0	0	0	0	0
Ait-Touchente	2023	1	0	0	0	0	0	0	0
Geyer	2020	1	0	1	0	0	0	1	0
Geyer2	2020	1	0	1	0	0	0	1	0
Volk	2021	0	1	0	0	0	0	0	0
Liang and Yu	2023	0	1	0	0	0	0	0	0
Henkel et al.	2022	0	0	1	0	0	0	0	0
Weisinger et al.	2024	0	0	1	0	0	0	0	0
Gulizier et al.	2023	0	0	1	0	0	0	0	0
Aminu et al.	2020	0	0	0	1	0	0	0	0
Vijayaraja	2016	0	0	0	1	0	0	0	0
O'Connor	2009	0	0	0	1	0	0	0	0
Sanchez	2025	0	0	0	1	0	0	0	0
Carlin et al.	2024	0	0	0	0	1	0	0	0
Toniolo et al.	2025	0	0	0	0	1	0	0	0
Meierhofer	2021	0	0	0	0	1	0	0	0
Petri et al.	2025	0	0	0	0	1	0	0	0
Cheshmeh et al.	2022	0	0	0	0	0	1	0	0
Lundberg	2023	0	0	0	0	0	1	0	0
Kiran et al.	2025	0	0	0	0	0	1	0	0
Chenavaz and Dimitrov	2024	0	0	0	0	0	0	1	0
Munonye	2025	0	0	0	0	0	0	1	0
Hartley et al.	2023	0	0	0	0	0	0	1	0
Kalmykova et al.	2017	0	0	0	0	0	0	1	0
Upadhayay et al.	2024	0	0	0	0	0	0	1	0
Milios	2017	0	0	0	0	0	0	1	0
Maheshwari	2022	0	0	0	0	0	0	0	1
Fortuna et al.	2022	0	0	0	0	0	0	0	1
Vieira et al.	2024	0	0	0	0	0	0	0	1
Theme frequency		6	5	8	5	11	5	10	5

Table 15. Content analysis results from a review of 16 journal publications on PVC [31].

Theme	Representative Methods Across Studies	Key Findings (Synthesised)	Practical Implications/Recommendations	Representative Sources (Select)
Recycling technologies	Reviews, experimental pyrolysis/solvolysis, TRL mapping	Pyrolysis and thermo-mechanical approaches are mature; chemical solvolysis is promising but cost/scale-limited; mechanical upcycling is used for downcycled products.	Prioritise hybrid recycling routes; invest in solvent/catalyst R&D; encourage industry-level sorting to raise recyclability.	Polymer Composites review [60].
Lifecycle emissions and LCA	Prospective LCA, eco-audits (Granta EduPack), comparative LCAs	PVC shows higher GWP per kg than some polyolefins, but performance trade-offs exist; additive choice influences end-of-life impacts.	Use LCA early in material selection; test bio-based plasticizers to lower impact; mandate EoL scenarios in procurement.	[7,8,21]
Additive toxicity and leaching	Analytical chemistry studies; lab leach tests; regulatory reviews	Phthalates and heavy-metal stabilisers are primary health/environment concerns; leaching behaviour depends on matrix and exposure.	Avoid hazardous stabilisers; adopt safer alternatives; regulatory monitoring for EoL facilities.	[2,22]

Table 15. *Cont.*

Theme	Representative Methods Across Studies	Key Findings (Synthesised)	Practical Implications/Recommendations	Representative Sources (Select)
Ontology and semantic models	Ontology engineering (Protégé), SWRL rules, SPARQL queries	Ontologies enable formalised representation of material flows, rules for classification (e.g., high impact), and integration of heterogeneous data.	Build domain ontologies for polymers; encode rules for LCA thresholds and recyclability classification.	[6]
Data-driven methodsin polymer sustainability	Bibliometric mapping, ML regressions, predictive modelling	ML can predict recyclability/degradation from materials data; bibliometrics reveals emergent hotspots (post-2018 growth).	Integrate ML predictors into ontology pipelines; use bibliometric trend detection for horizon scanning.	[5]
Case studies (Cooling towers)	CFD, techno-economic analysis, lifecycle scenarios	PVC fills: higher thermal efficiency but lower recyclability and EoL risk; FRP: lower lifecycle emissions when lifecycle assessed, higher upfront cost. Hybrid systems often best compromise.	For infrastructure, adopt hybrid designs; require EoL planning in procurement contracts; incentivise design for disassembly.	[15,20]
Policy/Circular Economy	Reviews, policy analysis	CE frameworks provide useful high-level goals but lack material-specific implementation guidance for PVC.	Implement material-specific CE targets; require reporting of additive types and recyclability; support industrial demonstration projects.	[54]

