School of Chemical and Environmental Engineering

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Integration of Innovative Energy Efficient Technologies in Buildings and Neighborhoods

A Thesis Submitted in partial fulfillment of the requirements for the degree of

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by

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During the preparation of this thesis, I utilized artificial intelligence tools to improve the readability, grammar, and formatting of the text. The use of these tools was strictly limited to language enhancement and did not extend to the creation or modification of the substantive content, ideas, data analysis, or conclusions presented herein. All intellectual contributions, including research methodology, interpretations, and arguments, remain entirely my own.

Περίληψη

Η παρούσα διατριβή αναπτύσσει και αξιολογεί μια καινοτόμο αρχιτεκτονική βασισμένη σε Γράφους Γνώσης (Knowledge Graph - KG), ενσωματωμένη σε ένα πλαίσιο Ψηφιακού Διδύμου (Digital Twin - DT), σχεδιασμένη για την ενίσχυση των δυνατοτήτων διαχείρισης δεδομένων και γνώσης σε κλίμακα κτιρίου και γειτονιάς. Κίνητρο αποτέλεσαν οι περιορισμοί των παραδοσιακών μεθόδων διαχείρισης δεδομένων, ιδιαίτερα στην αντιμετώπιση αποσπασματικής και δυναμικής αστικής πληροφορίας. Η προτεινόμενη αρχιτεκτονική αξιοποιεί προσαρμοσμένα οντολογικά μοντέλα που θεμελιώνουν διασυνδεδεμένες σχέσεις και ιεραρχικές δομές, επιτρέποντας σημασιολογική διαλειτουργικότητα, συγκειμενοποιημένη συλλογιστική και ενοποίηση στατικών και δυναμικών ροών δεδομένων. Ο βασικός πυρήνας της καινοτομίας έγκειται στην ενσωμάτωση σημασιολογικών Γράφων Γνώσης εντός ενός πλαισίου Ψηφιακού Διδύμου, ώστε να υποστηρίζεται η λήψη αποφάσεων από εμπλεκόμενους φορείς (stakeholders). Σε αντίθεση με τις συμβατικές προσεγγίσεις που δυσκολεύονται να διαχειριστούν ασύνδετα ή μη συμβατά δεδομένα, η αρχιτεκτονική KG-DT προσφέρει ένα δομημένο, μηχανικά αναγνώσιμο μοντέλο για τις διαδικασίες σε επίπεδο κτιρίου και γειτονιάς. Υποστηρίζει την πλήρη συγκειμενοποίηση δεδομένων, προηγμένα ερωτήματα και διαφανή ανάλυση σεναρίων ανακαίνισης. Κεντρικό χαρακτηριστικό αποτελεί η χρήση SPARQL, που επιτρέπει στους χρήστες να εξάγουν πληροφορίες για ιδιότητες υλικών, ενεργειακή απόδοση και αποτελέσματα σεναρίων χωρίς χειροκίνητο φιλτράρισμα ή επανεκτέλεση προσομοιώσεων. Δύο μελέτες περίπτωσης τεκμηριώνουν την πρακτική αποτελεσματικότητα της προσέγγισης. Η πρώτη αφορά την ενσωμάτωση παραφινικών υλικών αλλαγής φάσης (PCM) σε γυψοσανίδες και τσιμεντοσανίδες, συνδυάζοντας πειραματικές μετρήσεις με προσομοιώσεις EnergyPlus. Τα αποτελέσματα επιβεβαίωσαν βελτιωμένη θερμική απόδοση και εξοικονόμηση ενέργειας έως και 22,3% για γυψοσανίδες με υψηλή περιεκτικότητα σε PCM, ειδικά όταν λαμβάνονται υπόψη τα φαινόμενα υστέρησης. Η δεύτερη μελέτη περιλάμβανε αξιολογήσεις Κόστους Κύκλου Ζωής (LCC) και Περιβαλλοντικού Αποτυπώματος Κύκλου Ζωής (LCA) για 17 σενάρια εγκατάστασης φωτοβολταϊκών και μπαταριών σε πανεπιστημιακή πανεπιστημιούπολη. Το βέλτιστο σενάριο, με διπλής όψεως φωτοβολταϊκά πάνελ και αποθήκευση ενέργειας σε μπαταρίες ιόντων λιθίου υπό στρατηγική αυτοκατανάλωσης, πέτυχε την βέλτιστη ισορροπία μεταξύ οικονομικής αποδοτικότητας και περιβαλλοντικής επίδοσης. Και στις δύο περιπτώσεις χρησιμοποιήθηκαν προσαρμοσμένες οντολογίες: ένα ελαφρύ, υλικοκεντρικό μοντέλο για το Leaf House και μια επεκτάσιμη, αρθρωτή δομή βασισμένη στα Brick και SAREF για την περίπτωση της πανεπιστημιούπολης του Πολυτεχνείου Κρήτης (TUC). Ο KG εμπλουτίστηκε με πειραματικά δεδομένα, αποτελέσματα προσομοιώσεων, μεταδεδομένα αισθητήρων και βασικούς δείκτες απόδοσης (KPIs). Συνολικά, το KG-DT πλαίσιο παρέχει ένα επεκτάσιμο και σημασιολογικά

εναρμονισμένο σύστημα υποστήριξης αποφάσεων, επιτρέποντας διαφανή, τεκμηριωμένο σχεδιασμό για βιώσιμες ανακαινίσεις γειτονιών και εφαρμογές σε μελλοντικές έξυπνες πόλεις.

Abstract

This thesis develops and evaluates an innovative Knowledge Graph (KG)-based architecture integrated within a Digital Twin (DT) framework, designed to advance data and knowledge management capabilities at the building and neighborhood scale. Motivated by the limitations of traditional data handling, particularly in dealing with semantically fragmented and dynamic urban data, the proposed architecture leverages tailored ontologies that establish interconnected relationships and hierarchical structures. This enables semantic interoperability, contextualized reasoning, and integration of static and real-time data streams. The core innovation lies in uniting semantic KGs within a DT framework to support stakeholder-driven decision-making. Unlike conventional approaches that struggle with disconnected and incompatible data, the KG-DT architecture provides a structured, machine-interpretable model of building and neighborhood-level processes. It facilitates end-to-end data contextualization, advanced querying, and transparent analysis of retrofit scenarios. SPARQL-based querying is a central feature, allowing users to extract insights on material properties, energy performance, and scenario outcomes without manual filtering or simulation reruns. Two case studies demonstrate the approach's practical effectiveness. The first involved the integration of paraffin-based phase-change materials (PCMs) in gypsum and cement boards, combining experimental testing with EnergyPlus simulations. Results confirmed improved thermal performance and up to 22.3% energy savings for high-PCM gypsum boards, especially under hysteresis modeling. The second case study applied LCC and LCA analyses to evaluate 17 PV + battery scenarios at a university campus. The optimal configuration, combining bi-facial PV modules with lithium-ion battery storage under a self-consumption strategy, achieved the best balance between economic and environmental performance. Both cases required tailored ontologies: a lightweight material-focused model for Leaf House, and a modular, extensible structure based on Brick and SAREF for the TUC campus. The KG was populated using a combination of measured data, simulations, sensor metadata, and performance indicators. Overall, the KG-DT framework provides a scalable and semantically aligned decision support system, enabling transparent, data-driven planning for sustainable neighborhood renovations and future smart city applications.

Publications

Publications in scientific journals directly related to the PhD thesis

1. Lygerakis F, Kampelis N, Kolokotsa D. Knowledge Graphs' Ontologies and Applications for Energy Efficiency in Buildings: A Review. Energies. 2022; 15(20):7520. https://doi.org/10.3390/en15207520
2. Lygerakis F, Gioti C, Gournis D, Yentekakis IV, Karakassides M, Kolokotsa D. Enhancing Building Energy Efficiency with Innovative Paraffin-Based Phase Change Materials. Energies. 2024; 17(16):4155. https://doi.org/10.3390/en17164155
3. Lygerakis, F., Kampelis, N., & Kolokotsa, D. (2025). *Knowledge graph (KG) centric decision support for green building neighborhood renovation scenario modeling* (Patent No. GR1009891). Technical University of Crete.
4. Lygerakis F, Kampelis N, Kolokotsa D. Knowledge Graph–Based Architecture for Neighborhood Renovation Decision Support Integrating Life Cycle Costing and Life Cycle Assessment. Advanced Engineering Informatics. 2025 (under revision). Preprint: https://dx.doi.org/10.2139/ssrn.5346595

Publications in international scientific conferences

1. Kampelis N, Lygerakis F, Kolokotsa D. Towards the development of a knowledge graph-based decision support framework for Green Building Neighborhoods. In: Rajagopalan P, Soebarto V, Akbari H, eds. Proceedings of the 6th International Conference on Countermeasures to Urban Heat Islands (IC2UHI). RMIT University; 2023:1-11.
2. Kampelis N, Lygerakis F, Kolokotsa D. Towards a Digital Twin-based conceptual framework for Green Building Neighbourhoods. Presented at: 14th National Scientific Conference of Chemical Engineering; May 29-31, 2024; Thessaloniki, Greece.
3. Lygerakis F, Kolokotsa D, Drosou C, Gournis D, Yentekakis IV, Gioti C, Karakassides MA. Enhancing building energy efficiency with innovative paraffin-based phase change materials. Presented at: 14th Panhellenic Scientific Conference of Chemical Engineering; May 29-31, 2024; Thessaloniki, Greece.
4. Chytis, T. M., Kampelis, N., Lygerakis, F., Kolokotsa, D., & Diangelakis, N. A. (2023, July 5-7). Occupant behaviour optimisation towards thermal comfort and energy efficiency in

buildings. The 1st International Conference of Net Zero Carbon Built Environment, Nottingham, UK.

Other publications (not directly related to the PhD thesis)

Lygerakis, F., Gioti, C., Karakassides, M. A., Gournis, D. P., Yentekakis, I. V., & Kolokotsa, D. (2025). Impact of Accelerated Weather Aging on Building Energy Efficiency Using Cement and Gypsum Boards with Shape-Stabilized Phase Change Materials. Scientific Reports (accepted)

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Abbreviations & Symbols

Abbreviation	Description
AEC	Architecture, Engineering & Construction
AI	Artificial Intelligence
BACS	Building Automation and Control Systems
BAS	Building Automation System
BEDES	Building Energy Data Exchange Specification
BEO	Building Elements Ontology

BIM	Building Information Model
BPO	Building Products Ontology
BOT	Building Ontology Topology
BRoT	Ontology for Bridges
CBF	Sample Cement Board
ConFD	Conduction Finite Algorithm
CTF	Conduction Transfer Function
DER	Decentralized Energy Resources
DOT	Ontology for Damage Monitoring of Buildings and Built Structures
DSC	Differential Scanning Calorimeter
DSS	Decision Support System
DT	Digital Twin
EPD	Environmental Product Declaration
FM	Facility Manager
FOG	Ontology for Geometry Formats
FSO	Flow Systems Ontology
GBF	Sample Gypsum Board
gbXML	Green Building XML
GHG	Greenhouse Gas
GNN	Graph Neural Network
GWP	Global Warming Potential
HTO	Haystack Tagging Ontology
IEQ	Indoor Environmental Quality
IFC	Industry Foundation Class
IoT	Internet of Things
IRI	Internationalized Resource Identifier
KG	Knowledge Graph
KM4CITY	Knowledge Model for City
KPI	Key Performance Indicator
LBD	Linked Building Data
LCA	Life Cycle Analysis
LCC	Life Cycle Costing
LCOE	Levelized Cost of Energy
MEP	Ontology for Distribution Elements
MCDA	Multi-Criteria Decision Analysis
ML	Machine Learning
NBIMs	National Building Information Model Standard
NCC	Net Capital Cost
NPV	Net Present Value
OMG	Ontology for Managing Geometry
OneDM	One Data Model
OP	Occupant Profile
OPM	Ontology of Property Management
OWL	Web Ontology Language
P2P	Peer to Peer
PCM	Phase Change Material
PED	Positive Energy District
PV	Photovoltaic
RDF	Resource Description Framework
REC	RealEstate-Core

RES	Renewable Energy System
RSL	Reference Service Life
SAREF	Smart Applications REFerence
SEAS	Smart Energy Aware Systems
SPARQL	SPARQL Protocol and RDF Query Language
SSN/SOSA	Semantic Sensor Network/Sensor, Observation, Sample, and Actuator
UUID	Universal Unique Identifier
URI	Uniform Resource Identifier
VBIS	Virtual Buildings Information System
W3C	World Wide Web Consortium
WoT	Web of Things
SAM	System Advisory Model
SBOnto	Ontology of Smart Building
SWCNT	Single-Wall Carbon Nanotubes
TES	Thermal Energy Storage
TUC	Technical University of Crete
ZEB	Zero Energy Building
ZEN	Zero Energy Neighborhood

Symbols	Description
$GHG_{Emissions}$	the greenhouse gas emissions (kg $CO_{2\text{-}eq}$)
$GWP_{Interventions}$	the global warming potential of the interventions (kg $CO_{2\text{-}eq}$)
GHG_{Grid}	the greenhouse gas emissions from grid consumption during RSL (kg CO2-eq)
$PV\ Generated\ Energy$	the energy generated from the PVs during RSL for each scenario (kWh)
$EPD\ Factor_{PV}$	the environmental product declaration factor of the PV (kg $CO_{2\text{-}eq}$/kWh)
$Inverter\ Units$	the number of inverter units sized for the scenario, including replacements every 10 years
$EPD\ Factor_{Inverter}$	the environmental product declaration factor of the inverter (kg $CO_{2\text{-}eq}$/inverter unit)
$Battery\ Capacity$	the capacity of the battery, including replacements every 10 years (kWh)
$EPD\ Factor_{Battery}$	the environmental product declaration factor of the battery (kg $CO_{2\text{-}eq}$/kWh)
$Grid\ Energy\ Mix\ Factor$	the local distributor emissions factor (kg CO2-eq/kWh)
$Energy\ from\ Grid\ to\ Load$	the energy simulated in SAM that the grid gives to the load during RSL (kWh)
$CO_2\ Savings$	the $CO_{2\text{-}eq}$ savings in operational phase as a percentage compared to the baseline scenario (%)

$GHG_{Emmisions_{S0}}$	the operational phase greenhouse gas emissions of the baseline scenario (kg $CO_{2\text{-eq}}$)
$GHG_{Emmisions_{Si}}$	the operational phase greenhouse gas emissions of scenario i (kg $CO_{2\text{-eq}}$)
$Net\ GHG_{Emmisions}$	The total greenhouse gas emissions considering intervention impacts and grid energy savings (kg CO_2)
$GHG_{Grid-saved}$	the avoided emissions due to reduced energy import from the grid, calculated as the difference between the baseline and the intervention scenario, multiplied by the grid emission factor (kg CO_2)
$E_{G\to L_{baseline}}$	Energy imported from grid to load for the baseline scenario (kWh)
$E_{G\to L_{scenario-i}}$	Energy imported from grid to load for the scenario i (kWh)

1.Introduction

The central challenge this thesis addresses is the lack of an integrated, multi-scale semantic framework that can support sustainable renovation decisions across both building and neighborhood scales. Current methods remain fragmented, focusing either on isolated building simulations, material-level experiments, or neighborhood-scale models that lack interoperability and reusability. As a result, there is a clear need for a unifying framework that can semantically integrate real operational data, performance indicators, life-cycle assessments, and renovation strategies into a single, queryable, and extensible decision-support system.

To address this gap, the thesis proposes a novel Knowledge Graph-based Digital Twin (KG-DT) architecture that enables the semantic modeling, integration, and querying of heterogeneous renovation data, including material properties, sensor measurements, simulation outputs, and LCA/LCC results. This architecture is designed to support informed renovation decisions across scales by embedding domain knowledge into a dynamic, scenario-driven platform.

To evaluate and validate the proposed architecture, the thesis applies it in two complementary case studies. At the material and building scale, the Leaf House case study investigates the integration of paraffin-based Phase Change Materials (PCMs) into gypsum and cement boards, combining experimental thermal characterization with EnergyPlus simulations that incorporate a custom hysteresis model. At the neighborhood scale, the TUC Campus case study demonstrates the implementation of the KG-DT to integrate sensor data, renovation actions, and sustainability KPIs for cross-building scenario evaluation. Together, these studies test the architecture's effectiveness in both detailed material-level modeling and large-scale semantic integration for sustainable renovation planning.

In addition to these application-driven demonstrations, the thesis also incorporates findings from a systematic review of existing ontologies and knowledge graphs in the built environment. This review, published in a peer-reviewed journal, identifies modeling patterns, reuse limitations, and gaps in semantic interoperability. Its insights directly informed the design of the tailored ontologies used in this thesis and shaped the structure of the KG-DT framework.

1.1. Shift Towards Neighborhood Scale Renovation

Historically, energy retrofits have been tackled at one building at a time. However, recent research and policy have emphasized district or neighborhood-level renovation as a more effective strategy. Multibuilding retrofits can optimize shared infrastructure (e.g. district heating, on-site renewables) and exploit economies of scale to cut costs and emissions[1]. Empirical studies confirm that district-wide projects often achieve higher CO_2 reductions per euro and foster quality-of-life improvements across the community[1], [2]. For example, the authors in [1] note that district renovation drivers extend beyond energy savings, including enhanced comfort, health, and property value, and that economies of scale enable more ambitious measures (like community PV or heat networks) than would be feasible at the single-building level.

This district focus is reflected in the literature. A systematic review in [2] finds that achieving climate neutrality requires a shift from single-building retrofits to multi-building and mixed-use projects. They describe such projects as “lighthouse” initiatives for climate goals yet note that most research and guidelines are still nascent at this scale. Case studies (e.g. in Europe) show that district retrofits face novel challenges, split incentives among owners and tenants, complex stakeholder coordination, financing constraints, but also yield larger cumulative benefits[1], [3].

As illustrated in Figure 1, this shift toward the neighborhood scale introduces significant complexity in data and knowledge management. Diverse operations such as construction, renovation, and energy management generate large volumes of heterogeneous and unstructured data, often in various formats. These must be integrated to align operational practices with overarching targets such as low energy use, GHG emissions reduction, grid resilience, and renewable energy integration. This fragmentation of data sources and lack of interoperability pose a major barrier to systemic renovation planning and decision-making.

In short, sustainable city development will increasingly depend on integrated renovation at the neighborhood or district level, guided by holistic planning tools. This growing trend, driven by policy (e.g. EU Renovation Wave targets) and by the need for systemic solutions, motivates research on decision-support methods that span multiple buildings and accounts for urban context.

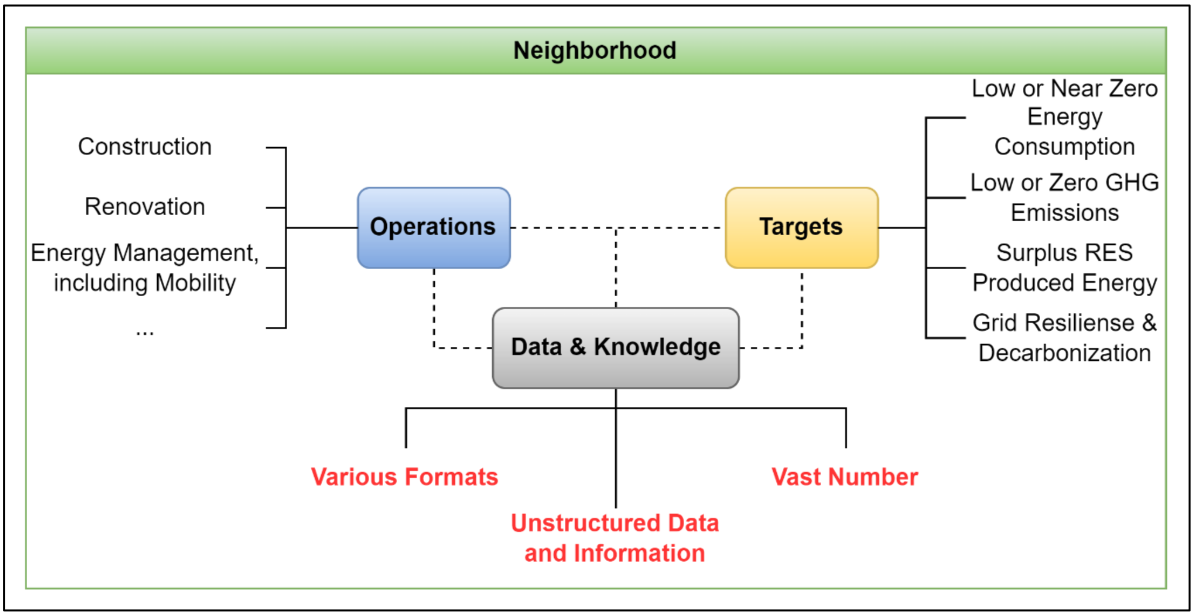


Figure 1: Neighborhood Data & Knowledge Management Challenge for the Various Operations that ensure the Targets

1.2. Knowledge Graphs for Built Environment Data Management

There are notable examples of KGs for data and knowledge management in built environments. In [4],the authors introduce Reno-Inst, an ontology for the building renovation domain. It maps domain knowledge (e.g. constraints on installing windows, insulation panels, radiators) by combining expert input with engineering documents. The ontology was validated via expert workshops and a case study and is designed to underpin applications that improve renovation planning and execution.

Moreover, in [5] the authors develop an ontology capturing surrounding geospatial and environmental data relevant to energy-efficient building renovation. This study identifies the knowledge framework by surveying renovation use cases and expert input. The resulting ontology maps geospatial/environmental concepts to specific renovation tasks, addressing the lack of a conceptual model for such data. By providing a common knowledge framework for this data, the work enables better BIM-GIS integration and informed renovation decision-making.

Furthermore, in [6], the authors propose a BIM-to-KG framework to automate BIM model auditing and quantity take-off. They define a BIM-KG schema capturing the necessary semantics for checking model correctness. BIM models are automatically transformed into a KG and embedded via KG embeddings. These embeddings are then used to detect modeling errors. Their data-driven KG approach successfully identifies intentionally inserted errors without manual rule-coding.

In addition, in [7], the authors present a method to federate multiple domain-specific BIM models into a unified KG. By integrating separate BIM ontologies and data sources, their approach bridges gaps in data exchange and significantly enriches the semantics of building models. A prototype “LBD-Online-Merge” application demonstrates the method in practice. The authors emphasize this framework’s role in achieving interoperable, semantically rich building information (e.g. for digital twins), especially by improving data preparation for a building’s operational phaser.

Also, in [8], the authors build a construction project management (CPM) KG with 36 subdomains and integrate it with large language models (LLMs) for QA. The KG includes multimodal information (text and images) about CPM. In experiments, CPM-specific KG augmentation raises LLM QA accuracy by approximately 30% on average (e.g. from 77% to 100% correct in some cases). This demonstrates how a domain-specific KG can significantly enhance decision-support tools in AEC project management.

Last but not least, in [9] the authors propose a KG approach to automate life-cycle assessment. The authors construct an ontology and KG from standardized LCA data to model flows and processes. They develop a two-stage recommendation method that uses the KG to suggest appropriate background inventory datasets for a given product system. A case study on an electrical product validates the approach. By leveraging a KG of LCA concepts, the method streamlines LCA data management and dataset selection for sustainability decision-making.

1.3. Digital Twins and Their Role in Urban Renovation

DTs have gained traction in urban planning and building management, among other, for their ability to simulate and visualize complex systems. A DT is generally defined as a dynamic virtual replica of a physical entity, with bidirectional data flows between the physical and digital sides[10], [11]. In the urban context, a city or neighborhood DT links real-time sensor feeds, historical databases, and analytic models into one platform. This enables planners and facility managers to monitor conditions continuously and to experiment with “what-if” scenarios before acting. Najafi *et al.* (2024) describe a city DT as an interactive model that “allows urban managers, planners, and other stakeholders to monitor changes and make informed decisions… in real time”[10]. Each object in the twin (buildings, infrastructure, etc.) carries a historical trace of past states, a current status updated from IoT data, and model-driven forecasts of future behavior[10], [11].

The advantages of urban DTs are well documented: improved situational awareness, streamlined asset management, advanced predictive control and maintenance, as well as higher levels of stakeholder engagement. For example, DTs allow facility operators to integrate the flood of IoT data (energy meters, weather stations, occupancy sensors) into coherent dashboards. They support *predictive analytics*: by fusing real-time data with physics-based, AI data-driven, statistical or hybrid models, a twin can forecast equipment failures or energy peaks. In heritage conservation, Hosamo *et al.* (2024) report that a DT linked to a KG allowed continuous monitoring of temperature, humidity and structural strain, enabling “early detection of vulnerabilities” and prediction of maintenance needs[12]. More generally, DTs have been used to optimize building energy use and automate maintenance: for example, DT-enabled smart facilities can continuously tune HVAC and lighting systems to meet comfort targets while minimizing energy[12]. In the context of urban renovation, digital twins can simulate the effects of retrofit measures on a community scale (e.g. running an energy model for an entire neighborhood or testing the impact of shared renewables). They also facilitate participatory planning by providing stakeholder with decision support and visualization functions of multi-criteria optimized different upgrade scenarios.