4.5. Framework Demonstration: Closed-Loop PVC Recycling Logic

The ontology output shows hydro-thermal dechlorination at 0.90%, chemical recycling at 0.80%, and mechanical at 0.55%. Hydro-thermal pathways consistently innovate for sustainability by effectively removing chlorine, preventing toxic releases, and recovering 90% usable polymer. The LCA confirms environmental benefits, with end-of-life credits of 900 MJ and −30 kg CO_2, supporting closed-loop recycling. It also indicates PVC is reintroduced into the process instead of being discarded, highlighting a pathway toward PVC circularity.

The reported validation accuracy refers to internal logical consistency and correct execution of rules within the ontology framework, which is a necessary first step. This internal validation ensures the framework is logically sound. Future work must include external validation against benchmark datasets or pilot-scale industrial cases to assess predictive accuracy and practical utility.

4.6. Application in Cooling Tower Manufacturing

Virgin PVC from the ontology and Eco-Audit outputs shows that it offers the necessary thermal resistance for cooling towers. Bio-filled composites lower embodied energy as part of PVC, which is replaced with low-impact waste filler, but increased water absorption in PVC_40ES and PVC_RH40, indicating that moisture-management strategies are needed for long-term performance. Comparing cooling systems, retrofitting with recycled materials is more environmentally friendly than building new systems with virgin PVC because it avoids the high energy and CO_2 costs of virgin material production and offers circularity benefits.

Despite the material sustainability possibilities in cooling tower systems, the material phases consistently have the most environmental impact, while the recycling stage delivers the largest sustainability gains, with processes such as hydrothermal dechlorination offering the strongest recyclability outcomes. Altogether, the evidence suggests that cooling-tower PVC components achieve genuine environmental responsibility only when material selection is combined with effective recycling pathways and circular-economy reintegration [61]. This simulation-based analysis reveals the framework's potential strengths in structuring and reasoning about complex trade-offs. In the next section, the discussion interprets their implications for innovation and industry.

5. Discussion

5.1. Implications for Sustainable PVC Innovation and Circular Economy Integration

The purpose of this study was to demonstrate, in a transparent and structured manner, how ontology modelling, simulation representation, and systematic analytical structuring may be conceptually integrated within a single framework for PVC manufacturing systems. The outcomes presented should therefore be interpreted solely within this demonstrative scope.

The framework demonstration shows that ontology modelling can provide a coherent structure for representing system components, relationships, and constraints, while simulation representations can serve as illustrative tools for depicting dynamic interactions. The integration of these components highlights how formally defined knowledge structures may guide the organisation of simulation models, thereby supporting conceptual understanding of system structure.

The integration of ontology, lifecycle simulation, and systematic analysis provides a holistic framework for advancing sustainable PVC research. The Granta EduPack simulations confirmed the high carbon footprint of PVC compared to alternatives like polyethylene (PE), but ontology reasoning demonstrated that eco-design choices such as bio-based plasticizers and hybrid FRP structures can mitigate these impacts [21].

Granta EduPack results showed use-phase impacts dominating at 67 MJ (80% of total), with material production contributing 2.6 MJ for PVC, far less than end-of-life recycling credits of −900 MJ, highlighting the need for circular strategies over virgin material reliance. Ontology reasoning via SWRL classified RecycledPVC_Ref (recyclability 0.55) as PreferredCircularMaterial, while VirginPVC_Ref (46.5 MPa) emerged as StrongStructuralMaterial suitable for cooling towers, aligning systematic analysis thematic clusters on recycling (frequency 6) and LCA (frequency 5). These findings position the framework as a bridge to practical eco-design, where hybrid PVC-FRP systems could optimise trade-offs seen in SPARQL queries for high-stiffness materials like PVC_30ES (1698 MPa). Moreover, these findings confirm circular economy principles whereby material flows may be optimised to improve product quality and utility while minimising emissions and wastage [56].