This thesis expands the concept of DTs in two key directions, each explored through a dedicated case study. At the building scale, the Leaf House case study develops a semantic digital twin that incorporates paraffin-based PCM properties, empirical testing data, and EnergyPlus simulation parameters. This enables dynamic modeling of passive thermal energy storage and links PCM configurations to energy and comfort KPIs via semantic queries. At the neighborhood scale, the TUC Campus case study implements a full semantic DT integrating real-time sensor streams, intervention records, and life-cycle assessment (LCA/LCC) metrics across multiple buildings. This two-level approach demonstrates how digital twins can support both material-level decision making and systemic renovation planning, embedded within a Knowledge Graph-based architecture that enables scalable, queryable, and evidence-driven scenario evaluation.

1.4 Phase-Change Materials for Energy Efficiency and Semantic Integration

Improving building energy performance remains a central goal in sustainable construction and climate mitigation strategies. Among passive energy-saving solutions, Phase-Change Materials (PCMs) have attracted significant attention due to their ability to store and release thermal energy through latent heat during phase transitions [13], [14], [15]. Paraffin-based PCMs, in particular, are valued for their thermal stability, chemical inertness, and compatibility with conventional construction materials, enabling their integration into wallboards, plasters, and composite systems [16], [17].

By melting and solidifying within a controlled temperature range, PCMs can reduce indoor temperature fluctuations, thus lowering HVAC demand. Case studies across various climates have demonstrated energy savings between 10% and 46% depending on PCM placement, climate conditions, and thermal loads [14], [18], [19]. However, many of these studies remain confined to laboratory-scale experimentation or single-zone simulations, often lacking real-scale deployment and integration with dynamic renovation frameworks [14], [20], [21].

In this thesis, the Leaf House case study explores the building-level application of paraffin-based PCMs through both empirical and simulation approaches. Composite gypsum and cement boards with embedded PCMs were thermally characterized in the lab and their performance evaluated in EnergyPlus, incorporating a custom hysteresis model to simulate latent heat storage. Multiple PCM configurations (e.g., 10%, 20%, 30% mass fractions) were tested under realistic boundary conditions to assess their seasonal energy-saving potential in the Mediterranean climate.

What distinguishes this work is the semantic modeling and integration of PCM-related data within a broader Knowledge Graph-based Digital Twin (KG-DT) architecture. Unlike prior work that models PCMs in isolated tools or spreadsheets, this thesis defines a custom ontology with classes such as PhaseChangeMaterial, PCM_CementBoard, and PCM_GypsumBoard. These are enriched with data properties like hasLatentHeat, hasMeltingTemperature, and hasThermalConductivity, and linked to time-series sensor or simulation inputs via hasSimulationInputID and hasTimeSeriesID. This enables formal semantic representation of both material characteristics and their corresponding performance data, making them queryable within the same KG infrastructure that supports LCA/LCC analysis and real-time sensor integration.

Recent literature has advanced ontology-based energy modeling and digital twin simulation, but material-level semantic integration remains underexplored. For instance, in [22] the authors introduced an ontology-based energy modeling framework for scalable and adaptable building digital twins, grounded in SAREF and its building extension SAREF4BLDG. Their work enables dynamic simulation of HVAC components but does not incorporate PCM thermal storage or link semantics directly to latent heat scenarios. Moreover, a follow-on study by the same group delivered a large-scale field demonstration of the energy modeling framework, showing interoperability and automation of digital twin model generation across building zones, but still without PCM-specific material semantic modeling[23]. Neither of these studies models phase-change materials explicitly nor embeds material definitions into dynamic renovation or simulation scenarios, highlighting the novelty of the current thesis.

Existing materials KGs such as MatKG and MKG provide extensive repositories of materials data across chemistry and manufacturing domains [24], [25], [26]. These efforts excel in representing physical properties and process metadata but do not target building simulation, nor do they enable scenario evaluation or energy model integration. Ontologies like the Materials Design Ontology (MDO) offer formal class structures for materials properties, but again, lack application-level connections to built environment use cases[26].

This thesis addresses that gap by developing a material-aware semantic layer that links PCM thermal properties directly to simulation models and renovation scenarios. The integration within the KG-DT allows for SPARQL-based querying of PCM-enhanced assemblies, comparison across material options, and cross-linking with LCA and cost assessments. To the best of the author’s knowledge, this is the first implementation of a PCM-integrated material bank semantically embedded into a KG-DT framework for building energy simulation and sustainable renovation planning.

1.5. Integrating LCA/LCC in Semantic Digital Twins

To enable sustainable renovation decisions, life-cycle thinking is essential. LCA quantifies environmental impacts (energy related emissions, embedded carbon, materials and natural resources, environmental pollutants etc.) across all phases of a building or neighborhood life span. LCC similarly tallies economic costs (construction, maintenance, operation, disposal). Integrating LCA/LCC into the design process has been explored at the building level. For example, in[27] present a BIM-based workflow that computes LCA and LCC during design: quantities extracted from the BIM model are multiplied by environmental impact factors and cost factors from databases. They automated this via a Dynamo script and dashboard, allowing designers to compare material or system alternatives in terms of embodied carbon and lifecycle cost. Other teams have linked BIM to LCA tools (like One-Click LCA, Tally) to produce color-coded 3D visualizations of impacts (e.g. mapping GWP to building components) during development stages[28], [29], [30].

However, these BIM-LCA-LCC methods have limitations. As noted in [27], creating fully automated, error-free workflows remains challenging, especially as detail levels rise. In particular, we observe two key gaps: (1) semantic interoperability, LCA databases and BIM often lack common ontologies, making data exchange brittle; and (2) operational data, traditional BIM-LCA covers mainly construction and materials impacts, but ignores actual usage. Here Digital Twins can help. In [31], the authors explain that whereas BIM supports LCA at the design stage, a DT can supply the operational data (energy, water, etc.) needed to complete and validate the life-cycle model. In their SemanticLCA project, they use ontologies to fuse sensor measurements and usage patterns from the DT with the as-built BIM data, closing the gap between predicted and real performance.

Recent work also shows the promise of KGs for LCA/LCC. In [32], the authors develop an ontology-driven KG for integrated life-cycle analysis and reporting. They argue that graph databases can unite diverse information requirements of LCA (materials, processes, policy rules) into a single searchable knowledge graph. Likewise, in[33] the authors propose a KG framework that enriches LCA data with domain knowledge and even AI-generated estimates, enabling early-stage design decision support. These studies demonstrate that semantic models can manage the complexity of life-cycle data, but they remain focused on products or single buildings.

In summary, the state-of-the-art includes BIM-based LCA/LCC integration and emerging KG-based LCA systems, as well as DT platforms for monitoring and simulation. However, to the best knowledge of the authors, no current approach seamlessly combines all these at the neighborhood scale. Existing BIM-LCA tools typically lack formal semantics and do not scale beyond individual projects. Urban DTs generally omit life-cycle impact assessment, and do not exploit ontologies for data integration. There is thus a clear gap: a KG-based Digital Twin architecture that links building and urban data and embeds LCA/LCC models for collective renovation planning has not yet been realized.

1.6. Research Gap and Contribution of This Work

Despite the growing interest in digital twins and knowledge graphs (KGs) for the built environment, most existing approaches remain focused on either operational monitoring or static design information for individual buildings. As highlighted in recent literature (e.g., [33], [34]), current BIM schemas and DT frameworks often lack the semantic expressiveness and integration required for comprehensive renovation support, particularly when it comes to combining materials intelligence, simulation workflows, and neighborhood-scale decision-making.

This thesis identifies two major research gaps in this domain, which are addressed through two complementary case studies:

(1) Lack of semantic integration of advanced materials like Phase-Change Materials (PCMs) into simulation and decision workflows. While PCMs are widely recognized for their thermal energy storage potential, they are typically modeled in building simulation tools like EnergyPlus through manual input and hardcoded configurations, disconnected from formal semantic representations. Existing material or energy ontologies rarely define thermal phase-change behavior, latent heat, melting point, or related KPIs in a machine-readable way. Moreover, there is currently no method for connecting empirical PCM material data, such as DSC measurements, to semantic building models, simulation scenarios, or retrofit decision-making processes. This results in fragmented data pipelines, poor traceability, and limited reusability of PCM modeling efforts.

(2) Limited scalability of renovation-focused semantic frameworks beyond single buildings, and absence of LCA/LCC integration in digital twins. Although several ontology-based digital twin prototypes exist, few extend to multi-building or neighborhood contexts. Even fewer integrate actual renovation records (e.g., inventories, material replacements, costs) with life-cycle KPIs such as LCA and LCC in a queryable, interoperable way. Most LCA/LCC workflows operate independently of KGs and are not integrated into decision-support systems for

neighborhood-scale planning. This limits the ability of planners to assess the long-term environmental and financial performance of renovation scenarios across multiple assets.

To address these gaps, this thesis develops a dual-case semantic architecture, implemented through two distinct but interconnected case studies:

- Case Study 1 - Leaf House (Material-Level Focus): A reusable material ontology is developed for PCMs, representing empirical and simulation attributes such as latent heat, melting range, and thermal conductivity. These semantic definitions are directly linked to EnergyPlus simulations through custom input mappings and scenario IDs, enabling SPARQL-based queries of PCM configuration outcomes. This represents the first known integration of empirical PCM data and simulation outputs within a queryable knowledge graph tailored for renovation planning.
- Case Study 2 - TUC Campus (Neighborhood-Level Focus): A scalable digital twin architecture is implemented for multiple buildings within the campus, linking BIM-derived data, sensor streams, and renovation interventions to life-cycle metrics. External LCA and LCC assessments are integrated into the KG and exposed via semantic queries to support cross-building evaluation and planning. The architecture supports dynamic data interaction and real-time scenario analysis across the renovation lifecycle.

Table 1 and Table 2 contextualize the novelty of this work by comparing it against recent literature. Table 1confirms that no prior approach semantically models PCM materials and links them to simulation workflows within a KG-DT environment. Table 2 demonstrates that no previous study integrates KG-based decision support with LCA/LCC reasoning at the neighborhood scale.

Table 1: Comparative Table of Semantic Modeling Approaches for Materials and PCM Integration in Building Simulation

Reference	Semantic Modeling of Materials	PCM Integration	Simulation Link (e.g., EnergyPlus)	Queryable via KG (SPARQL)	Case Study / Real Data
[22]	✔ **Based on SAREF/SAREF4BLDG**	❌ **Focus on HVAC components**	✔ **Energy modeling enabled**	❌ **No material-specific queries**	✔ **Demonstration model only**

[23]	✔ Interoperable DT with ontologies	❌ PCM not modeled	✔ Multi-zone DT simulation	❌ No SPARQL query support	✔ Large-scale field test
[24]	✔ Rich materials database	❌ Not building-focused	❌ No simulation linkage	✔ SPARQL-ready materials KG	❌ No built-environment case
[26]	✔ Ontology for materials design	❌ Not PCM-specific	❌ No energy modeling	❌ Static material metadata	❌ No case study
This Work (2025)	✔ Custom ontology (e.g., PhaseChangeMaterial, PCM_GypsumBoard)	✔ Empirical PCM data & 3 configurations (10/20/30%)	✔ Linked to EnergyPlus via KG inputs	✔ Scenario-based SPARQL (e.g., hasLatentHeat, hasSimulationInputID)	✔ Real case (Leaf House) with full semantic + simulation pipeline

Table 2: Comparative Table of Knowledge Graph and Digital Twin Frameworks for Neighborhood-Scale Renovation and LCA/LCC Integration

Reference	Knowledge Graph (KG)	Digital Twin (DT)	LCA / LCC Integration	Multi-Building / Neighborhood Scale	Queryable Scenario Evaluation (SPARQL)	Case Study Implementation
Amorocho & Hartmann (2021) - Reno-Inst [4]	✔ Ontology for renovation planning	❌	❌	❌ Single building focus	❌	✔
Daneshfar et al. (2022) [5]	✔ Geospatial ontology for renovation	❌	❌	❌	❌	✔
Liu et al. (2022) [6]	✔ BIM-to-KG for auditing/QTO	❌	❌	❌	❌	✔
Teclaw et al. (2024) [7]	✔ Federated BIM-based KG	❌	❌	✔ Multi-domain BIM	❌	✔
Zhou et al. (2025) [8]	✔ Multimodal KG with LLMs for QA	❌	❌	❌	✔ (QA only)	✔
Peng et al. (2024) [9]	✔ KG for LCA recommendation	❌	✔ LCA only	❌ Product-level focus	❌	✔

This Work (2025)	✔ Tailored KG from multiple ontologies (Brick, SAREF, KPI)	✔ Semantic DT for scenario evaluation	✔ Both LCA & LCC with dynamic simulation inputs	✔ Neighborhood-scale (TUC campus)	✔ SPARQL-enabled scenario and KPI queries	✔ Full implementation with real data

Together, these contributions form a first-of-its-kind dual-scale KG-DT framework that spans both material-level intelligence and multi-building renovation planning. It delivers:

- A semantic layer for PCM characterization and simulation scenario management,
- A queryable KG infrastructure that connects simulation inputs, outputs, and performance KPIs,
- A decision-support system that links material choices and renovation actions to life-cycle impacts at building and district scales.

This dual-case implementation offers a replicable foundation for integrated, sustainable renovation planning using semantic digital twins.

1.7 Research Objectives

Based on the identified challenges and research gaps, this thesis aims to achieve the following objectives:

1. To evaluate the energy performance and reliability of PCM, enhanced construction components by conducting experimental testing (including accelerated aging), material characterization, and dynamic building simulations under realistic boundary conditions.

2. To define and implement a multi-domain ontology capable of semantically representing diverse renovation-related data, including material properties, intervention strategies, sensor measurements, simulation identifiers, and performance indicators, across both building and neighborhood scales.

3. To develop a Knowledge Graph-based Digital Twin (KG-DT) architecture that enables semantic integration of heterogeneous data sources (e.g. sensor feeds, simulation results, renovation records, and life cycle analysis) into a unified, interoperable decision-support platform.

4. To support multi-scenario renovation decision-making through SPARQL-based semantic querying of key performance indicators (KPIs), using UUID mappings to link time-series data, interventions, and simulation outcomes.
5. To validate the proposed approach through two real-world case studies: (i) a building-scale PCM retrofit evaluation (Leaf House), and (ii) a neighborhood-scale semantic integration and sustainability analysis (TUC Campus).

This thesis focuses on semantic integration and decision support for sustainable renovation, limited to the domains of energy performance, environmental impact (LCA), and economic assessment (LCC). It does not address aspects such as real-time building control, social life cycle assessment (S-LCA), mobility systems, or broader urban governance mechanisms. While the developed KG-DT architecture is extensible, the current implementation is bounded to physical renovation components, material-level and neighborhood-scale KPIs, and does not yet include behavioral data or policy simulation layers.

2. Knowledge Graphs Ontologies and Applications in Buildings

2.1 Knowledge Graphs

2.1.1 Definition

Knowledge graphs are still evolving today, yet many different attempts have been made to provide thorough and concise definitions [34], [35]. According to a commonly used definition, a knowledge graph acquires and integrates information into an ontology and applies a reasoner to derive new knowledge [34]. This definition was given after research was conducted, in order to produce a working definition based on examples. As noted by Ehrlinger and Wolfram, considering that there are many diverse applications, a KG is more likely to be similar to an abstract framework than to a mathematical structure [34]. Another approach is that a knowledge graph describes real-world entities and their interrelations, organized in a graph. It does so by defining possible classes and relations of entities in a schema. In addition, it allows for other potentially interrelating arbitrary entities connection with each other, and covers various topical domains [36]. Similarly, a KG can be viewed as a graph of data intended to accumulate and convey knowledge of the real world, whose nodes represent entities of interest and whose edges represent relations between these entities [37]. KGs were first introduced in 1973; however, they were not used in a useful way until 2012, when Google announced its KG, which was the starting point for many other companies to introduce their own [38], [39]. Many applications have been developed since then and many papers have been published, all aiming at the core idea, which is to represent data using graphs in a manner to represent knowledge [40]. Graphs, contrary to a relational model or NoSQL approaches, are more coherent and direct, using edges to represent the relations between entities, and apply to various domains [37], [41]. A further aspect of a graph is that it provides the creator with the ability to delay the definition of its schema. In this way, the graph is more flexible to evolve and obtain more incomplete knowledge, resulting in a continuously updated database schema, or serving under an organization or a community as an ever-evolving shared form of knowledge [40].

2.1.2 Data Graphs

One of the first principles of a KG is the graph abstraction to data. Graphs are able to create primary data graphs, be represented by data models and be processed by query languages. Modeling a graph differs in every situation, although some graph data models can be adapted and customized. For example, a directed edge-labeled graph is compiled from a set of nodes and a set of directed labeled edges that connect these nodes [42], [43]. In KGs, nodes stand for entities and edges stand for the binary relations between them. This way of modeling a graph is more appropriate when adding new sources of data. The RDF is a model based on directed edge-labeled graphs and uses a variety of nodes[44], [45]. The most important nodes are the IRIs, which give access to entities through the Web. Other important nodes are literals, which represent strings and other datatype values. Finally, blank nodes are used in RDF graphs, which are anonymous nodes that are not assigned an identifier. In addition to literals, URIs can be used to uniquely identify all nodes and edges in a graph[46]. The simplicity of an RDF is based on the triplets it consists of, which are three-part statements that represent a relationship of subject, predicate and object (Figure 2)[47].

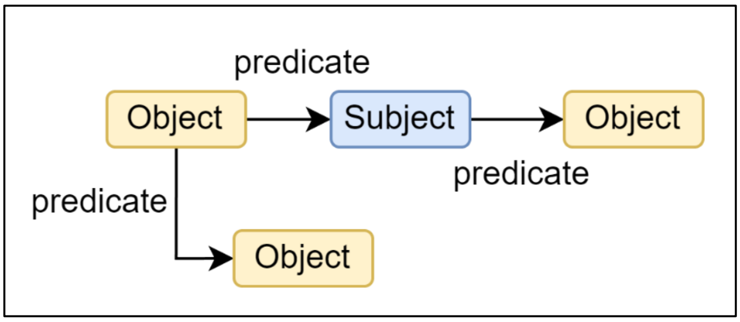


Figure 2: Structure of an RDF graph.

When querying a graph, many languages have been introduced, including SPARQL for RDF graphs [48]. Graph patterns are stationed at the center of a query language, which uses the same models as the data graph that is being queried [49]. Furthermore, graph patterns also add variables as terms, which are divided into constants [49]. Next, mappings are generated from the variables and constants of the data graph; thus, the graph pattern is included in the data graph. Moreover, since a graph pattern exports a table of results, and due to the need for relational algebra to work with these tables, more complex queries are being created [58]. Another aspect of graph query languages is that navigational graph patterns add path expressions in queries. This allows the matching of arbitrary length paths between two nodes, which are expressed as a regular path and are used in graph patterns to express navigational graph patterns [49].

2.1.3 Deductive Knowledge

A KG can be identified as a data graph enhanced with representations of schema, identity, context, ontologies and rules [37]. Schemata are used to mark the structure and semantics that a KG will be based on. However, it has been mentioned that the definition of a schema can be delayed even after the KG's configuration [37]. One type of graph schemata is semantics. Semantic schemata are used as a vocabulary for understanding terms used in a KG, while using these terms for reasoning the KG. RDF Schema is an example of a semantic schema, which introduces subclasses, sub-properties, domains and ranges for the classes and properties in an RDF graph [50]. Many more details and content about the semantics of KG terms is provided by the OWL standard for RDF graphs [51]. Contrary to semantic schemata, validating schemata certify existing graph data, using shapes. Shapes are responsible for targeting a set of nodes in a data graph and identifying their constraints [52], [53]. Both types of schemata need a domain expert to identify definitions and constraints. However, in a data graph, latent structures can be exported as an emergent schema. An emergent schema uses graphs as frameworks to separate quotient groups of nodes, while maintaining some structural properties of the graph [54], [55]. It is necessary to know the meaning of the terms that are used in order to apply entailment. This is achieved using ontologies, which provide a formal depiction of the meaning of the terms. A common definition of ontologies also states that an ontology is a "formal, explicit specification of a shared conceptualization" [56]. OWL is recommended by the W3C and is compatible with RDF graphs [37], [51]. In the process of interpretation, the data graph is changed to a domain graph. There, real-world entities and real-world connections are included and connected with the nodes and edges of the data graph, in addition to those of the domain graph, thus following the same model as the data graph. Linking particular patterns in the data graph with semantic conditions results in the features of an ontology language. These features result in entailments. Each axiom that is introduced from an ontology imposes some conditions on the interpretation of the graph that satisfies it, which are called graph models. One graph entails another if and only if the first is also a model of the last one or alternatively the former graph entails the latter. In this context, there is not an algorithm that can decide the correct true/false answer to the question of which graph entails the other [57]. Another approach is to always halt false with the correct answer, only receiving input ontologies with specific features, and the final approach is to only reply with correct answers for any input ontology, risking never halting on some inputs [58].

2.1.4 Inductive Knowledge

Inductive knowledge, unlike deductive reasoning, derives from generalized patterns in observed data to generate new but less precise predictions. Popular inductive techniques are summarized in Figure 3.

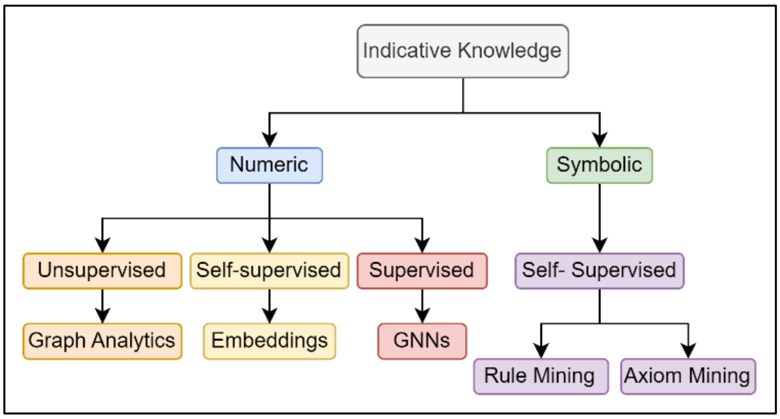


Figure 3: Conceptual overview of popular inductive techniques for knowledge.

Graph analytics involve discovering, interpreting, and communicating patterns inherent in data collections, where graph-specific analytics utilize techniques from graph theory and network analytics to deduce insights based on graph topology [59]. Machine learning has made significant strides recently, enabling direct refinement of KGs. KG embedding methods aim to compress the graph into a continuous, low-dimensional vector space to perform machine learning tasks around nodes and edges, while custom machine learning models tailored for graph-structured data, often based on artificial neural networks, offer another approach [60], [61]. GNNs are neural networks adapted to a data graph's topology, potentially replacing traditional algorithms[62], [63], [64]. Symbolic learning involves constructing interpretable models from KG-generated hypotheses in a symbolic language, aiding additional reasoning by clarifying positive and negative edges.

2.2 Existing Ontologies for Buildings

In this section, the most important ontologies for buildings are introduced and categorized, according to the phase they refer to, i.e., design or operational. An in-depth analysis of some of these key ontologies is conducted as it is necessary for the objectives of the review.

2.2.1 Ontologies in Building Design Phase

One of the most important tools, if not the most important, that is used as a base for many ontologies is the IFC schema, which has been combined in an approach with OWL, creating the ifcOWL ontology [65], [66]. ifcOWL ontology's complexion has driven the introduction of SimpleBIM, which is a much more simplified but powerful ontology [67]. Another ontology is gbXML, for which the main scope is the information exchange between BIM and AEC analysis software [68]. With streamlining, gbXML transfers BIMs from and to AEC models, aiming to design sustainable and energy-efficient buildings [69]. Another is Tubes, which supports a high-level description of building service systems and utilizes data principles to extract their topology from IFC models [70]. Two more ontologies are SimModel Ontology and EnergyADE, which focus on exchanging energy simulation data and are an extension to CityGML [71], [72], [73].

2.2.2 Ontologies on Building Operational Phase

An ontology that focuses on sensor networks is SSN/SOSA, which is not only specific to building sensors [74]. Other ontologies, such as WoT, oneM2M BaseOntology's and OneDM, focus on the representation of IoT objects [75], [76]. WoT is a model used to describe the virtual counterpart of physical objects in the Web of Things; oneM2M BaseOntology provides syntactic and semantic interoperability between oneM2M and external systems; and OneDM is a model used to support a common language for the Internet of Things. More ontologies that focus on smart buildings are Smart Energy Aware Systems (SEAS), ThinkHome, Building Ontology for Ambient Intelligence (BOn- SAI), DogOnt, SBOnto and SAREF [77], [78], [79], [80], [81], [82]. SEAS ontology represents entities in a smart building. ThinkHome is an ontology that includes concepts needed to realize energy-efficient and intelligent control mechanisms. BOnSAI is a smart building ontology for ambient intelligence, whereas DogOnt is a model for all devices being part of IoT inside a smart environment. SBOnto is a smart building ontology and SAREF matches existing assets in the smart application domain. SAREF ontology has many extensions that differentiate the classifications and concepts, which are able to be used together for a more specific approach. These extensions include SAREF4BLDG, a building domain extension. SAREF4ENER, an energy domain extension, SAREF4CITY, a smart cities domain extension, SAREF4ENVI, an environment domain extension, SAREF4INMA, an industry and manufacturing domain extension, SAREF4AGRI, a smart agriculture and food chain domain extension, SAREF4AUTO, an automotive domain extension, SAREF4EHAW, an e-health/ageing-well domain extension, SAREF4WEAR, a wearables domain extension, SAREF4WATR, a water domain extension, and SAREF4LIFT, a smart lift domain extension[83]. Next, some ontologies have building automation and monitoring as the center of their attention. These ontologies are Project Haystack 3, BASont, Project Haystack 4, HTO, Brick Schema, Google Digital Building Ontology, SBMS, CTRLont and Green Button [84], [85], [86], [87], [88], [89], [90]:

- Project Haystack 3 and 4 focus on the representation of buildings entities and concepts utilizing tagsets.
- BASont focuses on building automation and monitoring.
- HTO focuses on streamlining data from IoT based on Project Haystack.
- Brick focuses on metadata and data points from building advancement and needs to be based on end-use applications.
- GDBO represents structured information about buildings and building-installed equipment.
- SBMS is a BAS-protocol-independent model of intelligent building systems, and CTRLont is a model of control logic in BAS.

Another ontology that falls in the same category is that proposed by E. Meshkova, which has as its scope the representation of relations between devices and services regarding home automation [91]. Other ontologies have a broader perspective, such as REC, BOT, BACS, KM4City and EM-KPI Ontology [92], [93], [94], [95], [96]. REC focuses on usage analysis and optimization and presence analysis of a building structure; BOT focuses on the representation of physical and conceptual objects of a building and the connections between them; BACS supports the modeling control behavior in a BAS, physical devices of a BAS, and their location in the building and connection to technical equipment and appliances; KM4City is a representation model for a city and mobility; and EM-KPI focuses on the enhancement of energy management at district and building levels. Furthermore, other ontologies target their scope towards grid-interactive efficient building applications. These ontologies are Facility Smart Grid Information Model and RESPOND [97], [98]. FSGIM is an abstract information model representing a Smart Grid's perspective of a facility. RESPOND reuses BOT, SAREF and SEAS ontologies to create its ontology. Its main scope is to manage the dispatch of real-time optimal energy, considering both supply and demand, while considering all energy assets on-site [98]. Moreover, some ontologies concentrate on occupants' behavior, such as DNAs Framework (obXML), Occupancy Profile (OP) Ontology, Onto-SB and OnCom [99], [100], [101], [102]. DNAs Framework explains that, in order to describe the impact of the behavior of occupants on energy use in building, there has to be four core components i.e., drivers, needs, actions and systems. These components interact with the outside world and the inside world as human beings [103]. Onto-SB is a human profile ontology for energy efficiency in smart buildings, OP ontology is a semantic model for occupancy profile, and OnCom is an ontology for occupant thermal comfort and energy efficiency optimization. Finally, ontologies that emphasize asset management and audits are BEDES, VBIS and OPM [104], [105], [106].

All the ontologies are gathered in Table 14 Appendix I, and the most prominent are discussed in Section 2.2.4

2.2.3 Applications of Ontologies in Buildings

In this section, some applications of the ontologies reviewed in Section 2.2.1 and 2.2.2, as well as their reuse to create new applications, are presented. First, applications focusing on building performance improvement are discussed, followed by applications that target the facility management perspective. Using KPIs to assess a building's performance is common and that is why some ontologies have been taken into consideration. The first to be discussed was introduced by Corry et al. [107]. In it, ifcOWL, SimModel and SSN ontologies are reused to create an architecture that focuses on reducing the performance gap between the real and simulated data. This case study considered the simulated and measured KPIs in order to assess the thermal comfort conditions and the HVAC system performance. These considerations were supported by the selected ontologies. However, this architecture did not manage real-time data streaming. Hu et al. [96], [108] took the previous work one step further by creating an ontology-based architecture, which was based on two algorithms. The first gathers and prepares data streaming from various sources and the second calculates the building performance. Furthermore, a case study was examined with the use of the RDF schema and SPARQL query language integrated with OpenMath and Linked Data. The difference between these two cases is that the first did not use real-time data, whereas the second did. It was proved in the second case that it is essential to use real-time data, as it supports various procedures throughout the building's life cycle. An ontology-based architecture that focused on performance tracking at building and district levels was developed by Li et al. [107], and tested in a case study of a microgrid comprising 19 solar houses. This architecture consisted of the ifcOWL ontology, the SimModel ontology, for creating an XML-based building simulation model (to be used in EnergyPlus and OpenStudio), and the SSN ontology, which was used for semantically integrating sensor data [96], [107], [108]. In addition, an ontology-based architecture for building energy savings was proposed by Han et al. [109], which included the RDF schema, D2RQ ontology translator, OWLIM-RDF database and EnergyPlus as a simulation tool [110], [111]. The scope of the case study that was conducted was to identify any energy waste in the office zone. In the same context, InterfaceOnto was proposed by Kadolsky et al. [112]. Its main scope is to support the selection of efficient and best-cost HVAC systems. In addition, it focuses on the evaluation and prioritization of energy performance values (cooling/heating) consumption, through a platform called MonitoringLab. The case study aimed at the design phase, while the operational phase needs to be further researched. A more occupant-centric ontology is OPTIMUS, which is used in an architecture to target the occupants in a building and makes suggestions to reduce building energy by their behavior [113]. Two case studies were explored, where the first used the architecture to provide solutions for energy reduction and increased comfort based on the building's assessment; in the second, the architecture was applied in a lab in Athens where the building's energy was reduced relative to the year before the ontology was applied. The obFMU tool is a modeling tool that takes into consideration occupant behavior, as it is based on DNAs framework and obXML schema, which were discussed in Section 2.2.2 [114]. Moreover, these tools contain a co-simulation interface, a data model and solvers. Three examples were examined, where the first coupled obFMU with EnergyPlus to model occupant behavior lighting control; the second modeled the occupant behavior window action; and the last modeled HVAC control. Onto-SB ontology was used in another work, where an intelligent context-awareness Building Energy Management System was proposed [115]. The scope of this mechanism is to reduce building energy consumption by having occupant behavior changes as a top priority and covering their thermal comfort needs. Their case study is a residential building with four people, where they apply distinctive characteristics. After they integrate the proposed mechanism, they achieve a 40% reduction in energy consumption. Furthermore, Onto- SB ontology is also used in an approach where the main scope is the efficient control of appliances and devices in smart buildings, targeting the occupants' comfort and energy consumption reduction [116]. Two experiments were conducted. The first aimed to reduce energy consumption by altering different characteristics in the scenario and the second tried to make the simulation process quicker. Another occupant behavior-centric ontology is OnCom, which combines a wireless sensor network and an emotional state analysis from occupants to calibrate indoor thermal comfort [101]. A case study was conducted that tested eleven participants with different characteristics. Each participant responded to thesystem's actions in a different situation with respect to the indoor thermal comfort. The results showed that the majority of users agreed with the system's decisions. In another work, gbXML was used in an attempt to create a BIM-based system that automatically associates and updates thermal property measurements with BIM elements in a gbXML schema [69]. Based on two case studies, this application showed that the proposed method minimizes the gap between architectural information in BIM and the real data used for energy performance simulation. Furthermore, another work used a gbXML schema to convert semantic information from raw point cloud data and use it in energy simulation tools [117]. The applications were made in five existing buildings (three residential and two bank buildings) and, although some errors occurred, the overall integration was successful. Similar work also used a gbXML framework to store data from big buildings, such as factories, in gbXML format, to make it easier to import them into simulation tools [68]. Another work was proposed by Bottaccioli, where an ontology was created by reusing existing ontologies [118]. The architecture that was based on this ontology has the scope of providing modification options to facility managers. These options are addressed to the building, facility or energy managers. In addition, they include real-time visualization tools for energy consumption information and simulation of temperature trends, in addition to energy consumption tools. Moreover, the managers can access and assess the performance efficiency of the building, the users' energy behaviors and feasible refurbishment measures. The case study in this situation was conducted in an educational building and was able to apply real-time data in building energy simulation modifications. EESPA ontology is another approach, which combines SSN/SONA and BOT ontologies, in order to create semantic relationships between BMS data and building spaces [119]. The case study in this paper was performed on an educational building and supported its data analysis, although the lack of real-time data was found to be a challenge in HVAC system control. Another work that used BIM and BMS data connected with the semantic web in order to assist facility managers is ESIM ontology, but did not provide a case study [120]. Due to the problematic nature of creating ontologies that reuse a lot of complex existing ontologies, Uribe et al. [121] proposed a simpler ontology to be used in a context-awareness architecture for managing thermal energy in nZEBs. This ontology manages sensors and knowledge-based information in an nZEB. A case study based on this architecture was conducted, showing that SPARQL and Semantic Web Rule Language were compatible with decision making in this building. Similar to this simplification, the BACS ontology was proposed, based on EXPRESS, OSPH, SSN/SOSA, BOT and FSM ontologies, among others [94]. These ontologies were reevaluated instead of just being reused. The case study that was conducted for this work included a room and the automated control of the windows' shades using SPARQL queries. In another approach, an ontology called SPORTE2 was created, which combined an artificial neural network, genetic optimization algorithm, real-time sensors, actuator data and SWRL rules to optimize the performance in a swimming pool [122]. Having as each base the machine-readable semantics, Schachinger and Kastner put forward a similar work with SPORTE2, with a common scope to optimize building energy [123]. As the core of the ontology, both approaches had real-time sensors, numerical methods and actuators, which integrated online simulation to improve building performance. Having examined some notable applications of ontologies in buildings, other review papers are brought into the spotlight. Bergmann et al. [124] gathered the scope from different ontologies, including IFC, Brick, Project Haystack and other ontologies, having in mind the energy efficient buildings. In another review, Benndorf et al. [125] focused on semantic interoperability, fault detection and predictive control for energy performance optimization in buildings. Moreover, a survey on information modeling and ontologies in building automation was conducted by Butzin et al. [126]. Pritoni et al. [127] conducted a review of metadata schemas and ontologies for building energy applications. Finally, Gilani et al. [128] proposed a review of ontologies within the domain of smart and ongoing commissioning. Table 15 in Appendix I includes all the applications of ontologies in buildings that were presented in this section.

2.2.4 Prominent Ontologies for Buildings

2.2.4.1 IFC Related Ontologies

To every entity, an IFC schema gives spatial properties, and various other properties that are classified. ifcOWL is a complex ontology language, which is a translation from the IFC schema through the EXPRESS data modeling language into an OWL representation [129], [130]. The complexity is shown as a property set that assigns the properties using relational nodes. Two intermediate nodes are needed to insert the name and the value of the property. The EXPRESS datatype is used to express literals. SimpleBIM is an attempt to simplify this ifcOWL as it uses the most straightforward approach. Figure 4 shows the difference between them, as they represent the same entities. SimpleBIM also uses the Turtle serialization format for RDF data models [131].

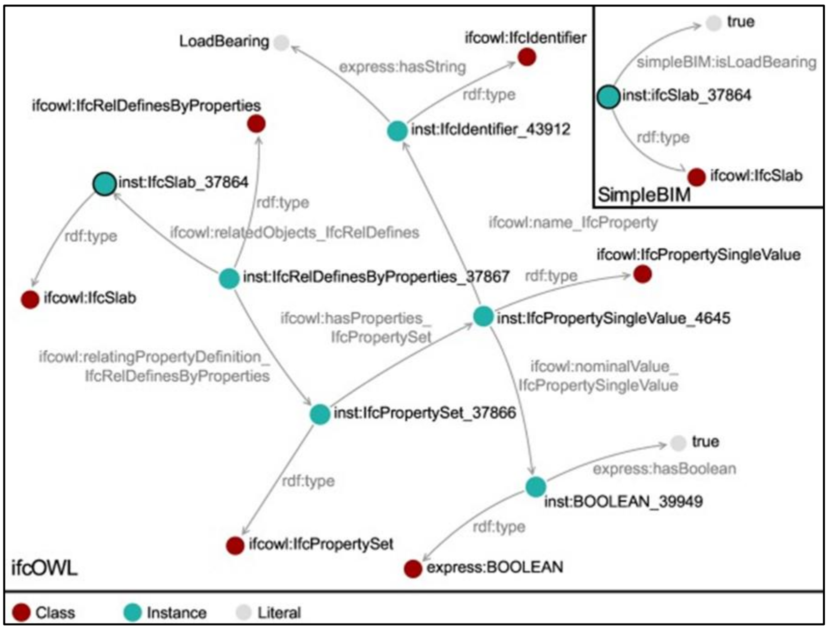


Figure 4: Visual complexity comparison of representing property assignment using ifcOWL and simpleBIM [74]

2.2.4.2 W3C Related Ontologies and Extensions

Due to IFC's extensive use, a less complex, extensible and modular ontology was required, and hence the W3C LBD community group was first created in order to provide solutions for these needs [132].

The main solution was BOT, introduced by Rasmussen in 2016. It constitutes a simple ontology based on the topology of a building and its physical and conceptual objects and the connections between them [133]. For this to happen, BOT sets some rules that subdivide the building into stories and spaces. Spaces are bound by building elements and spaces can contain building elements. It is an ontology that focuses on the building as a structure and does not cover the needs of the whole AEC domain, but can be used as a central ontology to link others [133]. As a result, BOT is a simple base ontology for building structures that can be easily connected with other ontologies to add more information, making the procedure more customizable and malleable in different situations. Having BOT as their core, many extensions to this ontology have been developed. Examples include domain ontology for building elements (BEO) and distribution elements (MEP); ontologies for damage monitoring of buildings and built structures (DOT); ontology for bridges (BrOT); a flow systems ontology (FSO); an ontology for building products (BPO); an ontology for geometry formats (FOG); an ontology for managing properties (OPM); and an ontology for managing geometry (OMG) [106], [134], [135], [136], [137], [138], [139], [140]. Moreover, extension ontologies such as QUDT, SSN/SOSA, O&M and time can be combined with BOT, enabling adaptation to specific needs [141], [142], [143].

OPM, which is of great interest among the rest of the extensions, offers the vocabulary for modeling complex entities in a design environment, and was proposed by Rasmussen in 2018 [65], [144]. These entities are defined as complex because they can alter through time. Their reliability can be based on assumptions and on other entities that can also change, causing an effect on them. OPM uses SEAS, schema.org and PROV-O ontologies as extensions, and can work alongside BOT, PROPS and PRODUCT ontologies of the W3C LBD Community Group [145]. To test OPM, a case study was developed to calculate the heating demand in a building through the ontology (Figure 5) [65], [146]. An OPM-REST application on the AEC-KG was then developed as a generic approach. The case study showed that OPM is a different way of working with building data and paves the way to access and utilize BIM models, exchanging information between stakeholders using the same tool.

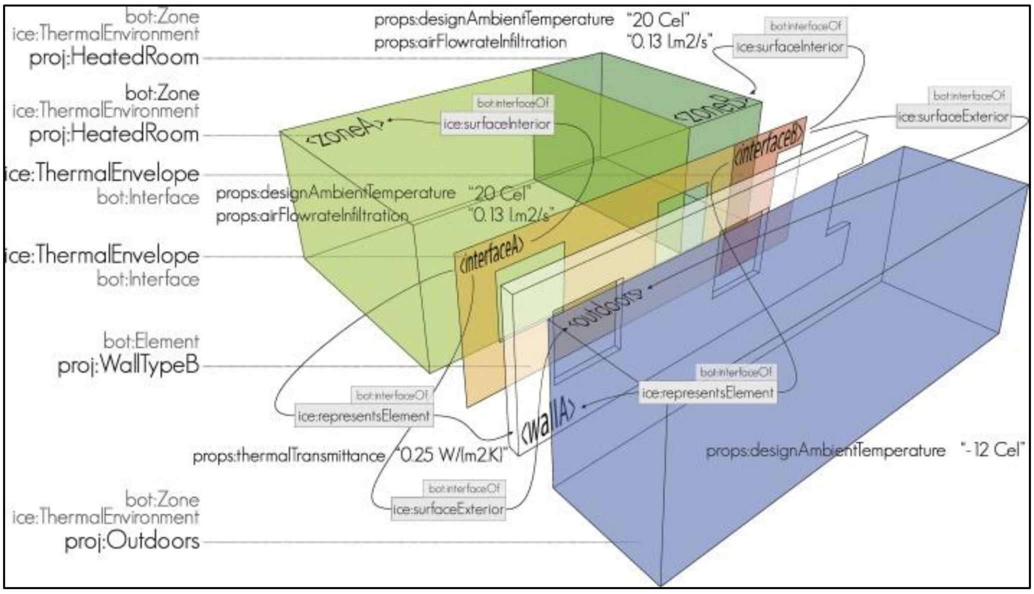


Figure 5: Visualization of the AEC-KG model for the heat-loss calculation case study [65]

2.2.4.3 Smart Building Related Ontologies

The first smart building-related ontology to be discussed is Brick [146]. Brick's main goal is concentrated on metadata and data points from building advancement and needs. These data points are based on end-use applications and consist of the main ontology that establishes the core concepts and the connections between them, in addition to a typology that enlarges the building's concepts [87]. Brick is a schema that addresses the problem of heterogeneity of building representation, and adds a quick and non-costly reaction to energy efficiency measures [147]. The concept of tags is adopted, based on Project Haystack, to add a more flexible means to annotate metadata. Then, these tags are altered with an ontology that boosts its concepts, creating a framework that establishes hierarchies, relationships and properties that are mandatory for building metadata [87], [148]. Furthermore, using an ontology provides the schema with the ability to manipulate the metadata using common tools. In the Brick schema, the tagset concept is introduced, which groups tags with similar properties [147]. In Figure 6a, the information concepts and the relationship to a data point are shown. Relationships are qualities that connect a point with other classes, with the major classes being the Location, the Equipment and the Measurements, also shown in Figure 6b, as well as their subclasses in Figure 6c depicts the example building. Based on this building, Figure 6d shows the relationships of it and it is understood that it represents an early visual of a KG. Brick models are making it easier to represent some subsystems in buildings, as they bypass their complex and heterogeneous character, and support the composition and hierarchies in the building [87]. Furthermore, Brick also stands out due to its ability to access open reference implementations on existing buildings, in order to authenticate the effectiveness of the solution.

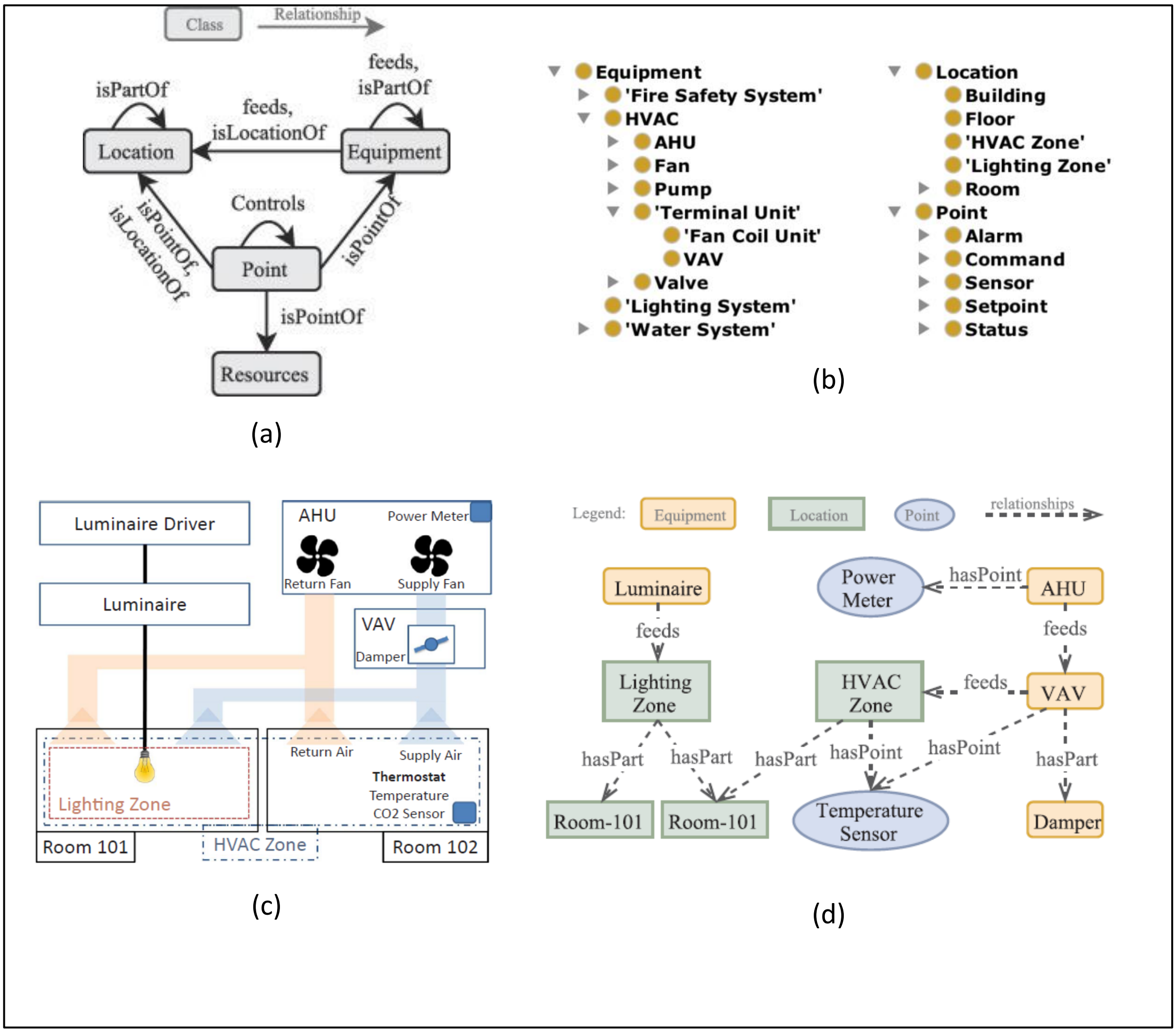


Figure 6: (a) Information concepts in Brick and their relationship to a data point, (b) A subset of the Brick class hierarchy, (c) A simple example building that highlights the components to be modeled in a building schema & (d) Brick classes and relationships for a subset of the example building in (c) [147]

HTO is an "open-source initiative to streamline working with data from the Internet of Things", based on Haystack [86]. Haystack is responsible for terminology and instance data representation. Its primary purpose is semantic data representation using depositories of name and value relations [148]. These names are called Tags and are used to describe instance data. The name-value pairs mentioned previously are called Defs, and the repositories are called libraries, where a group of them is utilized to describe instance data [148]. HTO is based on Haystack and utilizes semantic web technologies and organizes the tags' usage in parallel to enriching the current ontology [135]. HTO's structure is similar to the Brick ontology, and consists of site, equipment and points classes, which are also connected with an external weather class [149]. The tags are utilized to connect properties and product classes with any entity in the building structure.

Another important ontology is SAREF, which is "a tangible[89] object designed to accomplish a particular task in households, common public buildings or offices and in order to accomplish this task, the device performs one or more functions". SAREF4Building Ontology is an extension of SAREF, and is an ontology similar to BOT; however, the former includes sites, stories and a class of devices, whereas the latter does not [136].

The last ontology to be mentioned is REC, which has as its main role energy usage analysis and optimization, and the presence analysis of a building structure [150]. The ontology is based on two main and four secondary modules. The two main modules include the metadata and the core. The metadata module contains annotation properties, used for ontology documentation. The core module gathers high- level classes and properties that are frequently reused in REC modules. In addition, the core module imports the metadata module. Energy usage analysis and optimization refer to the fact that a facility that is more sustainable and planned energy usage is automatically applied. REC can support a BMS in different ways [106]. One is by controlling and analyzing energy usage by locating broken or misaligned sensors and by altering the HVAC and lighting system to the users' needs. Moreover, support can be given by anticipating future needs and loads and using thermo-dynamic effects. Presence analysis refers to the ability of the system to detect occupancy in the building. This detection is achieved with measurements such as the actual number of people in different rooms, the people flows in a building and the activity of these people [106]. REC's structure is close to that of BOT and SAREF4Building, except for some classes and a difference in component classification.