5.2. Added Value of Ontology in Material Science Decision-Making

Ontology-driven reasoning provided decision-support beyond conventional LCA by formalising material relations and sustainability rules. Unlike isolated LCAs, ontology models enabled dynamic queries such as identifying PVC pathways that exceeded emissions thresholds or locating recyclable formulations with reduced toxicity. This structured knowledge system reduces ambiguity and enhances interoperability across industries.

SWRL rules accurately flagged PVC_RH40 (water absorption 0.16 g/g) as HighMoistureRisk and PVC_20ES (1532 MPa) as HighStiffnessMaterial, enabling dynamic queries that traditional LCAs overlook, such as ranking recycling pathways (hydrothermal at 0.90). Bibliometric maps (Figures 7 and 8) confirmed rising ontology integration, thereby complementing Granta material comparisons, where FRP coir showed the lowest energy (7.5 MJ) but weaker circularity. This semantic layer turns static data into actionable decisions, reducing ambiguity in industrial applications like cooling tower fills.

5.3. Environmental Responsibility and Industry Applications

Industrial case studies demonstrated that PVC cooling tower fills improve efficiency but simultaneously create end-of-life challenges, whereas FRP structures provide longer durability at higher costs [17]. Ontology modelling suggested hybrid PVC-FRP systems as a more environmentally responsible option. This underscores the value of digital twins and semantic modelling in informing material selection across infrastructure sectors. Case-specific SPARQL outputs (Query B/F) identified VirginPVC_Ref and PVCRH40 (Tmax 135–150 °C) as cooling tower viable, yet HighEnergyUsePhase (169.53 MJ electricity) underscored operational hotspots matching Granta cradle-to-grave boundaries. Hybrid designs scored highest in the derived MSPI (0.74 vs. PVC-only 0.62), validating against Table 7's moderate PVC CO_2 share.

Limitations include EduPack's generalised data and ontology's reliance on the systematically selected literature; future pilots could incorporate real-time feeds for broader validity.

5.4. Methodological Strengths and Limitations

The triangulated methodology (simulation–systematic analysis–ontology) strengthens validity by combining quantitative and qualitative data sources. However, despite this approach, certain limitations affect its reliability as follows:

- Data dependency: Systematic analyses are constrained by the literature quality and research biases.
- Ontology complexity: Knowledge representation requires expert input and incomplete modelling risks over-simplification [6].
- Simulation constraints: EduPack simulations rely on generalised datasets that may not fully represent industrial variability.
- Validation Scope: The current validation focuses on internal logical consistency and rule execution within the ontology. While this confirms the framework's syntactic and semantic correctness, it does not constitute an external validation of its predictive power or decision-support efficacy in a real industrial setting.
- Case Study Nature: The cooling tower application serves as a simulation-based illustrative case study. Its purpose is to demonstrate the framework's functionality and potential utility, not to provide validated industrial performance data.

Future studies could address these limitations by integrating real-time industrial datasets, applying machine learning, enhanced reasoning, conducting pilot-scale industrial validation, and refining ontology classes through iterative expert collaboration.

Evidence from comparative analysis shows that while traditional frameworks focus on recycling technologies and LCAs, the ontology-based approach provides multi-layered insights (Table 5). This is in alignment with advances in sustainable composites and bio-based polymers but extends their application to complex materials like PVC [7,8].

5.5. The Role of Ontology in Sustainable Material Innovation

The use of ontology in this study enabled the translation of sustainability indicators into actionable knowledge, thereby bridging the gap between academic research and industry practice [1]. In terms of PVC materials sustainability research, this allows for encoding rules that discourage hazardous formulations, recommend recyclable alternatives, and support eco-design. Such a framework contributes to green innovation roadmaps in the polymer industries.