2.2.4.4 Occupant Behavior Related Ontologies

DNAs Framework is a powerful approach to represent the impact of occupants' behavior on the building's energy efficiency [103]. It separates that impact into four components, i.e., drivers, needs, actions and systems, which comprise the outside and inside world (see Figure 7). Drivers are the environmental elements that impact the occupants' psychological or physical needs in the inside world. The categories of this topology include building (component, properties, location), occupant (attributes, attitudes, location, state), environment (climate, indoor, outdoor, weather), system (properties, state) and time (day, week, month) (Figure 8a). Needs refer to the physical and non-physical necessities to satisfy the occupants in the inside world. Physical needs refer to biological needs (food, drink, bathroom, hygiene, sleep) and the need for comfort (thermal, acoustic, visual, IAQ) (Figure

8b). Actions refer to the interactions between the occupant and the systems or activities in which an occupant can participate to change environmental comfort. These actions are interactions with the systems, movement, and reporting discomfort or inaction (Figure 8c). Finally, systems refer to equipment or mechanisms an occupant can interact with to change environmental comfort. These systems are windows, shades/blinds, lights, thermostats, space, equipment, clothing and prompts/feedback (Figure 8d). The overall field of DNAs Framework's applications addresses questions regarding the types of behaviors it covers, why this framework is valuable, in which types of buildings it can be applied, who can use it, when it can be used and how it can represent energy-related behavior (Figure 9).

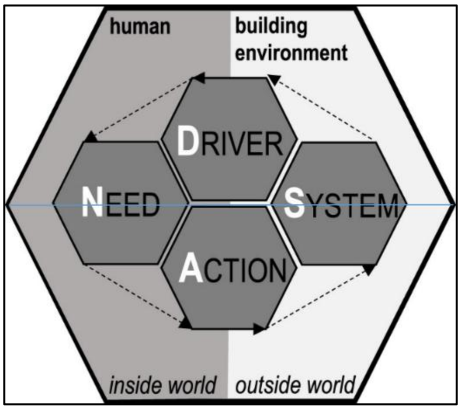


Figure 7: DNAs Framework Components [103]

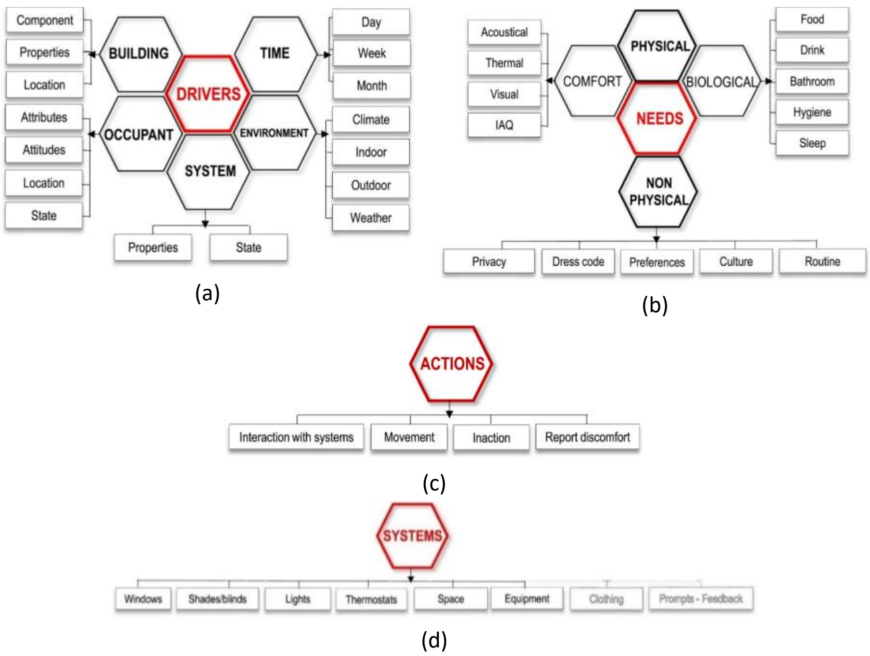


Figure 8: (a) Drivers that impact energy-related occupant behavior, (b) Needs of occupants that can impact the building energy use, (c) Actions taken by occupants to cover their needs & (d) Systems that an occupant can interact with and change the building energy usage [103]

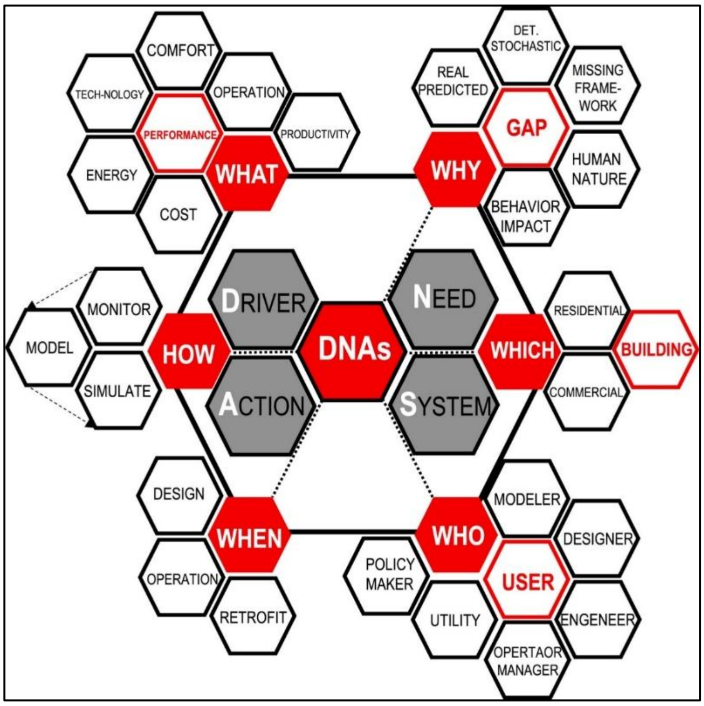


Figure 9: DNAs Framework Applications [103]

obXML is an attempt to implement DNAs Framework in the form of an XML schema, which resulted in a successful schema [99]. In its success, the obXML schema can describe occupant behavior in a structured way, to researchers and different stakeholders. Moreover, the schema provides a platform to describe the occupant behavior and assess the reaction between occupant behavior and building energy modeling. Furthermore, its design means it can be easily adapted and modified to include more elements in the schema. The DNAs framework is implemented in the obXML schema, linking three core elements which refer to the Building, the Occupants and the Behaviors. In addition to these core elements are the elements of Time of Day and Seasons. obXML has in its core DNAs Framework. obXML's trees categorize the core elements and the drivers, needs, actions and systems [99]. In Figure 10, an example of applying priority indicators for possible multiple actions taken in a Drivers-Needs-Actions-System framework is shown [99]. In this example, the indoor air temperature overheating is the driver, and the thermal comfort is the need. Moreover, the three actions to choose from are to close the blinds, turn on the HVAC, or open the window, and the system that it reacts with is the HVAC system.

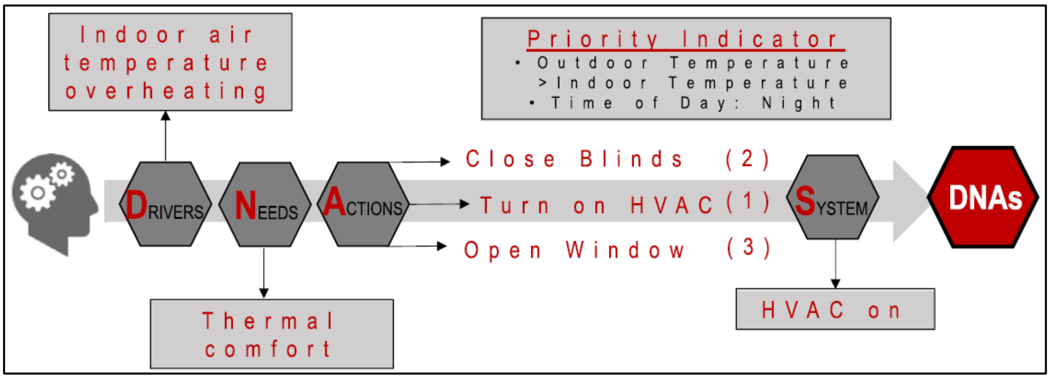


Figure 10: Example of priority indicators in DNAs Framework [99]

Next, another powerful ontology that considers human behavior is Onto-SB, which is a domain ontology for smart buildings [102]. This ontology considers factors of a smart building, namely humans, environment, services, devices, places, context-awareness, energy sources, profiles, etc. One of the core concepts of this ontology is the building concept. The building concept includes relationships with other concepts such as location, environmental parameters, actors and energy sources. Moreover, the activity concept is important and is divided into scheduled and inferred activities that a human can do in a smart building. Consequently, the human concept is also important for this ontology and includes characteristics such as name, age, weight, height and gender. Many concepts are also connected to the human profile, to create a better representation of the human concept in a smart building. This is rooted in the fact that human needs are responsible for the comfort in the building, which alters the energy consumption. The actors' concept is another and represents the residents of the smart building. The residents are divided into groups (family, friends, brothers, etc.) and individuals (Human and Nonhuman (pet, robot)) categories. This concept is connected with others, such as the human profile. Moreover, there is a service concept, which is connected with the appliances and devices concepts and has a type, grounding and model. This concept relates directly to the appliance that the user made the decision about. Furthermore, there is the time concept, which is divided into three classes, namely time-temporal, time-instant and time-interval. These classes include characteristics of time (hour, minute, second). Next, the concept of environmental parameters is also important and every location in a smart building is connected with that concept. Another important concept is the appliance concept. It includes categories of different devices, sensors and actuators. All three of these are connected with their location, the service they provide and the properties (ID, type, values, protocol) that defines them. The source concept is also a core concept and refers to the energy sources (renewable and nonrenewable) that can exist in a smart building. Finally, the place concept has a key role and represents different places in a smart building. This concept connects places with appliances, actors and the environment. It is also divided into indoor and outdoor places. Many other concepts are included in this ontology, but these are mostly the concepts that interact with human behavior.

2.3 KGs Data & Knowledge Management in Built Environment DTs

Over the past decades, the AEC industry has embraced digital tools, collectively referred to as DSSs, to facilitate planning, designing, constructing, operating, maintaining, and recycling in buildings, aiming to enhance collaboration among stakeholders and professionals for timely and effective decision-making to ensure the achievement of energy efficiency goals [151]. DSSs play a pivotal role in increasing efficiency and identifying optimal solutions across all stages of a building's life cycle, including renovation, by aiding stakeholders in selecting steps to improve energy efficiency while considering factors like IEQ, intervention costs, and overall environmental impact [152].

In this context, BIMs serve as digital representations of built structures, complementing the role of such a DSS. The National Building Information Model Standard (NBIMS) defines BIMs as digital resources that provide comprehensive information about a facility, supporting informed decision-making throughout its life cycle [153]. BIM facilitates data storage, information management, and data exchange among various users and tools like IFCs and gbXML [154], [155], [156]. Embracing the principle of continuous digital information usage throughout a structure's life cycle, BIM enables effective data sharing and exchange among collaborating stakeholders, surpassing traditional document-centric methods [154], [157]. BIM's capabilities extend to modeling BAS devices, enhancing semantic interoperability, and supporting FM by improving commissioning and operational phases [158], [159]. Moreover, BIM serves as a foundation for various intelligent applications through integration with domain knowledge and specific methodologies, leading to the development of data platforms and the utilization of semantic technologies for enhanced data integration and utilization [160], [161], [162], [163]. Additionally, the combination of different knowledge domains and reasoning with BIM can lead to the development of knowledge graphs.

DTs, resembling BIM in representing physical structures digitally, are distinguished by their integration with IoT technology, enabling real-time data collection from sensors installed in buildings for creating virtual representations [164], [165]. While BIM primarily aids error prevention, communication enhancement, and efficiency improvement during the design and construction phases, DTs focus on predictive maintenance, resource optimization, occupant comfort improvement, and knowledge transfer to future projects during the operational phase [166], [167], [168]. Stakeholders, including architects, engineers, constructors, and facility managers, utilize BIM and DTs at different stages of a building's life cycle, with BIM also holding valuable information for demolition processes [169], [170], [171].

Overall, digital tools such as BIM and DT based ones, generate a vast amount of data, encompassing planning, design, construction, operation, maintenance, and demolition/recycling processes, as well as sensor data from installed systems, aiming to enhance building energy efficiency [169], [172], [173]. However, challenges such as the complexity of data types, compatibility issues between software, and proprietary information hinder efficient data exchange and knowledge extraction among stakeholders with diverse backgrounds [164]. Stakeholders involved in various phases of a building's life cycle include architects, engineers, construction teams, facility managers, occupants, policymakers, and governance entities. The utilization of the semantic web, incorporating knowledge graphs and linked data, has been suggested and investigated to address data exchange and multi-stakeholder decision-making challenges, aiming to enhance communication and coordination [174]. Ontologies form the foundation of semantic web design, characterized by their formal nature, machine-readable capability, and interoperability [175].

DTs serve as DSS for buildings, potentially integrating knowledge graphs to tackle these challenges, effectively bridging the physical and cyber layers within a DT-KG architecture [176]. This architecture relies on runtime data and environmental parameters, transmitted from the physical to the cyber layer, to enable automatic adjustments or user-driven decision-making. A service interface is proposed to access synchronized digital models, including a Digital Twin-Physical Asset Awareness module facilitating ongoing parameter changes. Additionally, a metamodel such as an ontology plays a crucial role in the DT-KG architecture, establishing static and dynamic relationships between entities and connecting them to relevant data accessed by the physical asset. This ontology facilitates the creation and operation of the knowledge graph using digital data and models within DTs [176]. Proposed applications of knowledge graphs in DTs include internal linking and referencing, knowledge completion, error detection, collective reasoning, and semantic querying, as supported by existing literature [176], [177].

2.4 Neighborhood- level Decision Support (DS) Functions

Neighborhood-scale decision support systems integrate multiple disciplines to enhance sustainable urban planning and energy efficiency. A comprehensive review of ZENs and PEDs highlights the importance of key thematic areas such as energy systems, ICT, stakeholder engagement, urban morphology, LCA, social aspects, and microclimate dynamics [178], [179].

By structuring energy, economic, and environmental data within a semantic framework, KGs enhance MCDA, allowing urban planners to compare renovation scenarios and optimize trade-offs between cost, energy efficiency, and stakeholder preferences[180]. Moreover, KGs enable the seamless integration of LCA and LCC assessments, improving decision transparency and traceability[181], [182]. When integrated into AI-driven Digital Twins, KGs enable predictive analytics by structuring historical and real-time data. This enhances automated reasoning, allowing DSSs to anticipate energy trends, optimize urban planning, and minimize uncertainty in scenario planning[183], [184].

Decision support frameworks rely on LCA to assess the environmental impact of design and renovation choices, while LCC evaluates the long-term economic feasibility of green investment projects[181], [182]. Energy management strategies, such as mobility planning and smart grids, help balance demand and supply at the neighborhood scale. Building interconnections are increasingly significant in energy assessments, as hourly load analyses help evaluate interactions between buildings, EVs, and energy storage systems[185], [186]. LCA and LCC further support financial and environmental assessments, ensuring energy systems align with sustainability goals[181], [182].

With growing urban complexity, data-driven decision support tools are essential for optimizing energy efficiency and cost-effectiveness. DTs simulate real-world scenarios, allowing stakeholders to evaluate energy and renovation strategies before implementation[183], [184]. Advances in AI and ML further enhance urban energy analysis, using structured knowledge from KGs to improve predictive modeling [183], [184], [187]. Reinforcement learning-based adaptive DTs have shown notable improvements in energy efficiency and resource optimization, while KG-driven reasoning helps refine automated risk and sensitivity analyses, reducing uncertainty in decision-making[184].

Neighborhood-level decisions require collaboration among municipalities, urban planners, energy providers, and residents. Decision support systems integrate MCDA to evaluate economic, social, and environmental priorities[180]. Stakeholder-driven scenario exploration aligns decisions with local policies, while participatory governance frameworks ensure greater acceptance and long-term sustainability[188], [189]. These approaches foster co-creative planning, supporting equitable and adaptable urban transitions.

Modern decision support frameworks also incorporate smart grids and distributed energy systems. DERs such as solar PV and wind turbines enhance local energy independence[190]. Battery storage solutions and demand-side flexibility optimize energy use while increasing grid resilience[186]. Additionally, P2P energy trading allows communities to exchange surplus energy, reducing reliance on centralized grids[191]. Blockchain-enabled trading and battery-sharing in microgrids further enhance cost-effectiveness and grid stability by minimizing energy waste and dependence on traditional power infrastructures[192], [193].

By integrating these innovations, decision support systems enhance energy autonomy, optimize costs, and strengthen resilience. However, further research is needed to refine real-time data analytics, stakeholder engagement frameworks, and regulatory structures for effective cross-sectoral energy planning[184], [189]. As DSSs evolve, the integration of KGs with DTs will be pivotal in bridging disconnected datasets, supporting semantic reasoning, and ensuring informed, knowledge-driven decision-making[180], [184]. Moving forward, leveraging KGs as a core component of AI-enhanced DSSs will unlock new potentials in predictive urban planning, resource optimization, and climate-resilient city strategies[183], [184].

3. Methodology & Proposed Solution

3.1 Methodology

The methodology followed in this thesis is illustrated in Figure 11. Initially, the framework is introduced by defining the challenge, the scope, and the state-of-the-art. Next, a thorough investigation of the technical aspects is conducted, establishing the solution and methodology which introduces and reviews KGs, DTs, and ontologies within the built environment context. The developed KG-based architecture is proposed as a collaborative solution for structured data and knowledge management, supporting stakeholders in decision-making processes. This architecture is validated through two distinct case studies. The first is at the building scale, examining paraffin-based phase change material PCM interventions for energy efficiency improvements at Leaf House. The second case study addresses a neighborhood scale, exploring PV and battery interventions at the TUC campus, assessed through LCC and LCA. Both case studies illustrate the practical application of the KG-based architecture, tailored to represent physical entities and their relationships in digital twins. Ontologies tailored specifically to each case study facilitate structured integration and reuse of available data, scenarios, and assessment KPIs. Finally, enriched KGs from the case studies effectively provide stakeholders with structured and interconnected knowledge, ultimately supporting informed and optimized decision-making.

3.2 Interventions Assessment Plan

As it was already explained, the focus of this work is to provide support for the decision-making processes linked with designing renovations in a neighborhood. Often, the goal of these processes is to ensure access to affordable energy and low to zero emissions. To accomplish that, an assessment plan is required, that delineates how the goals towards lower emissions can be achieved. As shown in Figure 12, the first thing that is required is to establish the assessment scenarios, including the baseline and the interventions scenarios. The next step is to conduct the scenarios assessment. Each scenario can be thought of as a sequence of actions taking place in consecutive life cycle stages e.g. planning, design, operation etc. As part of this process, the use of assessment tools or decision support functions is necessary alongside the definition and evaluation

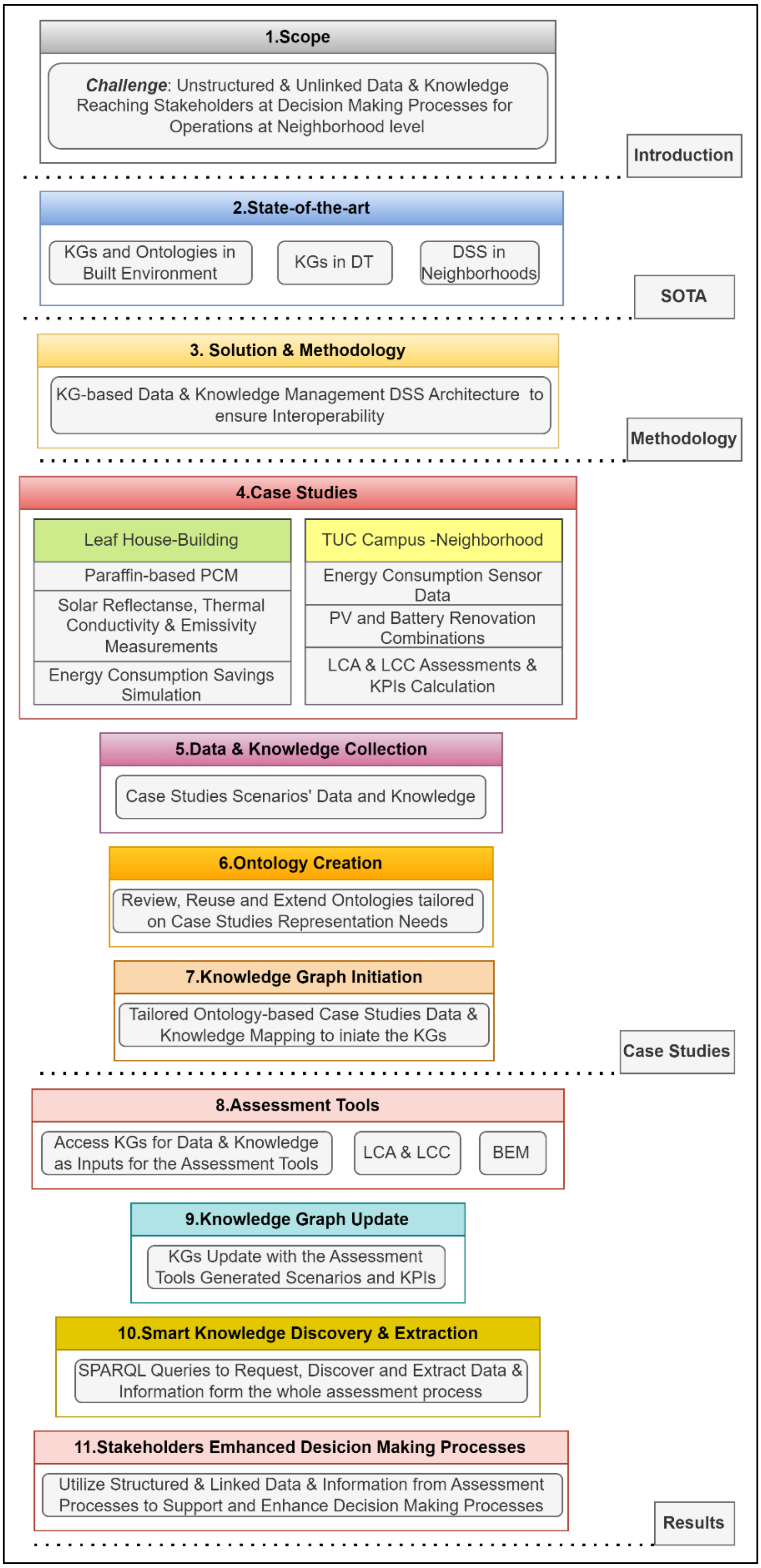


Figure 11: Thesis Methodology

of KPIs. The selected tools are parameterized based on neighborhood data normally referred to as inputs, in order to calculate and produce useful KPIs and possible other complementary types of outputs. The main challenge identified here is that the variety and large volume of neighborhood data, numerous scenarios, and diverse KPI outputs associated with each scenario and assessment tool pose complexities for structured storage and management, making it challenging to support stakeholders effectively in their decision-making processes. To tackle that, a KG-based data and knowledge management DSS architecture at neighborhood-level is proposed in Section 3.3.

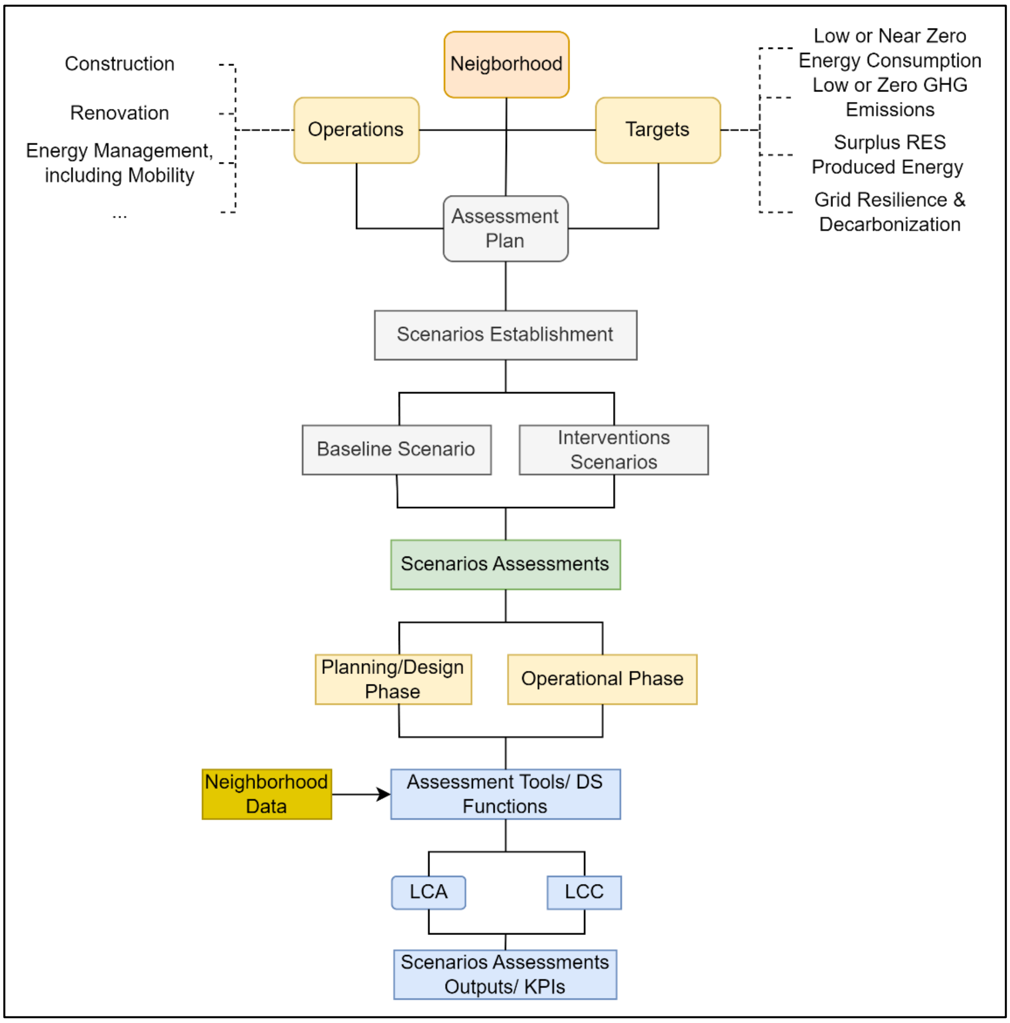


Figure 12: Neighborhood Interventions Assessment Plan

3.3 KG-based DT Architecture for Stakeholders Decision Support at Neighborhood level

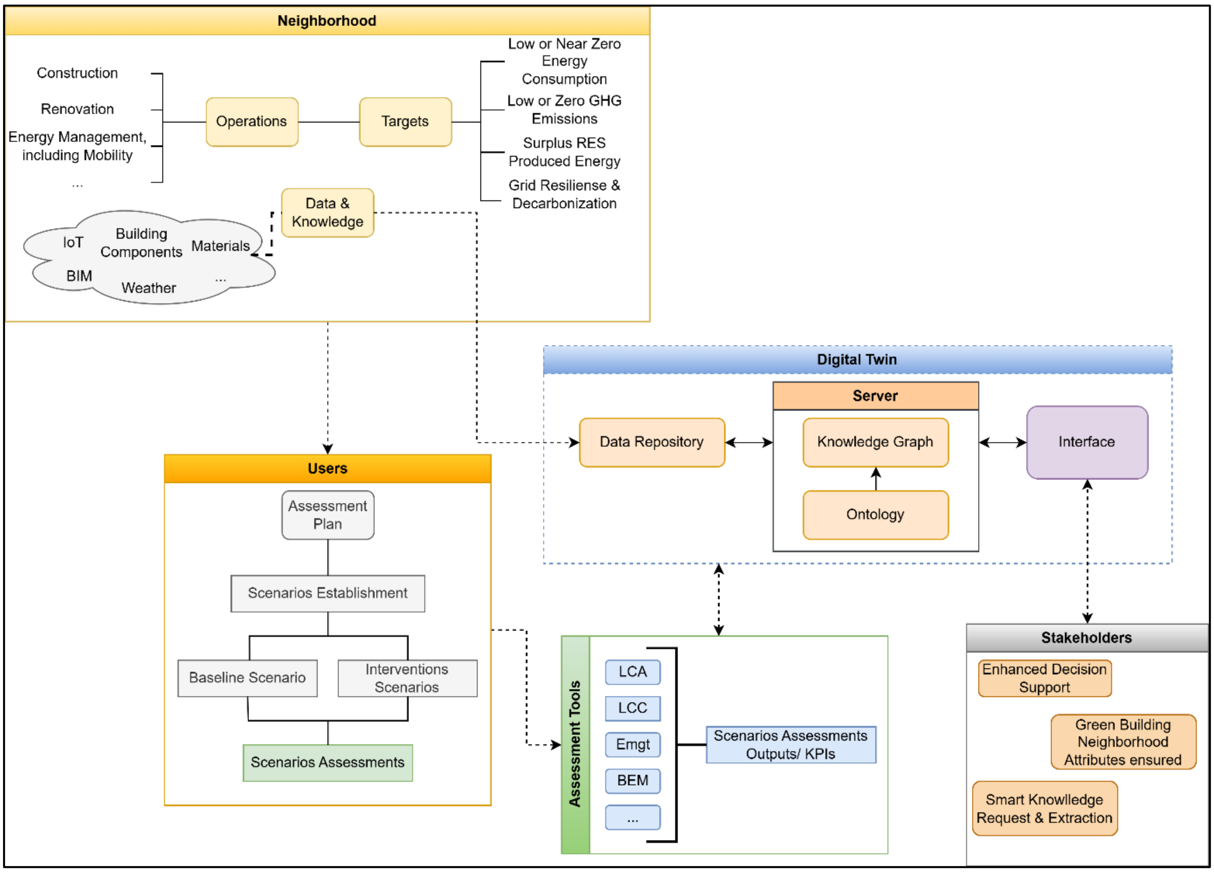


Figure 13: Proposed Innovative Solution Concept

This novel architecture's aim is to cover the need for data and knowledge management at neighborhood level, created from the interventions assessment plan, to manage and structure the different data and knowledge connected to the intervention scenarios, and hence supporting stakeholders through decision support process. In Figure 14, the KG-based DSS architecture is shown. Starting with the various kind and large amount of neighborhood data, the KG is able to structure them under the tailored case study ontology, which is able to represent the different classes associated with the neighborhood data and the intervention scenarios, as well as the relationships between them. The KG is then able to provide structured information to different processes through discovery and extraction queries.

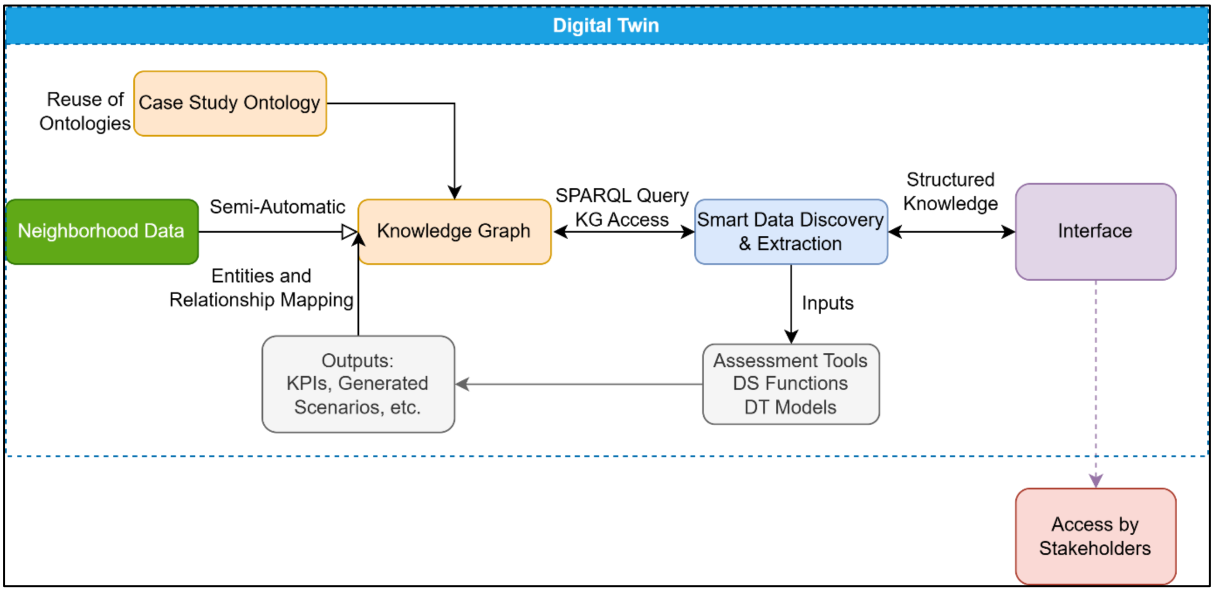


Figure 14: KG-based Data & Knowledge Management DSS Architecture

One of the processes that will require the data from the KG as inputs, is the feed of assessment tools or DS functions. The tools will generate new outcomes and KPIs based on the inputs from the KG. So, the new data and knowledge can then be integrated in the KG and be structured and connected alongside the neighborhood data and the established scenarios.

Another process to use the structured information through data and knowledge discovery and extraction, is after having integrated the assessment tools' outcomes to the KG and having connected them to the scenarios. Then, the intervention scenarios connected with their neighborhood data, as well with the assessments' KPIs, are able to support stakeholders during decision making. However, these scenarios might of a great number, hence returning to the initial challenge, being a lot to be handled by stakeholders during decision making processes. So, the scenarios outcomes would still create confusion.

4.Case Studies

4.1 Enhancing Building Energy Efficiency with Paraffin-Based PCMs: Leaf House Case Study-Building level

4.1.1 Phase Change Materials in Buildings

In the quest for sustainable development and climate change mitigation, improving building energy efficiency is a primary objective. Innovative paraffin-based PCMs offer a promising solution in this regard. PCMs have the unique capability to store and release large amounts of thermal energy during phase transitions, effectively regulating indoor temperatures [14]. Thermal Energy Storage includes various methods, such as utilizing latent heat, the sensible heat capacity of materials, or the exothermic and endothermic chemical reactions of materials [13]. PCMs are a Thermal Energy Storage method and are known for storing or releasing thermal energy through latent heat storage [16]. This fact has proven particularly promising over the past few decades, as PCMs have a significant latent heat capacity, making them highly effective for man-aging a building's thermal environment. By transitioning between solid and liquid phases, PCMs can efficiently absorb and release heat, thus reducing heating and cooling loads and shifting peak energy demands [194]. During the day, PCMs absorb excess solar energy, minimizing heat penetration into the building. At night, when temperatures drop, PCMs release stored heat, maintaining indoor thermal comfort [195].

PCMs contribute significantly to the sustainability goals of green building certification systems like LEED and BREEAM by enhancing energy efficiency, reducing green-house gas emissions, and improving indoor environmental quality [196]. By incorporating PCMs into building materials, energy consumption for heating and cooling can be substantially decreased, leading to lower operational carbon footprints. This aligns with LEED and BREEAM credits for energy optimization and reduction of environmental impacts. Additionally, the improved thermal regulation provided by PCMs enhances occupant comfort and indoor air quality, contributing to credits related to health and wellbeing. The use of PCMs also supports the efficient use of resources and materials, a key aspect of these certification systems. In general, paraffin-based PCMs help buildings achieve higher performance in energy efficiency, sustainability, and occupant comfort, thus sup-porting the comprehensive goals of green building certification systems. Buildings designed with PCMs contribute to reducing overall energy consumption, thereby mitigating environmental impact and promoting resource conservation. Furthermore, integrating PCMs supports the advancement of net-zero energy buildings, offering significant eco-nomic and environmental benefits for society [18]. As PCM technology continues to evolve and gain traction, its implementation represents a critical step toward achieving energy-efficient and environmentally sustainable buildings [197]. For example, integrating PCMs into the outer face of south-side brick walls resulted in a 13.4% energy savings, although a 30-year life cycle analysis indicated that this might not be cost-effective. Similarly, PCM dry walls significantly improved energy efficiency in a Mediterranean climate like Coimbra, Portugal, with gains of up to 62%, though effectiveness varied in other climates, showing energy efficiency improvements ranging from 10% to 46% [14], [198], [199].

Figure 15 illustrates the categories of PCMs, focusing on paraffin-based types and their various applications in building components. The diagram categorizes PCMs into solid-solid and solid-liquid transitions, with paraffin-based PCMs highlighted for their use in construction materials [15]. Paraffin-based PCMs, derived from organic compounds, are used due to their high latent heat storage capacity and compatibility with different building materials. The organic category encompasses fatty esters, fatty acids, alcohol/polyols, and paraffins. Compared to other PCM types such as salt hydrates and fatty acids, paraffin-based PCMs generally offer superior thermal stability and a more consistent phase change temperature, which translates to more reliable performance over time. While salt hydrates can have higher latent heat capacities, they often suffer from issues like subcooling and phase separation, which can reduce their effectiveness and reliability. Fatty acids, on the other hand, are biodegradable and environmentally friendly but may not provide the same level of thermal stability as paraffin-based PCMs. Paraffin-based PCMs strike a favorable balance between energy savings, thermal regulation, and long-term stability, making them a competitive choice compared to salt hydrates and fatty acids for building applications. The applications depicted in the figure include integration into floors, bricks, walls, roofs, and windows, showcasing the versatility of paraffin-based PCMs in enhancing the thermal performance of buildings . This integration helps in reducing energy consumption by improving the thermal regulation of indoor environments, thus contributing significantly to energy-efficient building designs. The figure encapsulates the potential of paraffin-based PCMs to transform conventional building practices by incorporating advanced materials that support sustainable and energy-efficient architecture.

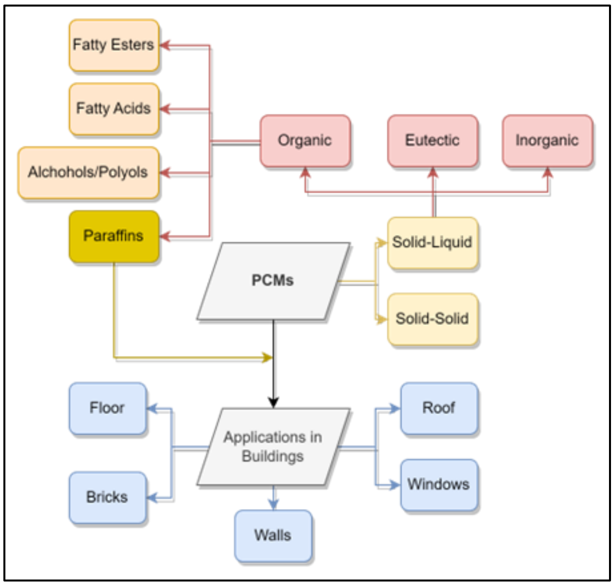


Figure 15: Paraffin-based-focused PCM categories, and their applications in Buildings

Advancements in PCM technology, particularly in encapsulation and the development of composite materials, have significantly enhanced the effectiveness of paraffin-based PCMs in building applications. Encapsulation techniques, such as microencapsulation and macroencapsulation, are crucial for improving the thermal stability, pre-venting leakage during phase transitions, and enhancing the durability of PCMs when integrated into building materials. According to [17], incorporating additives such as expanded graphite into paraffin can increase its thermal conductivity by up to 6.5 times, addressing the low thermal conductivity that is typically a limitation of paraffin-based PCMs. Additionally, another review highlights that encapsulating PCMs within building elements not only improves their thermal performance but also facilitates easier integration into various construction materials, leading to better energy efficiency and indoor thermal comfort [200]. The use of encapsulated PCMs in building elements helps maintain stable indoor temperatures by effectively absorbing and releasing heat, thereby reducing the load on heating and cooling systems. These advancements make paraffin-based PCMs more practical for a wide range of applications in sustainable building design, offering substantial benefits in both energy savings and improved indoor environmental quality.

Extensive research has explored the use of paraffin PCMs within building components, leading to emerging alternatives like biobased PCMs [199]. However, much of this research has been limited to simulation studies or laboratory-scale experiments. The un-tapped potential lies in implementing PCMs in real-life building environments to evaluate their thermal performance in real-time scenarios. Current studies predominantly emphasize singular applications [17], [19], [20], [200], [201], [202], [203]. However, by diversifying integration across multiple building elements, like walls, ceilings, and floors, there is potential for varied outcomes that enhance building performance, aligning with sustainable efforts to transition conventional structures into net-zero energy buildings [199].

Specifically, within civil engineering, PCM applications focus on energy-saving through temperature regulation, particularly in building walls, roofs, ceilings, and floors. For instance, research by Rathore et al. [21] embedded PCM-filled tubes in walls, achieving a moderate reduction in peak temperatures and energy savings. Yan et al. [204] integrated PCM systems with nocturnal sky radiators, significantly reducing indoor temperatures and energy consumption during hot weather. Lee et al. developed PCM thermal shields that reduced peak [205]heat fluxes and delayed temperature peaks. These examples underscore PCM's efficacy in enhancing building thermal performance and reducing energy consumption [206], [207].

Recent studies have shown significant advancements in passive thermal management of buildings through the integration of PCMs, particularly when these materials are enhanced by innovative techniques. For instance, the use of PCM microcapsules enhanced by SWCNTs has been demonstrated to improve thermal performance significantly, offering better heat storage and release characteristics, which is crucial for maintaining indoor thermal comfort [208]. Furthermore, the scaling laws for fluid transport phenomena in porous PCM media have been extensively studied, providing insights into the permeability and porosity relationships critical for optimizing PCM-based systems in building applications [209].Moreover, PCM applications extend be-yond traditional materials like concrete walls to include innovative uses such as PCM-enhanced gypsum boards [210], [211], wooden composites [212], and PCM-filled double-glazed windows [210], [211], [212], [213], [214], [215], [216]. These applications illustrate the potential for PCM integration to improve thermal insulation and regulate indoor temperatures effectively [210], [211], [212], [213], [214], [215], [216]. The integration of PCMs in low-scale personal cooling systems has been experimentally validated, demonstrating enhanced efficiency and operational autonomy [217].

In challenging environments, PCMs have been explored for their ability to mitigate temperature fluctuations and enhance structural integrity in materials like concrete and pavement [218], [219], [220], [221]. These studies highlight PCM's potential in diverse applications ranging from construction materials to pavement maintenance and beyond.

However, despite these advancements, practical challenges remain, including high costs, technical complexities in integration, and the need for standardized assessment methods [217], [222], [223]. Further research and development are crucial to overcome these challenges and promote wider adoption of PCM technologies in building applications.

While paraffin-based PCMs significantly enhance thermal performance by improving energy storage and temperature regulation in building materials, their integration can present trade-offs with other critical material properties such as mechanical strength and fire resistance. The inclusion of paraffin-based PCMs in cementitious composites can lead to a reduction in mechanical strength due to the softer and more flexible nature of PCMs compared to the host matrix, which may weaken the material under stress [224]. Additionally, paraffin-based PCMs are organic and inherently flammable, potentially compromising the fire resistance of building materials. This presents a significant safety concern, especially in applications where fire resistance is critical. However, advancements such as the incorporation of fire-resistant additives or encapsulation methods have been developed to mitigate these risks, enhancing the fire performance of PCM-enhanced materials [225]. While these strategies can help balance thermal benefits with safety and structural integrity, they underscore the need for careful material design and selection when integrating PCMs into building applications.

The innovative application of paraffin-based PCMs for building energy efficiency can be paralleled with advancements in hydrogen storage materials. Recent advancements in PCMs, such as the integration of multi-wall carbon nanotubes to enhance photothermal conversion and storage, have shown promising results [226]. For example, the addition of metal oxide catalysts to organic hydrogen storage materials has shown promising results in reducing dehydrogenation temperatures and enhancing thermal stability [227]. Similar to the use of paraffin-based PCMs in building energy efficiency, the integration of metal oxide additives to improve thermal stability in hydrogen storage materials is another area of active research.

4.1.2 Case Study Building: LeafHouse

Leaf House, located in Angeli di Rosora, Ancona, Italy, serves as the case study building, owned and operated by the Loccioni Group (Figure 16). This facility functions as a hub for research and innovation in various sectors, including energy and sustainability. The Leaf House is a residential apartment complex with a rectangular layout, showcasing an innovative bioclimatic design and advanced technologies. It features six highly insulated apartments with a total floor area of around 470 m^2. The building is equipped with a ventilated roof, solar tubes, smart monitoring and control systems, building-integrated photovoltaics, geothermal air preconditioning with heat pumps, solar thermal collectors, electrical storage, and a user-friendly energy management system [228]. That study further validates the energy performance of the Leaf House through dynamic simulation models and real-time operational data, highlighting its success in integrating renewable energy technologies and advanced energy management practices.

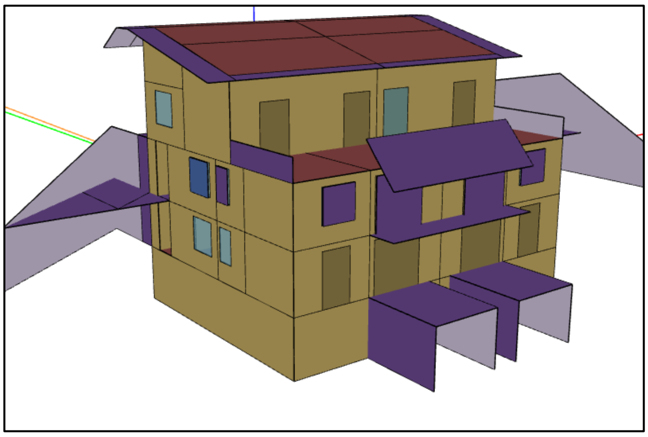


Figure 16: Leaf house case study building model in OpenStudio.

3.4.1.3 Leaf House Case Study Methodology

The methodology employed in this research is illustrated in Figure 17. The material samples used in this study consist of mixtures of N-octadecane, which has a melting point of 28 °C and serves as the phase change material, and a lightweight ceramic/carbon foam [51] acting as the shape stabilizer. These composite PCM/foam materials are used as thermal energy storage additives in cement and gypsum boards (Figure 18). Initially, the thermal conductivity and specific heat of these boards are measured using the Hot Disc TPS 1500, their solar reflectance with the UV Carry 5000, and their emissivity with an Emissometer equipped with a Scaling Digital Voltmeter Model AE1 RD1 (Figure 18). These measured characteristics, along with other inputs, are then simulated as components in the external roofs and walls of the case study building. The building simulation is conducted using the EnergyPlus simulation tool, where various scenarios and their energy savings results are evaluated (Figure 19).

The measured samples included various compositions: cement boards with 0%, 10%, 20%, and 30% v/v PCM/foam, and gypsum boards with 0%, 10%, 15%, 20%, and 30% w/w octadecane mixtures PCM/foam.