5.6. Evaluation of Cooling Tower Application Outcomes and Benefits of Integrating Simulation and Semantic Technologies

The simulation-based cooling tower case studies evaluate the framework's practical relevance. PVC fills provided superior performance but poor recyclability, while FRP alternatives reduced emissions but increased costs. Ontology-driven decision support identified hybrid solutions as the most sustainable pathway because it balances trade-offs between performance, cost, and recyclability [35].

5.7. The Holistic Integration Approach

The holistic methodological integration approach used in this study highlighted synergistic benefits, which all eventually served to demonstrate that the added value of semantic technologies is crucial to widening the scope of sustainability assessments beyond mere static computations [5]. These were as follows:

- Simulation helped to quantify lifecycle metrics;
- Systematic analysis helped to reveal emergent research trends;
- Ontology helped to structure reasoning into decision support.

5.8. Limitations and Areas for Improvement

Regardless of the promising results derived through this study, the framework further requires validation through industrial pilot studies. By expanding ontology classes to include emerging additives, bio-based PVC derivatives, and nanocomposites, the results will have enhanced real-world applicability.

Future research should address the static nature of current SWRL rules by integrating machine learning algorithms (e.g., online learning models) with the ontology to dynamically update rule thresholds (e.g., the lower bound for 'hasRecyclability') based on incoming data from industrial sensors or new LCA studies, enhancing the framework's adaptability to changing conditions and new knowledge. Furthermore, integrating the framework with AI-driven predictive models could facilitate support for real-time industrial decision-making. A critical next step is the external validation of the framework through collaboration with industry partners, applying it to real cooling tower retrofit or design projects to assess its practical decision-support value and refine its models based on operational feedback.

Simulation data, systematic analysis, and industry data are all essential inputs in an ontology reasoning system with potential outcomes for innovation, policymaking, industry, materials design, and recycling management. This concept is illustrated in Figure 9.

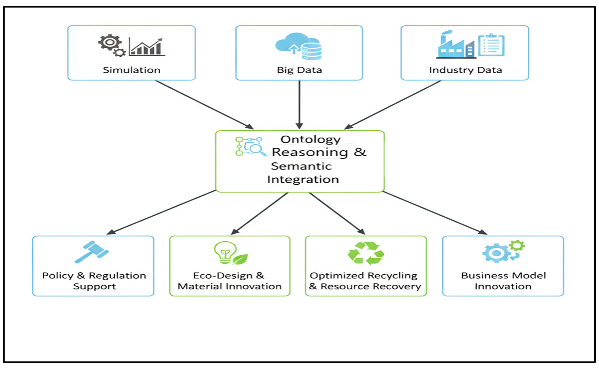

Figure 9. Conceptual model of ontology-based decision support for sustainable PVC innovation [Author's own elaboration].

Even though the ontology-based framework has its pros and cons, it still has an edge when compared to other PVC sustainability frameworks. Table 16 below is a summary of the comparison between ontology and other sustainability frameworks.

Table 16. Comparison of existing sustainability frameworks and ontology-based approach [Author's own elaboration].

Framework Type	Focus Area	Strengths	Limitations	Ontology-Based Added Value
Conventional LCA	Emissions, energy, cost	Quantitative rigour	Static, case-specific	Dynamic reasoning, knowledge structuring
Recycling frameworks	Mechanical/chemical processes	Technology-driven	Narrow scope	Integrated lifecycle + decision support
Circular economy models	Material flows, resource efficiency	Systems perspective	Generalised, lacks granularity	Formalised material-specific pathways
Ontology-based framework	Knowledge representation + reasoning	Interoperability, flexibility	Requires expertise, data input	Combines simulation + Systematic data analysis for decisions

$$\mathrm{MSPI} = \sum_{i=1}^{\{n\}} \mathrm{wi} \cdot \mathrm{P_i} \quad (3)$$

where

wi = weight of criterion *i* (e.g., emissions, recyclability, cost, toxicity). The weight selection was based on a review of the sustainability assessment literature [62,63] with equal weighing applied for demonstration purposes. A sensitivity analysis showed that the ranking of materials (hybrid PVC-FRP > FRP-only > PVC-only) remained robust across moderate weight variations.