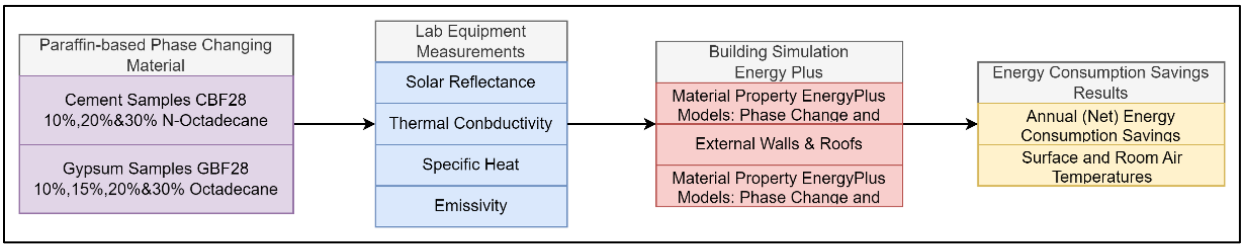


Figure 17: Leaf House Case Study Methodology

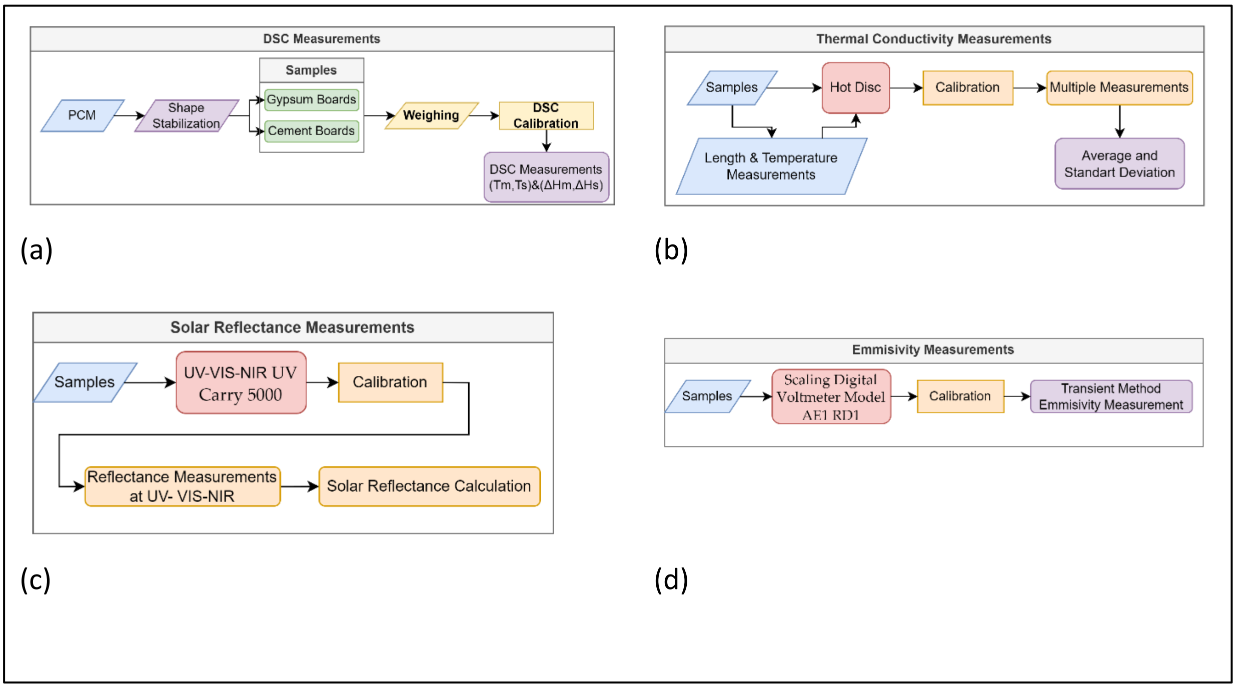


Figure 18: Experiments setup. (a) Differential Scanning Calorimeter (DSC), (b) Thermal conductivity, (c) solar reflectance, and (d) emissivity

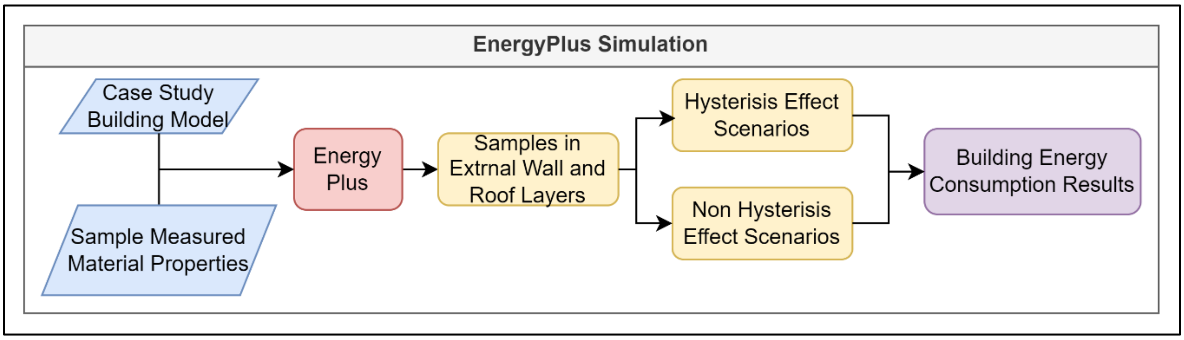


Figure 19: EnergyPlus building simulation model with measured PCM material properties

4.1.3 EnergyPlus PCM Simulation in Buildings

The building energy simulation in EnergyPlus utilizes PCM materials, simulated using the MaterialPropert:PhaseChanging and MaterialPropert:PhaseChangingHysterisis types. Incorporating these types necessitates an additional algorithm. The CTF is the default method for computing conduction heat transfer in building cooling/heating loads and energy calculations in EnergyPlus. It simplifies calculations by efficiently computing surface heat fluxes in a straightforward and linear manner, without requiring detailed temperature and flux data within the surface. However, it assumes constant properties and lacks results for the interior of the surface, limiting its applicability in dynamic thermal scenarios involving phase-changing materials.

In contrast, the CondFD solution algorithm is designed for complex constructions like those utilizing PCMs. It complements the CTF method by accommodating cases of variable thermal conductivity and material properties. The CondFD method determines the number of nodes in each layer of the surface based on Fourier stability criteria, making it particularly suitable for short zone time steps. The MaterialPropert:PhaseChanging defines material properties for phase changes assuming a constant phase change temperature, while MaterialPropert:PhaseChangingHysterisis includes hysteresis effects, allowing for different temperatures during melting and solidification. This feature captures the non-linear behavior of materials during phase transitions.

4.2 LCA & LCC Neighborhood-level Assessments: TUC Campus Case Study

4.2.1 TUC Campus Case Study

The proposed framework will be tested in a case study example in the TUC campus. TUC (1977) is located in Chania, Crete, Greece and is home to five school departments, and facilitates more buildings for administrative and other activities. In its premises, there are also a group of dorm buildings, a restaurant, athletic facilities and a library. There are 19 electric power meters installed all over the campus, and its load can be showed in different timesteps thought the day in TUC's website[229], as shown in Figure 20.

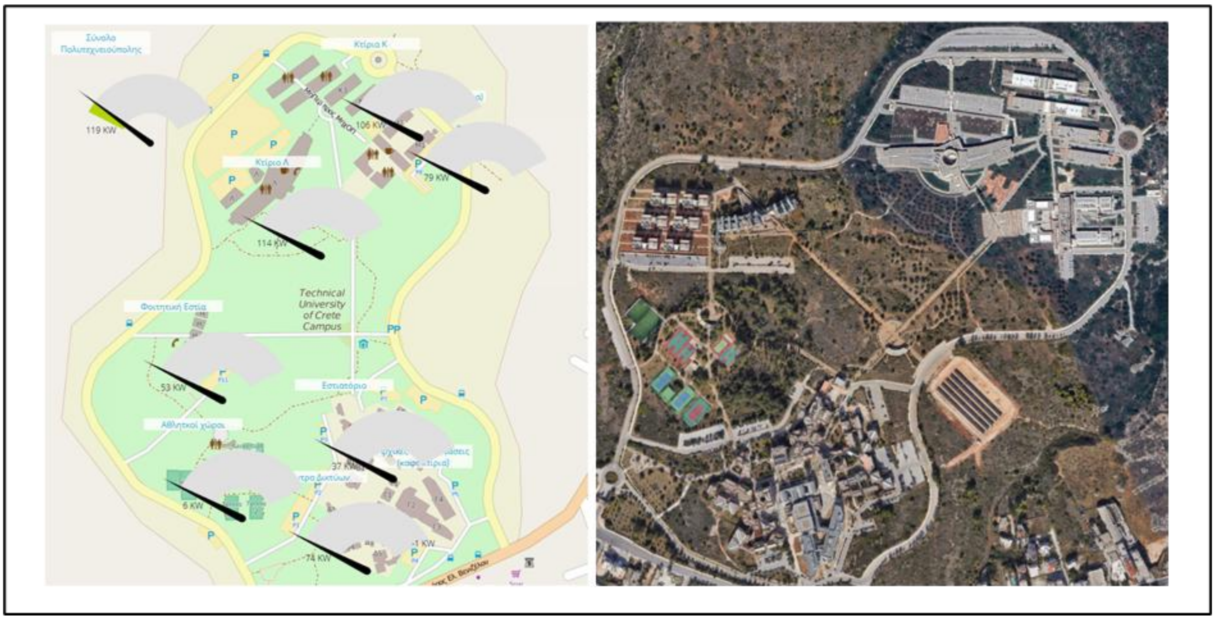


Figure 20: Screenshot of TUC in a specific time, including different neighborhoods power (kW) measurements.

The data from the electric power meters are stored in a mySQL database and include hourly measurements for each of the 19 meters that are installed (2014-2023). The first action for the case study is to structure the meters data inside the KG, in addition to the building clusters and the devices that are connected with the sensors. This takes place under the tailored case study ontology described in Section 5.2.1. In order to create the ontology as well as move it to a KG, the Protégé[230] tool is used. After mapping the different buildings, devices and sensors, a link from the database to the sensors needs to be established. Mapping all the timeseries measurements from 2014 until 2023, would create a chaotic KG with timestamps and measurements, hence hiding the true knowledge, enlarging the file's size and creating longer duration processes. So, to avoid that, universal unique identifiers (UUIDs) are given to the database and to each different sensor. Therefore, when requesting data from a KG, someone would only reach the sensor, which holds information to a specific UUID in database (Figure 21)After that, requesting the measurements for a specific time period, the associated values will be returned by the database. The query request is written in SPARQL language in order for the understanding of the RDF triples by the KG (Figure 22). Following this process, the power measurements for the whole TUC campus were extracted for 2022 (Figure 23), and the annual electric energy requirements were calculated to be 2.44 GWh. The aim of this case study is to create intervention scenarios that will include RES to cover different percentages of the electrical load of TUC.

pm_id	pm_host_id	pm_dev_id	pm_meas_id	pm_meas_value	pm_meas_timestamp	UUIDS
6406255	6	4	1	14785.56934	1/24/2022 7:14	452499d2-5daa-4165-85f8-5fc379e3c63e
6406258	3	1	1	92762.51563	1/24/2022 7:17	ae3bf630-17c7-4b79-a3be-32cf30053d2d
6406269	5	1	1	164137.9063	1/24/2022 7:20	94e8eda7-c0ed-4979-b334-ea4df1cc8e7a
6406267	6	2	1	0	1/24/2022 7:20	cf9fd61f-2064-4523-8941-254146dcbea7
6406293	5	1	1	12074.46606	1/24/2022 7:21	a06966f3-86c5-4bd4-851d-ff743aee5b33
6406309	6	3	1	38663.3677	1/24/2022 7:30	2d9df46e-2f64-41b2-9a99-cf34dd508d1b
6406311	2	1	1	5773.526785	1/24/2022 8:08	14e47980-1a6f-4cec-b156-5717db02d631
6406317	5	1	1	59209.46094	1/24/2022 8:06	37456790-0bec-48f5-a325-4f5fb6177626
6406330	6	1	1	108719.2266	1/24/2022 8:07	780c77f9-bbce-4fac-ac1c-bd1630766e59
6406331	3	1	1	25112.10742	1/24/2022 8:18	b93e7876-2d52-4d14-8134-5eba6fbf305a
6406335	5	1	1	4261.015152	1/24/2022 8:13	c3deb979-9c78-4954-bc95-9a1008c0a936
6406337	2	1	1	8010.219727	1/24/2022 8:13	1b38d24c-ef7f-4104-a9cd-b773030c4ae4
6406351	5	1	1	13808.52539	1/24/2022 8:14	452499d2-5daa-4165-85f8-5fc379e3c63e
6406354	3	1	1	66798.94531	1/24/2022 8:17	ae3bf630-17c7-4b79-a3be-32cf30053d2d
6406365	5	1	1	103616.2422	1/24/2022 8:20	94e8eda7-c0ed-4979-b334-ea4df1cc8e7a
6406367	6	2	1	1	1/24/2022 8:20	cf9fd61f-2064-4523-8941-254146dcbea7
6406383	5	1	1	15340.49023	1/24/2022 8:52	a06966f3-86c5-4bd4-851d-ff743aee5b33
6406399	6	3	1	38663.36766	1/24/2022 8:30	2d9df46e-2f64-41b2-9a99-cf34dd508d1b
6406407	2	1	1	5408.526172	1/24/2022 9:08	14e47980-1a6f-4cec-b156-5717db02d631
6406413	5	1	1	69168.60938	1/24/2022 8:06	37456790-0bec-48f5-a325-4f5fb6177626
6406425	6	1	1	119645.4922	1/24/2022 8:07	780c77f9-bbce-4fac-ac1c-bd1630766e59

Figure 21:Measurement table exported from MySQL Workbench. Column labels correspond to: 1) TUC Neighborhood ID, 2) Device ID, 3) Measurement ID (Power Active in W), 4) Measurement Value, 5) Measurement Timestamp, 6) UUIDs (Universal Unique Identifiers for each device).

```
SELECT DISTINCT ?g ?pm ?ud ?n
WHERE {
  ?pm brick:isPointOf ?g .
  ?g a brick:Energy_Generation_System .
  ?pm a brick:Electric_Power_Sensor .
  ?pm brick:hasTimeseriesId ?ud .
  ?n a s4city:Neighbourhood .
  ?n brick:hasPart ?g .
}
```

Figure 22: SPARQL query example asking data from the KG connected to the Database.

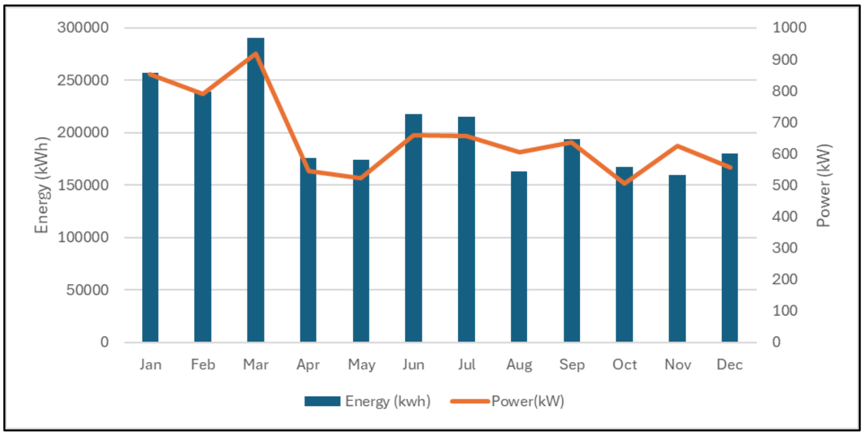


Figure 23: Load Timeseries data for TUC meters for 2022

The scenarios include two different types of bi-facial PV modules, one type of inverter and the option to have a Li-ON Battery as an energy storage system with self-consumption dispatch capabilities. In the current work, these scenarios are going under LCA and LCC assessments. Therefore, once the first the scenarios are established, the proposed systems are sized and the LCC assessment is being conducted. System Advisor Model (SAM)[231] is used for conducting a 25-year period analysis, as well as producing KPIs, such as Net Capital Cost (NCC), Net Present Value (NPV), Levelized Cost of Energy (LCOE) as well as nominal & real payback period. In addition, an LCA is conducted based on the sizing of the systems for each scenario. The LCA is conducted with the aid of Environmental Product Declarations (EPD) for each of the RES components.

After the assessments are completed, the scenarios and their KPIs are mapped in the KG based on the case study ontology. Lastly, SPARQL queries are proposed for scenarios and KPIs extraction, in addition to a more user-friendly approach under Protégé tool. Stakeholders are then able to assess the scenarios with all the KPIs from the different assessments. More details of the procedures and assessments, as well as their results, will be explored in Section 5.

4.2.2 TUC Campus Case Study Methodology

Figure 24, depicts the methodology that is followed in this work. First, the research challenge is highlighted, being the data and knowledge management through different operations at neighborhood-level. Following, the proposed solution is established, being the neighborhood level KG-based DT DSS architecture, that involves the tailored case study ontology. Moreover, the architecture is tested in Technical University of Crete (TUC) campus, involving an LCC and an LCA assessment for a number of renovation intervention scenarios. The results of the assessments are then integrated into the KG, again based on the case study ontology, and a series of prewritten queries for DT are examined, aiming to support stakeholders in decision making processes.

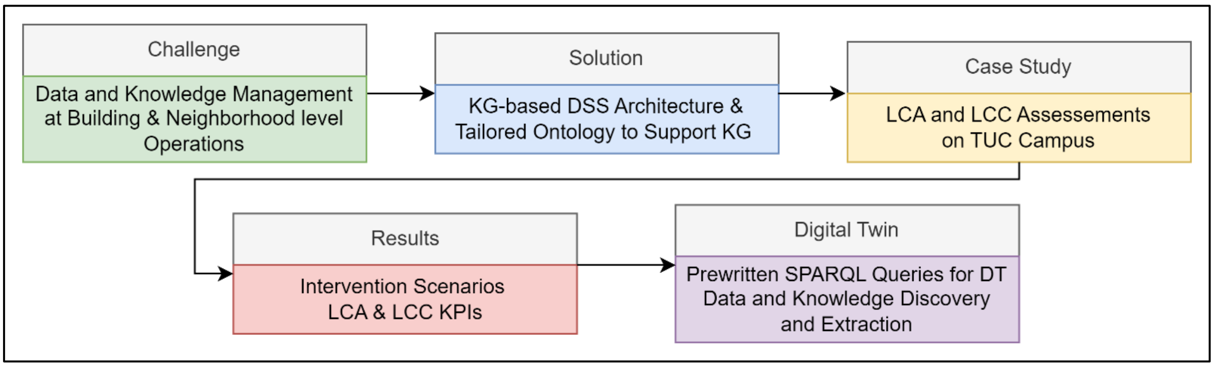


Figure 24:TUC Campus Case Study Methodology

5.Results

5.1 Leaf House Case Study-Building level

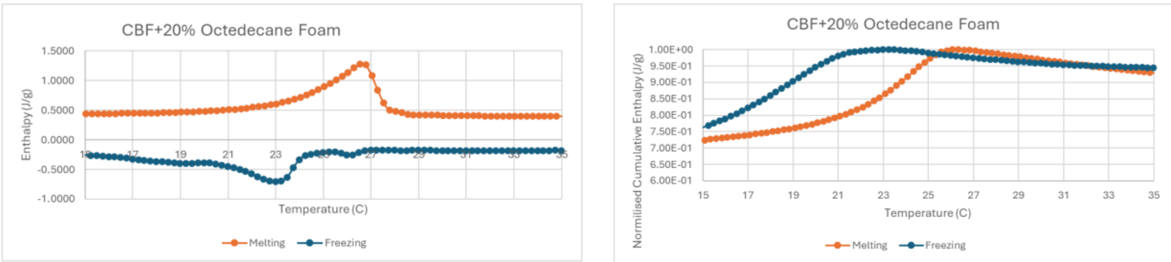
5.1.1 Material Characteristics Measurements

5.1.1.1 DSC Enthalpy Diagrams

In

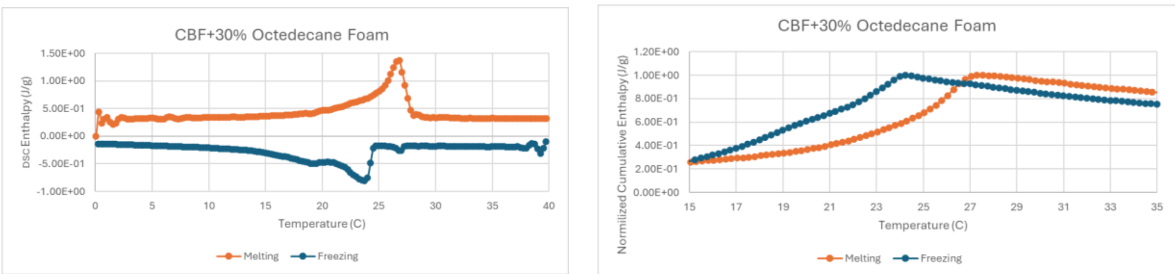
Figure 25-Figure 31, the results from the DSC measurements are depicted in enthalpy (J/g) over temperature (C) for all 7 material samples. In this context, enthalpy represents the amount of heat absorbed or released by the material as its temperature changes, reflecting the phase change behavior of the PCM within the composite. For both board types, the higher the percentage of PCM foam, the more the material's enthalpy tends to imitate the enthalpy curve of PCM. Hence, with these mixtures, construction materials like cement and gypsum acquire PCM characteristics without losing their own.

*Figure 25:*Cement board with 10% *v/v* PCM/foam: (a) DSC enthalpy diagram over temperature of melting and freezing curves; (b) normalized cumulative enthalpy diagrams of melting and freezing curves.



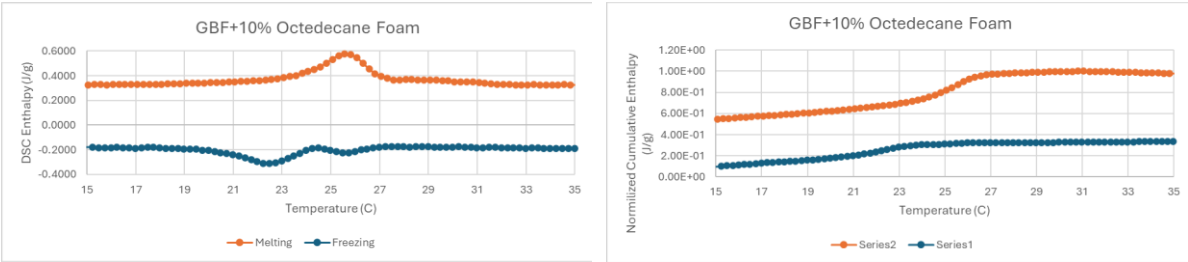
(a) (b)

*Figure 26: Cement board with 20% v/v PCM/foam: (**a**) DSC enthalpy diagram over temperature of melting and freezing curves; (b) normalized cumulative enthalpy diagrams of melting and freezing curves.*



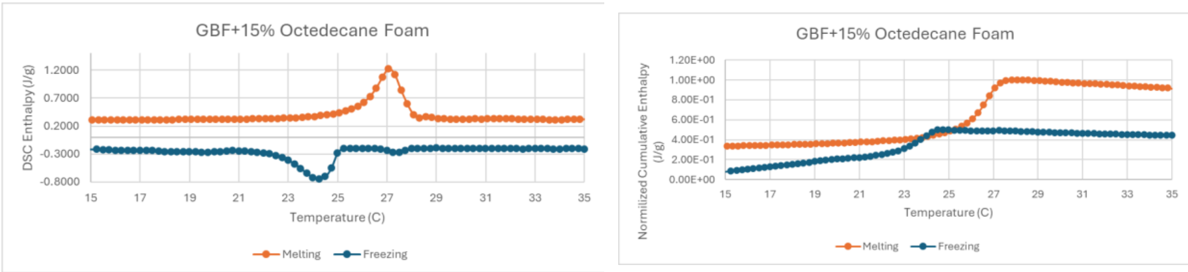
(a) (b)

*Figure 27: Cement board with 30% v/v PCM/foam: (**a**) DSC enthalpy diagram over temperature of melting and freezing curves; (b) normalized cumulative enthalpy diagrams of melting and freezing curves.*



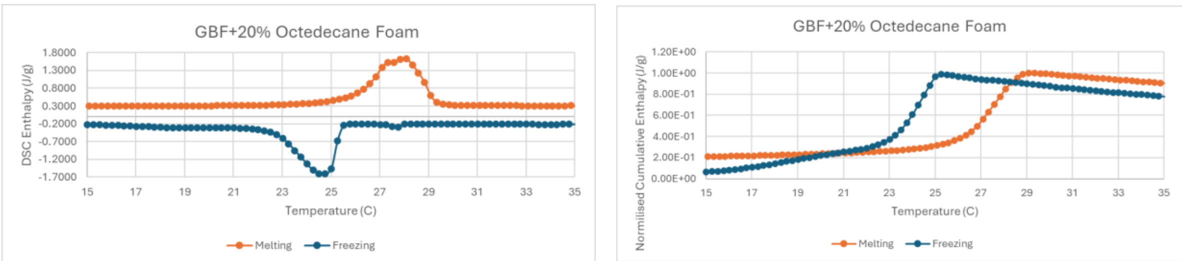
(**a**) (**b**)

*Figure 28: Gypsum Board with 10% w/w PCM/foam: (**a**) DSC enthalpy diagram over temperature of melting and freezing curves; (b) normalized cumulative enthalpy diagrams of melting and freezing curves.*



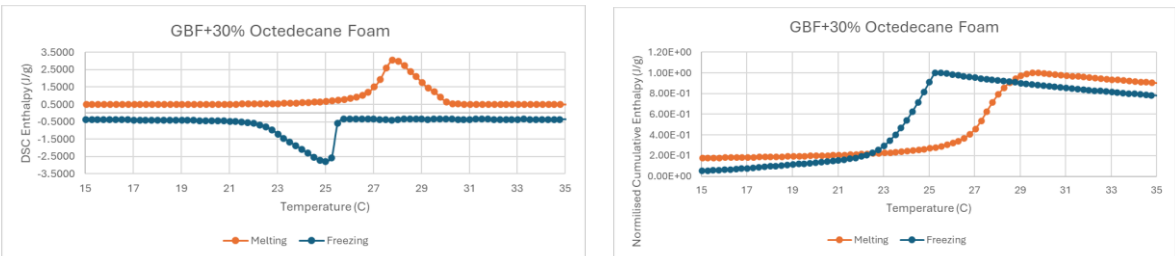
(**a**) (**b**)

*Figure 29:Gypsum board with 15% w/w PCM/foam: (**a**) DSC enthalpy diagram over temperature of melting and freezing curves; (b) normalized cumulative enthalpy diagrams of melting and freezing curves.*



(**a**) (**b**)

*Figure 30: Gypsum Board with 20% w/w PCM/foam: (**a**) DSC Enthalpy Diagram over Temperature of Melting and Freezing Curves; (**b**) Normalized Cumulative Enthalpy Diagrams of Melting and Freezing Curves.*



(**a**) (**b**)

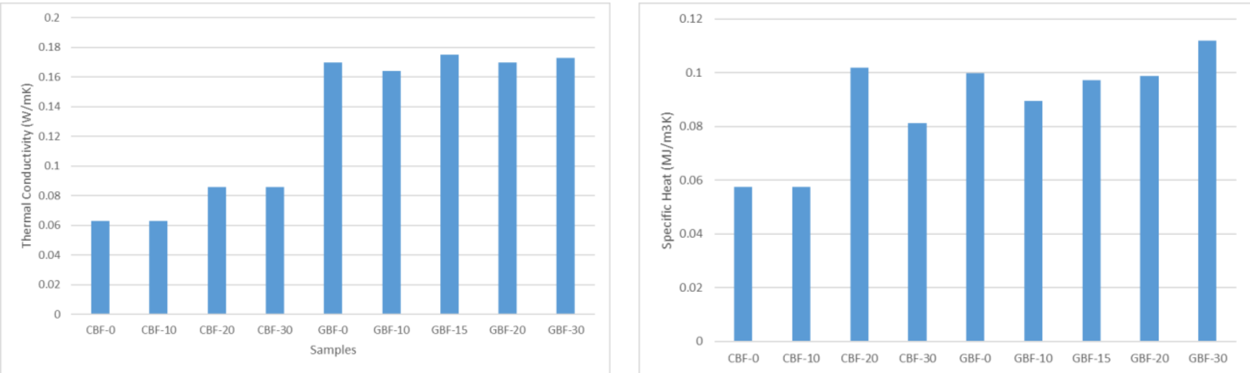
Figure 31: Gypsum board with 30% w/w PCM/foam: (a) DSC enthalpy diagram over temperature of melting and freezing curves; (b) normalized cumulative enthalpy diagrams of melting and freezing curves.

4.1.1.2 Thermal Conductivity Hot Disc

Hot Disc TSP 1500 equipped with Kapton 4922 sensor (diameter: 29.2 mm, resistance: 6,851,777 Ω) was used to measure the thermal conductivity and specific heat of all seven samples. The results are shown in Table 3 and Figure 32. Lowest thermal conductivity value is measured on cement board with 10% PCM/foam, while highest value is measured on gypsum board with 15% PCM/foam.

Table 3: Thermal conductivity and specific heat measurements for the cement (CBF) and gypsum (GBF) board samples taken with Hot Disc.

Sample	Thermal Conductivity (W/mK)		Specific Heat (MJ/m^{3}K)	
	Average	STD	Average	STD
CBF-10	0.063	0.001	0.057	0.005
CBF-20	0.086	0.002	0.057	0.005
CBF-30	0.086	0.007	0.102	0.022
GBF-10	0.164	0.001	0.089	0.007
GBF-15	0.175	0.002	0.097	0.007
GBF-20	0.170	0.003	0.099	0.005
GBF-30	0.173	0.001	0.112	0.009



(a) (b)

Figure 32: Hot disc measurements: (a) thermal conductivity (W/mK) for every sample; (b) specific heat (MJ/m3K) for every sample.

5.1.1.3 Solar Reflectance UV Carry 5000

The reflectance (%) measurements were taken with UV Carry 5000 spectrophotometer with the 2500 200 DRA reflectance.MSW method (Figure 33 & Figure 34) and were used to calculate the solar reflectance (%) at UV, VIS and NIR (Table 4).

Table 4: Solar Reflectance (SR %) at UV, VIS and NIR for the cement (CBF) and gypsum (GBF) board samples calculated from reflectance measured in Cary 5000 UV-Vis-NIR Spectrophotometer.

Sample	SR (%)	SR UV (%)	SR VIS (%)	SR NIR (%)
CBF28 10%	44.88	29.52	41.76	47.60
CBF28 20%	44.79	32.73	44.53	44.79
CBF28 30%	42.70	26.54	42.26	43.68
GBF28 10%	70.31	55.43	66.75	73.31
GBF28 15%	67.98	50.25	65.16	70.61
GBF28 20%	56.31	34.32	51.95	60.14
GBF28 30%	48.59	34.99	46.20	50.76

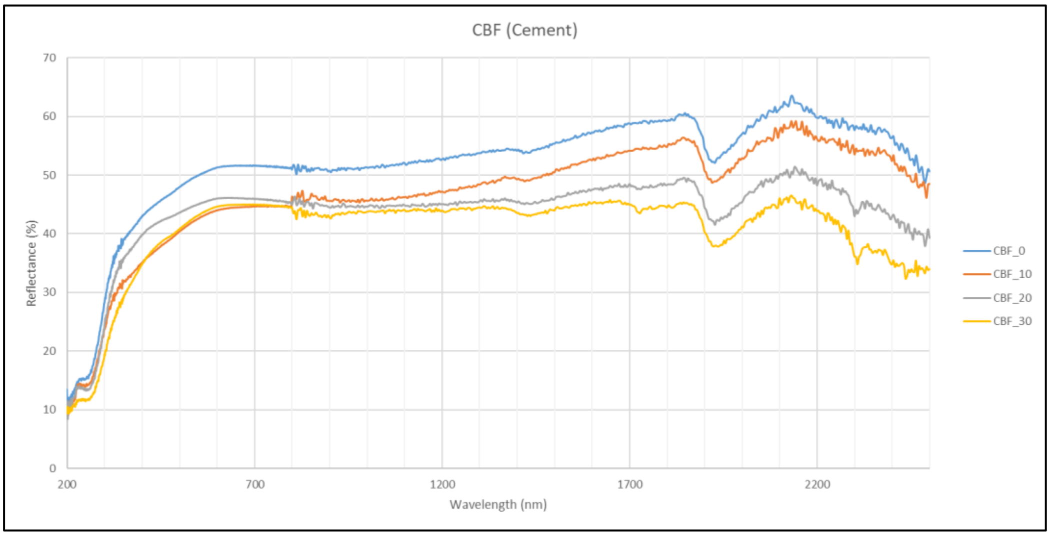


Figure 33: Cary 5000 UV-Vis-NIR Spectrophotometer measured reflectance (%) over 200-2500 wavelength (nm) for cement (CBF) board samples.

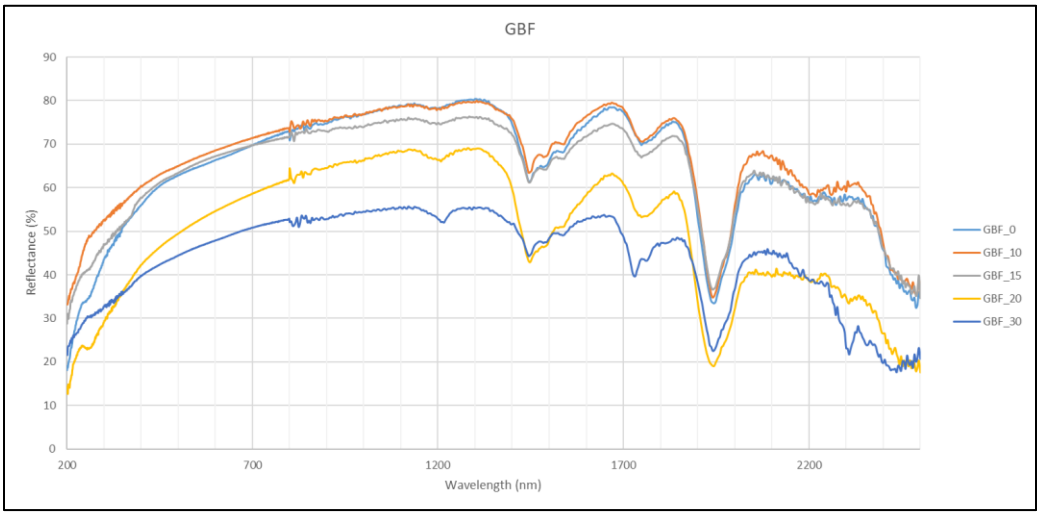


Figure 34 Cary 5000 UV-Vis-NIR Spectrophotometer measured reflectance (%) over 200-2500 wavelength (nm) for gypsum (GBF) board samples.

5.1.1.4 Emissivity

The emissivity measurements were taken with Emissometer with Scaling Digital Voltmeter Model AE1 RD1. The transient method was used to calculate the emissivity values (Table 5) for all seven material samples, as shown in Figure 35 and Figure 36.

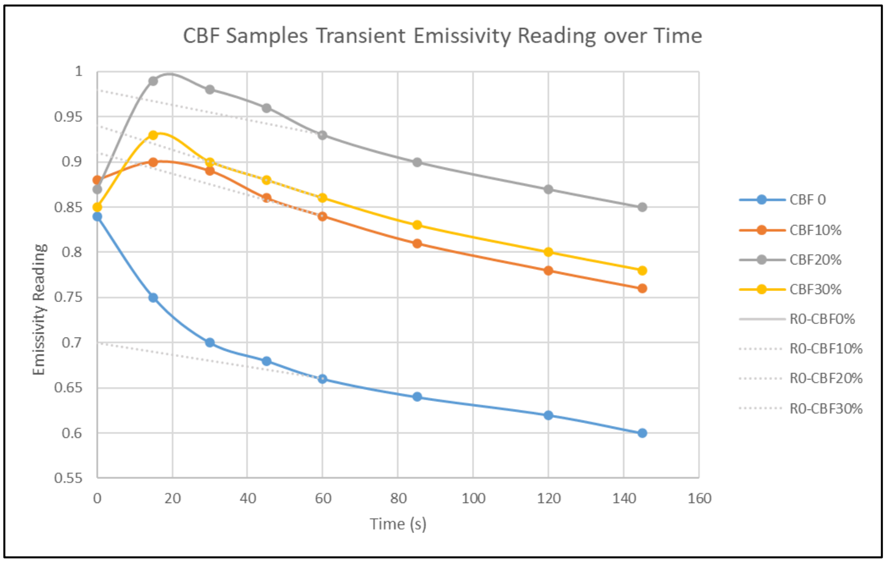


Figure 35: Cement board samples emissivity measurements with transient method.

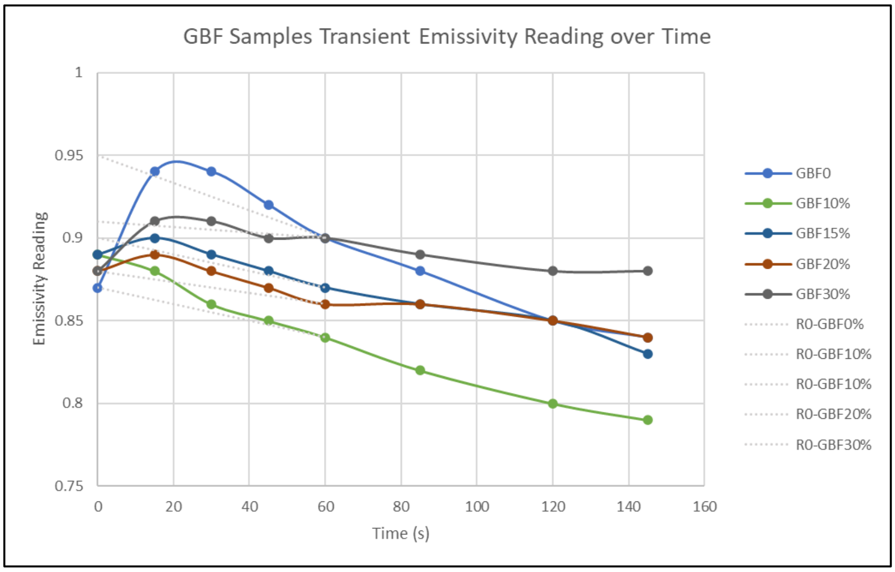


Figure 36: Gypsum (GBF) board samples emissivity measurements with transient method.

Table 5: Emissivity measurements (transient method) and visual extrapolated values for the cement (CBF) and gypsum (GBF) board samples.

N/N	Time (s)	CBF1 0%	CBF20%	CBF30%	GBF10%	GBF15%	GBF20%	GBF30%
1	0	0.88	0.87	0.85	0.89	0.89	0.88	0.88
2	15	0.9	0.99	0.93	0.88	0.9	0.89	0.91
3	30	0.89	0.98	0.9	0.86	0.89	0.88	0.91
4	45	0.86	0.96	0.88	0.85	0.88	0.87	0.9
5	60	0.84	0.93	0.86	0.84	0.87	0.86	0.9
6	85	0.81	0.9	0.83	0.82	0.86	0.86	0.89
7	120	0.78	0.87	0.8	0.8	0.85	0.85	0.88
8	145	0.76	0.85	0.78	0.79	0.83	0.84	0.88
E = 1*R0 extrapolated (vis)		**0.91**	**0.98**	**0.94**	**0.87**	**0.9**	**0.88**	**0.91**

5.1.2 Energy Plus Simulation Results

The measured characteristics were used as inputs for Energy Plus simulations (Table 16 Table 17 Table 18 in Appendix II). All seven samples were tested in the construction set of the external walls and roof. The scenarios include the baseline scenario without the samples; the samples run with MaterialProperty:PhaseChange and Hysterisis models at heating and cooling setpoints at 20 and 26 OC, as well as heating and cooling setpoints at the melting and freezing points of each sample. These parameters conclude in 36 scenarios, with their simulated annual building energy consumption and results shown in Table 6. In addition, the net annual energy building consumption is included, as LeafHouse has PVs installed, and the results are shown in Table 7. Furthermore, the savings of the PCM scenarios are calculated based on their baseline scenarios.

Table 6: EnergyPlus simulation annual energy consumption results for the cement (CBF) and gypsum (GBF) board samples at 20oC and 26oC cooling and heating setpoints, respectively.

N/N	Scenario	Annual Energy Consumption (kWh)	kWh/m2	Savings (%)
S0	**Baseline Setpoint 20-26**	**88,679**	**121.6**	**-**
S1	CBF10% nonHysterisis External Wall + Roof	84,862	116.4	4.3
S2	CBF10% Hysterisis External Wall + Roof	80,570	110.5	9.1
S3	CBF20% nonHysterisis External Wall + Roof	82,198	112.7	7.3
S4	CBF20% Hysterisis External Wall + Roof	79,476	109.0	10.4
S5	CBF30% nonHysterisis External Wall + Roof	85,204	116.9	3.9
S6	CBF30% Hysterisis External Wall + Roof	80,148	109.9	9.6
S7	GBF10% nonHysterisis External Wall + Roof	85,924	117.9	3.1
S8	GBF10% Hysterisis External Wall + Roof	79,098	108.5	10.8
S9	GBF15% nonHysterisis External Wall + Roof	85,946	117.9	3.1
S10	GBF15% Hysterisis External Wall + Roof	78,742	108.0	11.2
S11	GBF20% nonHysterisis External Wall + Roof	85,879	117.8	3.2
S12	GBF20% Hysterisis External Wall + Roof	78,817	108.1	11.1
S13	GBF30% nonHysterisis External Wall + Roof	85,682	117.5	3.4
S14	**GBF30% Hysterisis External Wall + Roof**	**77,323**	**106.1**	**12.8**

Table 7: EnergyPlus simulation annual energy consumption results for the cement (CBF) and gypsum (GBF) board samples at materials' melting and freezing points, cooling and heating setpoints, respectively.

N/N	Scenario	Annual Energy Consumption (kWh)	kWh/m2	Savings (%)
S15	**Baseline Setpoint MP-FP CBF10%**	114,073	156.45	-
S16	CBF10% nonHysterisis External Wall + Roof	109,500	150.18	5.2
S17	CBF10% Hysterisis External Wall + Roof	**105,517**	**144.72**	9.6
S18	**Baseline Setpoint MP-FP CBF20%**	113,078	155.09	-
S19	CBF20% nonHysterisis External Wall + Roof	105,475	144.66	6.7
S20	CBF20% Hysterisis External Wall + Roof	104,003	142.64	8.0
S21	**Baseline Setpoint MP-FP CBF30%**	117,671	161.39	-
S22	CBF30% nonHysterisis External Wall + Roof	113,634	155.85	3.4
S23	CBF30% Hysterisis External Wall + Roof	108,759	149.16	7.6
S24	**Baseline Setpoint MP-FP GBF10%**	110,581	151.66	-

S25	GBF10% nonHysterisis External Wall + Roof	107,470	147.40	2.8
S26	GBF10% Hysterisis External Wall + Roof	101,825	139.65	7.9
S27	**Baseline Setpoint MP-FP GBF15%**	123,238	169.02	-
S28	GBF15% nonHysterisis External Wall + Roof	120,349	165.06	2.3
S29	GBF15% Hysterisis External Wall + Roof	113,659	155.89	7.8
S30	**Baseline Setpoint MP-FP GBF20%**	124,215	170.36	-
S31	GBF20% nonHysterisis External Wall + Roof	121,465	166.59	2.2
S32	GBF20% Hysterisis External Wall + Roof	114,331	156.81	8.0
S33	**Baseline Setpoint MP-FP GBF30%**	128,969	176.88	-
S34	GBF30% nonHysterisis External Wall + Roof	126,032	172.86	2.3
S35	GBF30% Hysterisis External Wall + Roof	118,657	162.74	8.0

5.1.3 Leaf House Tailored Ontology and Knowledge Graph Creation

To cover this case study's needs for data and knowledge representation, the custom ontology shown in Figure 37 and Figure 38 is created from classes and relationships of already established ontologies. The measurements data of section 4.1.1 are mapped under this ontology for all the samples, hence creating a KG that works as material bank. In Figure 39, an example of that KG as a Material Bank is shown, with the external wall construction of Leaf House, its layers, its materials and their properties.

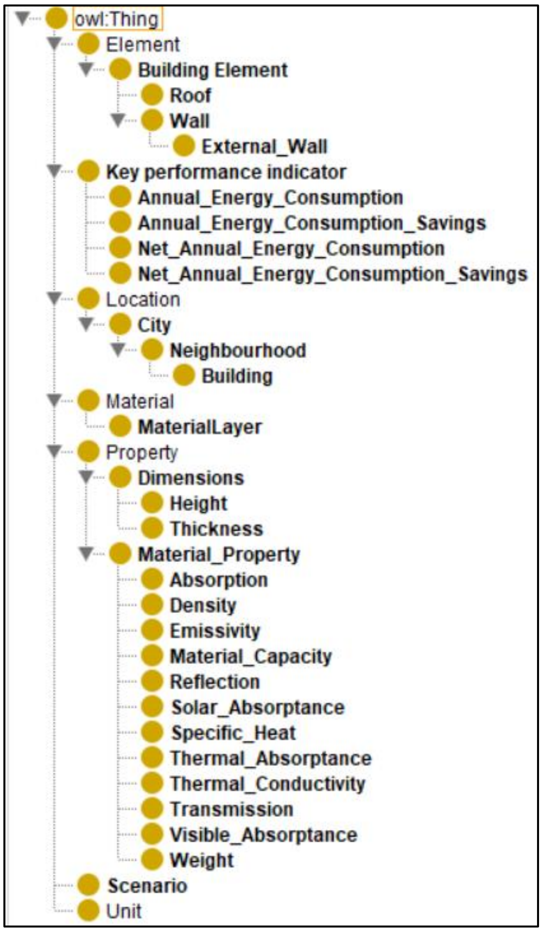


Figure 37: Leaf House Case Study Tailored Ontology- list

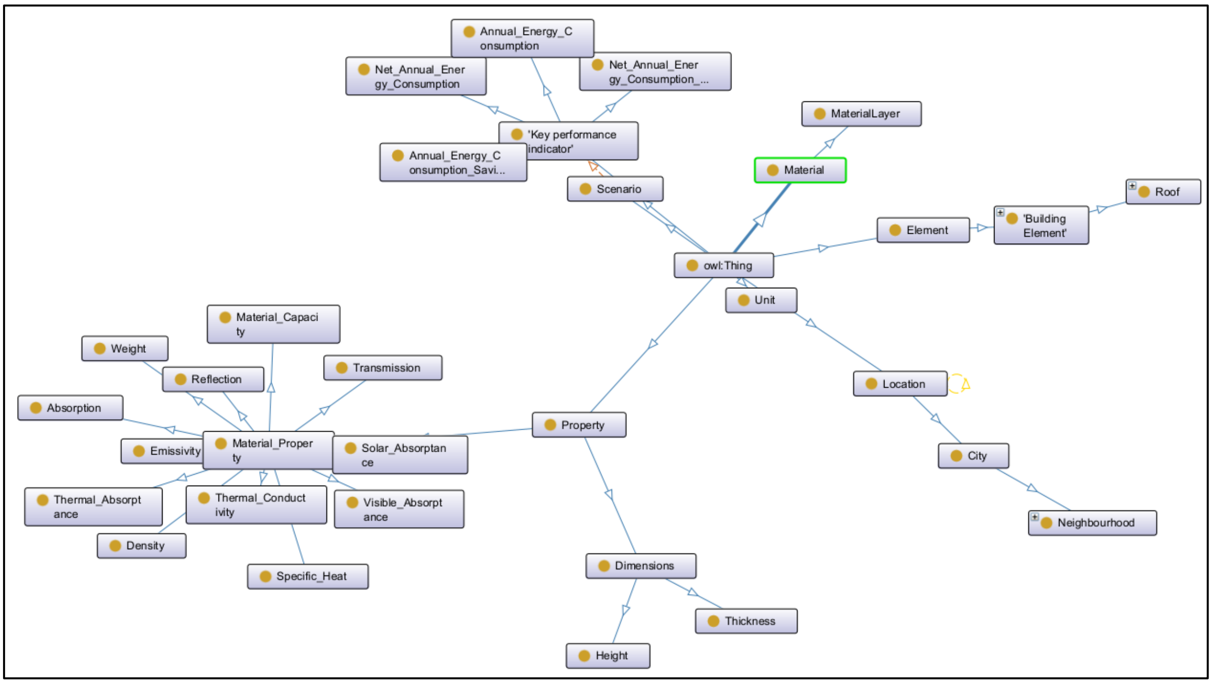


Figure 38: Leaf House Case Study Tailored Ontology- graph

So, all material information is hierarchically structured in the KG and can be queried to be accessed by stakeholders for further assessments. In addition, in Figure 40 a part of the KG of Leaf House case study is shown and focuses on the Energyplus scenarios. There the calculated KPIs are mapped under each scenario, and every scenario is linked with a sample material, a description and the relevant building components. In this context, the various scenarios outputs are now hierarchically structured under a KG, interconnected with all the available information about the case study, ready to be accessed by stakeholders to support decision making processes at neighborhood level.