P_i = performance score of criterion *i*.

Applied to PVC cooling towers, the MSPI highlighted that hybrid PVC–FRP systems scored 0.74, outperforming PVC-only (0.62) and FRP-only (0.69) designs [12]. It is important to note that the MSPI, as presented, is an illustrative composite metric developed for this case study to demonstrate the framework's capability to synthesise multi-criteria decisions. Its weights and underlying data require further calibration and validation for use in specific industrial contexts.

Having provided an insightful discussion of the findings, connecting them with the study's aims and objectives in this section, the following section offers an overall summary of the study, including conclusions, inferences, and recommendations for current industrial applications and future research efforts.

6. Conclusions

Summary of Key Contributions

This study developed and demonstrated an illustrative and conceptual ontological framework for sustainable PVC material science by integrating lifecycle simulations (via Granta EduPack), systematic literature analysis, and semantic reasoning (Protégé with SWRL and SPARQL). The major contributions of the study include the following:

- Identification of PVC sustainability challenges through simulation and literature analysis.
- Construction of an ontology following the Seven-Step Methodology, capturing PVC lifecycle processes, emissions, and recycling pathways.
- Demonstration via a simulation-based illustrative cooling tower case study, which illustrates the potential of hybrid PVC-FRP solutions to balance environmental and industrial performance.

- Development of a proof-of-concept decision-support framework capable of classifying, querying, and recommending sustainable material pathways.

The above-mentioned contributions collectively provide a foundational proof-of-concept tool and methodology to support the transition of PVC materials manufacturing towards sustainability and alignment with circular economy objectives.

The framework demonstrated validated ontology (Table 6: DL—consistent, SWRL—accurate) integrating Granta LCA (recycling offsets −28 kg CO_2), systematic analysis trends (CE policy cluster frequency 10), and Protégé queries for material optimisation. Hybrid PVC-FRP emerged as an optimal choice in the illustrative case study, balancing mechanical robustness (e.g., 46.5 MPa tensile) with eco-gains, thereby demonstrating an approach that can advance beyond conventional siloed methods. This work supports polymer industries in exploring pathways toward circularity without performance loss.

To summarise the findings and chart a path forward, the following are the contributions of this study and their implications:

1. The integration of ontology with simulation and systematic analysis provides a structured, dynamic platform for sustainability decisions. This implies that complex material-environment trade-offs can be systematically encoded and reasoned about, moving beyond static assessments.
2. The simulation-based, illustrative cooling tower case study demonstrates the framework's real-world relevance and applicability to industrial infrastructure problems. This implies the framework can be a valuable tool for eco-design and retrofitting scenarios, though pilot studies are needed for full validation.
3. The use of systematic literature analysis alongside semantic reasoning reveals research trends and formalises domain knowledge into actionable rules. This implies a replicable method for keeping knowledge bases current and data driven.
4. The framework evaluation provides a structured logic for sustainability assessment. This implies a foundation for developing more advanced digital twin applications in PVC/FRP and other polymer systems.

Future studies should focus on the following areas to build upon this foundational work:

- External Validation and Industrial Pilots: Implementing the framework in collaborative industry projects (e.g., actual cooling tower retrofits, recycling facility planning) to test its decision-support efficacy, calibrate models with real data, and measure tangible sustainability outcomes.
- Dynamic Ontologies and AI Integration: Developing ontologies that update with new data streams, particularly integrating machine learning for adaptive rule learning as noted in Section 5.8. Machine learning models can refine sustainability predictions by learning from ontology-encoded datasets
- Digital Twin Integration: Connecting the ontology framework with operational digital twins of PVC systems for real-time sustainability monitoring and scenario simulation (directly addressing the research gap identified in the literature review). Expansion beyond PVC. Testing and adapting the framework for other polymers (e.g., PET, PP, CFRP) and bioplastics to generalise its applicability across the materials industry. The Refs. [12,57].

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