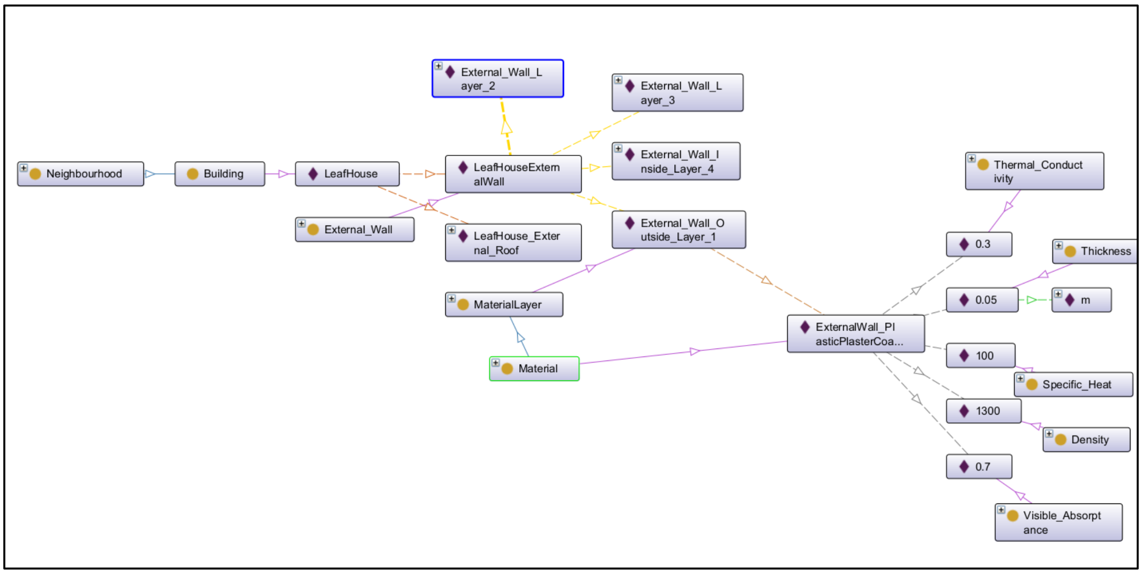


Figure 39: Leaf House Case Study part of KG example of Materials, Layers & Properties for Material Bank

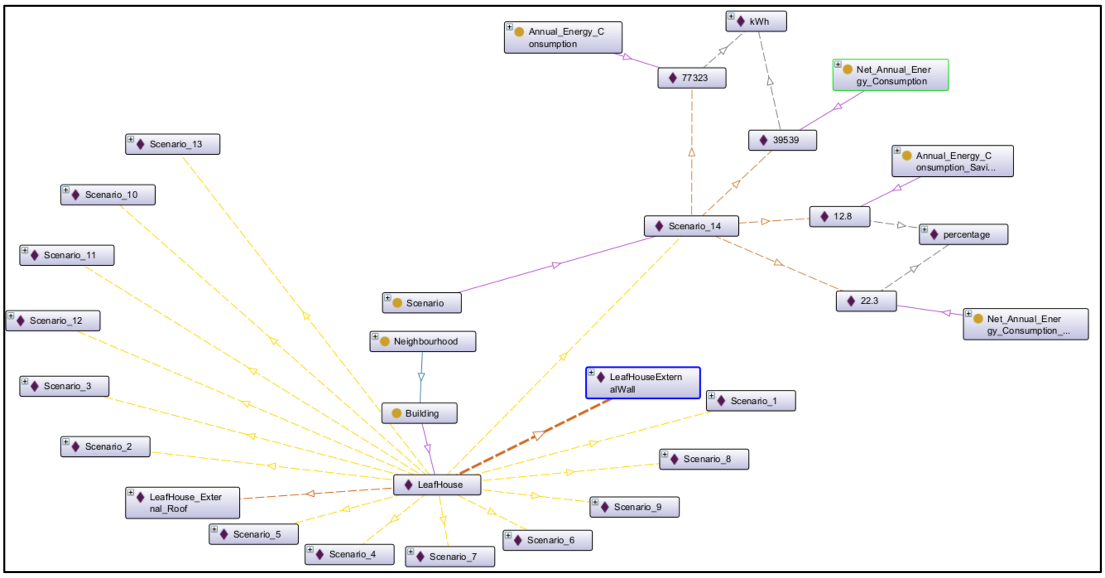


Figure 40: Example of Leaf House KG showing Scenario 14 and the calculated KPIs

5.2 TUC Campus Case Study- Neighborhood level

5.2.1 TUC Tailored Ontology and Knowledge Graph Creation

The KG for TUC case study is initially based on the information that is available and relevant to the assessments that are planned to happen. So, the KG starts with the buildings, neighborhoods, generators, transformers, and electric power sensors that are installed on them. After that, intervention scenarios and KPIs form the assessments are going to be available. To structure all the data and information, the case study ontology needs to be established.

5.2.1.1 Tailored Case Study Ontology

Having recognized the first neighborhood data and information that need to be structured in the KG, a set of appropriate ontologies are selected for the representation of them. The goal of the ontology is to be able to represent components and processes during construction renovation and energy management operations, putting emphasis on the renovation domain for this case study. Using the Protégé tool, the classes and relationships that are needed from each ontology are extracted and connected in the case study ontology. The selected ontologies to cover these needs are Brick[232], SAREF[233] and its extensions SAREF4ENER[234], SAREF4CITY[235], and KPI[236] Ontology. In Figure 41 and Figure 42 , the classes and subclasses of the ontology in OWL are shown, with the use of Protégé and OWLviz tools, respectively.

Brick focuses on semantically representing physical, logical, and virtual assets in a building, as well as the relationships between them. It is a well-known ontology that provides an analytic view on building representation with high level of detail, complementing the work of BOT. SAREF core ontology focuses on matching existing assets in the smart applications domain. There are several extensions for building, environment, and other domains, however the needs for this case study require the use of the extensions on city and energy domains. Last, but not least, the KPI ontology is part of the BIMERR ontologies[237], which

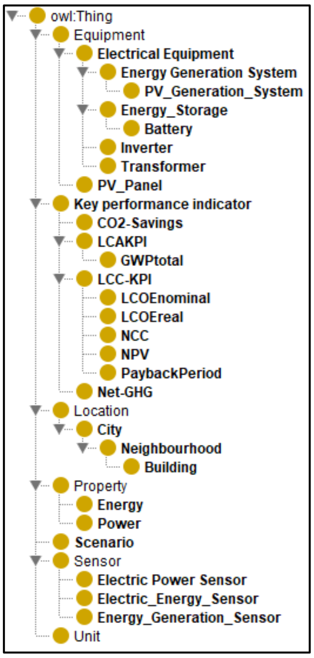


Figure 41:TUC Case Study Ontology Classes in OWL (Protege tool)

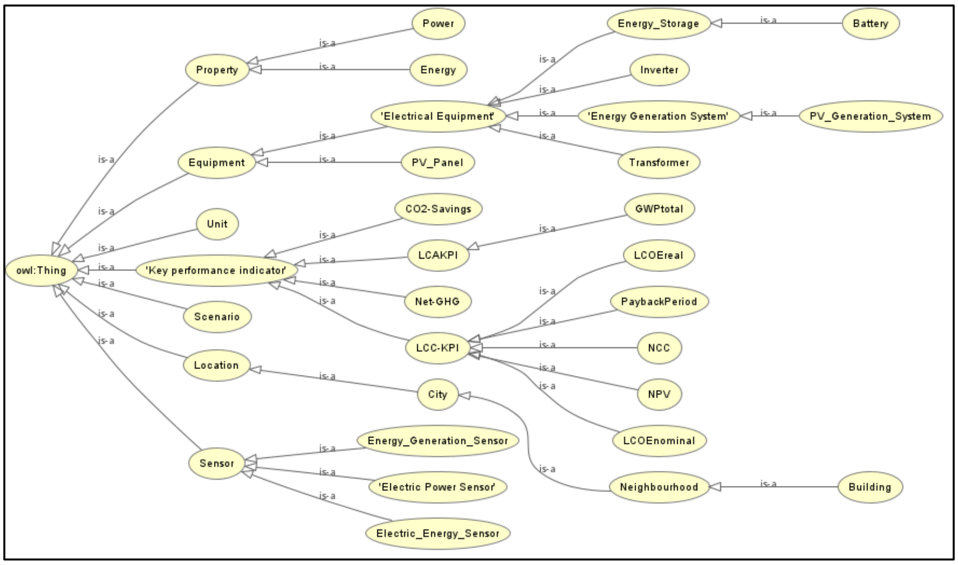


Figure 42: TUC Case Study Ontology in OWL, visualized in OWLviz[238]

are developed under H2020 BIMERR project[239], and focuses on key performance indicators representation. Reusing parts of these ontologies results in a appropriate combination for the TUC case study. However, some classes are created to cover the needs of the case study, like LCA-KPI and LCC-KPI subclasses. It is important to note that the reuse of the whole ontology is avoided, as this would create a vast combined ontology with many classes and relationships that do not exist in this case study. Therefore, the current data and information shape the ontology that is used. However, if and when new needs for representation appear, there is the ability to update and extend the current ontology to each main goal, hence representing processes and components for construction, renovation and energy management.

5.2.1.2 Knowledge Graph Creation

Based on this ontology, the KG is starting to be created, by adding new instances of the classes and connecting them with relationships, based on the information that are available, i.e., neighborhoods, buildings, generators, transformers, and sensors. In addition, the UUIDs from the database are established as information in the sensors' instances, as explained in Section 4.2.1. This will give the ability for timeseries data extraction, when querying the KG. An example of this creation of instances is shown in Figure 43, and this is a part of the whole KG.

Instances integration in the KG can be done on Protégé tool as well, however a more univerasl approach is by using python to add triplets in the KG directly. Furthermore, the instances can be added manually or semi-automatic, with the latter being available through data in a csv file. This latter method is also available through protégé tool.

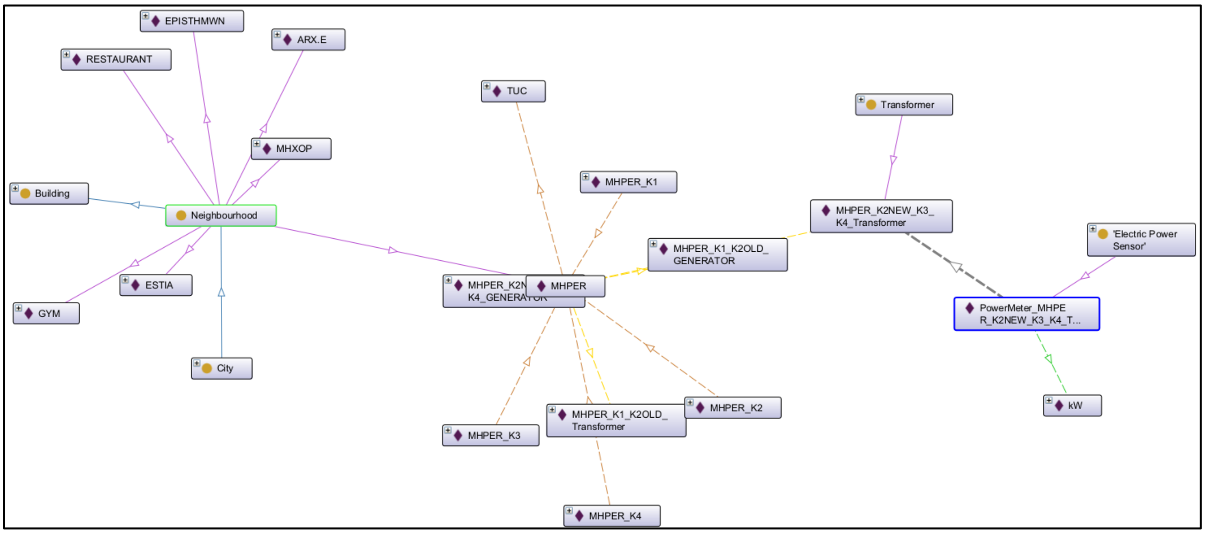


Figure 43: First Instances in KG. Example of TUC Neighborhoods, Buildings, Equipment, Sensor in OntoGraf[240]

5.2.1.3 Knowledge Graph and DS Tools

After having integrated some of the data and information that exist in the TUC campus and are relevant to the case study, we are able to query this information either by using the Ontograf extension in Protégé tool, or by working on python and writing SPARQL queries to request data. This data will be used for the assessments later on. In this way we can provide input information for the assessment tools. In the following section, the assessment processes will be explained, in addition to the integration of the calculated KPIs in the KG.

5.2.2 Neighborhood level Life Cycle Cost (LCC) including Life Cycle Analysis (LCA)

In accordance with the LCC assessment, the System Advisor Model (SAM) tool is employed to compute LCC KPIs for various scenarios spanning a 25-year period. For the LCA, the scenarios and sizing determined in the LCC assessment will be integrated with EPDs for the equipment under examination, namely PV panels, inverters, and lithium-ion batteries.

5.2.2.1 Goal and Scope Definition

The objective of the case study is to address the electric load requirements derived from the TUC campus power meters for the year 2022. The KG has been used to extract the data and inform the simulation load in SAM. The total load demand for 2022 is calculated to be 2.44 GWh, and the goal is to fulfill this demand through a combination of PV panels and batteries. Two types of bi-facial PV modules will be evaluated either independently or in conjunction with a lithium-ion battery operating in a self-consumption dispatch mode. This dispatch strategy aims to minimize the reliance on power imports or exports to the grid, thereby achieving 24/7 carbon-free energy provision. The PV coverage scenarios examined include 25%, 50%, 75%, and 100% of the electric load (Table 8). These scenarios are modeled in SAM using the "Detailed Photovoltaic Commercial" model for PV-only setups and the "Detailed Photovoltaic - Battery Commercial" model for PV combined with battery configurations. The primary LCC KPIs of interest in this study are Net Capital Cost (NCC), Net Present Value (NPV), Levelized Cost of Electricity (LCOE) in nominal and real terms, and the payback period.

Table 8: TUC LCC/LCA Case Study Interventions Scenarios

Scenarios	Description
0	Baseline Scenario- No Interventions
1	25% Coverage of the Load with PV Module 1
2	50% Coverage of the Load with PV Module 1
3	75% Coverage of the Load with PV Module 1
4	100% Coverage of the Load with PV Module 1
5	25% Coverage of the Load with PV Module 2
6	50% Coverage of the Load with PV Module 2
7	75% Coverage of the Load with PV Module 2
8	100% Coverage of the Load with PV Module 2
25	25% Load Coverage PV Module 1 + Li-ON Battery and Self Consumption Dispatch
26	50% Load Coverage PV Module 1 + Li-ON Battery and Self Consumption Dispatch
27	75% Load Coverage PV Module 1 + Li-ON Battery and Self Consumption Dispatch
28	100% Load Coverage PV Module 1 + Li-ON Battery and Self Consumption Dispatch
29	25% Load Coverage PV Module 2 + Li-ON Battery and Self Consumption Dispatch
30	50% Load Coverage PV Module 2 + Li-ON Battery and Self Consumption Dispatch
31	75% Load Coverage PV Module 2 + Li-ON Battery and Self Consumption Dispatch
32	100% Load Coverage PV Module 2 + Li-ON Battery and Self Consumption Dispatch

Subsequent to the LCC assessment and scenarios sizing, the outputs are combined with EPDs for PV panels, inverter, and battery to calculate the total Climate Change (GWP_{100}), which serves as the primary LCA KPI under focus. The EPDs for the equipment are sourced from EPD Italy[241] (Table 9). The functional unit for the PV EPD is 1 kWh of generated energy, for the inverter is 1 equipment unit, and for the battery is 1 kWh of capacity.

Table 9: Inputs from EPDs

Equipment	Functional Unit	Climate Change (GWP_{100}) (kg CO2 eq)
PV Module 1	1kWh Generated Energy	1.83E-02
PV Module 2	1kWh Generated Energy	1.79E-02
Inverter	1 unit	1.94E+04
Battery	1 kWh Capacity	2.67E+01

5.2.2.2 LCC & LCA KPIs calculation

The LCC KPIs are computed using SAM, and the findings are presented in Table 10 , showcasing various metrics such as power (kW), the generated energy (kWh), the power inverter units, the inverter power (kW), the battery capacity (kWh), the battery power (kW), NCC (€), NPV (€), LCOE nominal and real (cents/kWh), and payback period (years) across all scenarios.

For the LCA KPIs, Equation (1) outlines the calculation of GHG emissions by summing the interventions' Climate Change (GWP_{100}) with GHG emissions due to energy imported from the grid in each scenario[242].

$$GHG_{Emissions} = Interventions' \; Climate \; Change \; (GWP_{100}) \; + GHG_{Grid} \; (1)$$

where:

- $GHG_{Emissions}$, the greenhouse gas emissions (kg $CO_{2\text{-eq}}$)
- Interventions' Climate Change (GWP_{100}) , the global warming potential of the interventions (kg $CO_{2\text{-eq}}$)
- GHG_{Grid}, the greenhouse gas emissions due to energy imported from the grid (kg $CO_{2\text{-eq}}$)

Equation (2) enables the calculation of the GWP (kg CO_2) of the interventions for each scenario (Table 11) using the energy generated, power inverter units, battery capacity, and EPD factors from (Table 9).

$$Interventions \; Climate \; Change \; (GWP_{100}) \; = (PV \; Generated \; Energy * EPD \; Factor_{PV}) + (Inverter \; Units * EPD \; Factor_{Inverter}) + (Battery \; Capacity * EPD \; Factor_{Battery}) \; (2)$$

where:

- $Interventions' \; Climate \; Change \; (GWP_{100})$, global warming potential of the interventions for each scenario (kg $CO_{2\text{-eq}}$)
- $PV \; Generated \; Energy$, the energy generated from the PVs during RSL for each scenario (kWh)
- $EPD \; Factor_{PV}$, the environmental product declaration factor of the PV (kg $CO_{2\text{-eq}}$/kWh)

- $Inverter\ Units$, the number of inverter units sized for the scenario, including replacements every 10 years
- $EPD\ Factor_{Inverter}$, the environmental product declaration factor of the inverter (kg $CO_{2\text{-}eq}$/inverter unit)
- $Battery\ Capacity$, the capacity of the battery, including replacements every 10 years (kWh)
- $EPD\ Factor_{Battery}$, the environmental product declaration factor of the battery (kg $CO_{2\text{-}eq}$/kWh)

Moreover, Equation (3) calculates CO_2 emissions from grid consumption using SAM-calculated values of electricity imported from the grid and the CO_2 emissions factor for the grid network [243].

$$GHG_{Grid} = Grid\ Energy\ Mix\ Factor * Energy\ from\ Grid\ to\ Load \quad (3)$$

where:

- GHG_{Grid}, the greenhouse gas emissions from grid consumption during RSL (kg CO2-eq)
- $Grid\ Energy\ Mix\ Factor$, the local distributor emissions factor (kg CO2-eq/kWh)
- $Energy\ from\ Grid\ to\ Load$, the energy simulated in SAM that the grid gives to the load during RSL (kWh)

Table 10: LCC & Sizing KPIs from SAM

	RES					Storage		LCC			
Scenario	**Power (kWp)**	**Energy Generated (10^7 kWh)**	**Power Inverter Units**	**Inverter Power (kW)**	**Net Capital Cost (€)**	**Capacity (kWh)**	**Power (kW)**	**NPV (€)**	**LCOE nominal (cents/kWh)**	**LCOE real (cents/kWh)**	**Payback Period (years)**
0						-					
1	350	1.57	1	330	6.81E+05	-		5.11E+06	8.25108	6.43775	1.7
2	700	3.13	2	660	1.36E+06	-		1.02E+07	8.25108	6.43775	1.7
3	1050	4.70	3	990	2.04E+06	-		1.53E+07	8.25108	6.43775	1.7
4	1400	6.26	4	1320	2.72E+06	-		1.82E+07	8.25108	6.43775	2.0
5	350	1.56	1	330	6.86E+05	-		5.44E+06	8.32981	6.49918	1.6
6	700	3.12	2	660	1.37E+06	-		1.06E+07	8.32981	6.49918	1.7
7	1050	4.63	3	990	2.03E+06	-		1.56E+07	8.32505	6.49581	1.7
8	1400	6.19	4	1320	2.72E+06	-		1.87E+07	8.32617	6.4966	1.9
9	350	1.57	1	330	1.51E+06	2,721.31	378.11	4.01E+06	25.1149	17.1141	3.7
10	700	3.13	2	660	2.94E+06	5,296.08	661.02	7.90E+06	24.9455	16.9999	3.7
11	1050	4.70	3	990	3.70E+06	5,558.08	696.11	1.26E+07	20.1911	14.0973	3.1
12	1400	6.26	4	1320	4.38E+06	5,558.08	696.11	1.59E+07	17.2524	12.2903	3.1
13	350	1.56	1	330	1.51E+06	2,719.48	377.3	4.23E+06	26.7701	17.1901	3.5
14	700	3.12	2	660	2.94E+06	5,270.72	660.68	8.14E+06	26.5217	17.0431	3.6
15	1050	4.63	3	990	3.69E+06	5,565.94	697.91	1.30E+07	21.5641	14.2709	3.0
16	1400	6.19	4	1320	4.38E+06	5,565.94	697.91	1.67E+07	18.2878	12.4241	3.0

Table 11: Scenarios' LCA KPIs and Savings

Scenarios	Interventions Climate Change (GWP_{100}) (kg CO_2 eq)	Electricity from Grid to Load (10^7 kWh)	Grid CO_2 Emissions (kg CO_2)	CO_2 Savings (%)	CO2 emissions of Avoided Grid Consumption (kg CO2)	net GHG (kg CO2)
0	0	6.10	2.46E+07	0.00%	0	-
1	4.0E+05	5.45	2.20E+07	9.04%	2.63E+06	1.98E+07
2	7.9E+05	4.52	1.82E+07	22.73%	6.40E+06	1.26E+07
3	1.2E+06	4.17	1.68E+07	31.68%	7.81E+06	1.02E+07
4	1.6E+06	3.98	1.61E+07	34.76%	8.57E+06	9.10E+06
5	3.9E+05	5.45	2.20E+07	10.59%	2.61E+06	1.98E+07
6	7.8E+05	4.52	1.83E+07	25.87%	6.38E+06	1.27E+07
7	1.2E+06	4.18	1.69E+07	31.45%	7.75E+06	1.03E+07
8	1.5E+06	3.99	1.61E+07	34.59%	8.53E+06	9.14E+06
9	6.15E+05	5.45	2.20E+07	8.10%	2.61E+06	2.00E+07
10	1.21E+06	3.67	1.48E+07	34.98%	9.83E+06	6.20E+06
11	1.48E+06	2.17	8.77E+06	58.41%	1.59E+07	-5.62E+06
12	2.00E+06	1.32	5.31E+06	70.34%	1.93E+07	-1.20E+07
13	6.06E+05	5.46	2.21E+07	7.95%	2.57E+06	2.01E+07
14	1.19E+06	3.69	1.49E+07	34.71%	9.74E+06	6.35E+06
15	1.57E+06	2.24	9.03E+06	56.98%	1.56E+07	-5.01E+06
16	1.95E+06	1.35	5.45E+06	69.96%	1.92E+07	-1.18E+07

Finally, Equation (4) computes CO_2 savings as a percentage compared to the baseline scenario 0.

$$CO_2\ Savings\ (\%) = (GHG_{Emmisions_{S0}} - GHG_{Emmisions_{Si}})/(GHG_{Emmisions_{S0}})\ (4)$$

where:

- $CO_2\ Savings$, the $CO_{2\text{-eq}}$ savings in operational phase as a percentage compared to the baseline scenario (%)
- $GHG_{Emmisions_{S0}}$, the operational phase greenhouse gas emissions of the baseline scenario (kg $CO_{2\text{-eq}}$)
- $GHG_{Emmisions_{Si}}$, the operational phase greenhouse gas emissions of scenario i (kg $CO_{2\text{-eq}}$)

The net GHG emissions are determined by Equation (5), where the GHG emissions saved by interventions are subtracted from the sum of Equation (1). Negative values indicate the neighborhood has generated enough energy to have a positive impact[244], [245].

$$Net\ GHG_{Emissions} = GWP_{Interventions} + GHG_{Grid} - GHG_{Grid-saved}\ (5)$$

where:

- $Net\ GHG_{Emmisions}$, The total greenhouse gas emissions considering intervention impacts and grid energy savings (kg CO_2)
- $GWP_{Interventions}$, the global warming potential of the interventions (kg $CO_{2\text{-eq}}$)
- GHG_{Grid}, the greenhouse gas emissions from grid consumption in (kg CO_2)
- $GHG_{Grid-saved} = \left(E_{G\to L_{baseline}} - E_{G\to L_{scenario-i}}\right) * Grid\ Factor$
    - $GHG_{Grid-saved}$, the avoided emissions due to reduced energy import from the grid, calculated as the difference between the baseline and the intervention scenario, multiplied by the grid emission factor (kg CO_2)
    - $E_{G\to L_{baseline}}$Energy imported from grid to load for the baseline scenario (kWh)
    - $E_{G\to L_{scenario-i}}$Energy imported from grid to load for the scenario i (kWh)
    - $Grid\ Factor$, is the emissions factor for the grid (kg/kWh)

5.2.2.3 Outcomes Integration in KG

Figure 2These assessments have provided vital insights crucial for decision-making. To effectively organize and integrate this data with relevant components, it will be mapped onto the TUC campus KG using the case study ontology. In Section 4.2.1, timeseries data were linked within the KG using UUIDs connected to the database, rather than mapping every individual timeseries value. This approach results in a less dense KG focused on identifying classes and relationships rather than historical sensor data. However, UUIDs offer a practical method for accessing timeseries information.

Conversely, KPI outputs related to scenarios are valuable additions to the KG as distinct entities. This facilitates a direct linkage between scenarios and KPIs from various assessments. Consequently, KPIs computed in the assessments, as illustrated in Table 10 and Table 11, are integrated into the KG using the case study ontology through the Protégé tool and its addons. While a programming approach, such as Python, could also achieve this, the tool-based method offers a more user-friendly experience conducive to assessment methodologies.

Figure 44 displays the KG with integrated information. While initially appearing dense, zooming in on the scale reveals a comprehensible level of detail and interconnection among represented entities (Figure 45). There, the nodes around Scenario S16 are depicted along with their relationships, such as the "haKPI" relationship between the S16 scenario and the GWP total KPI.

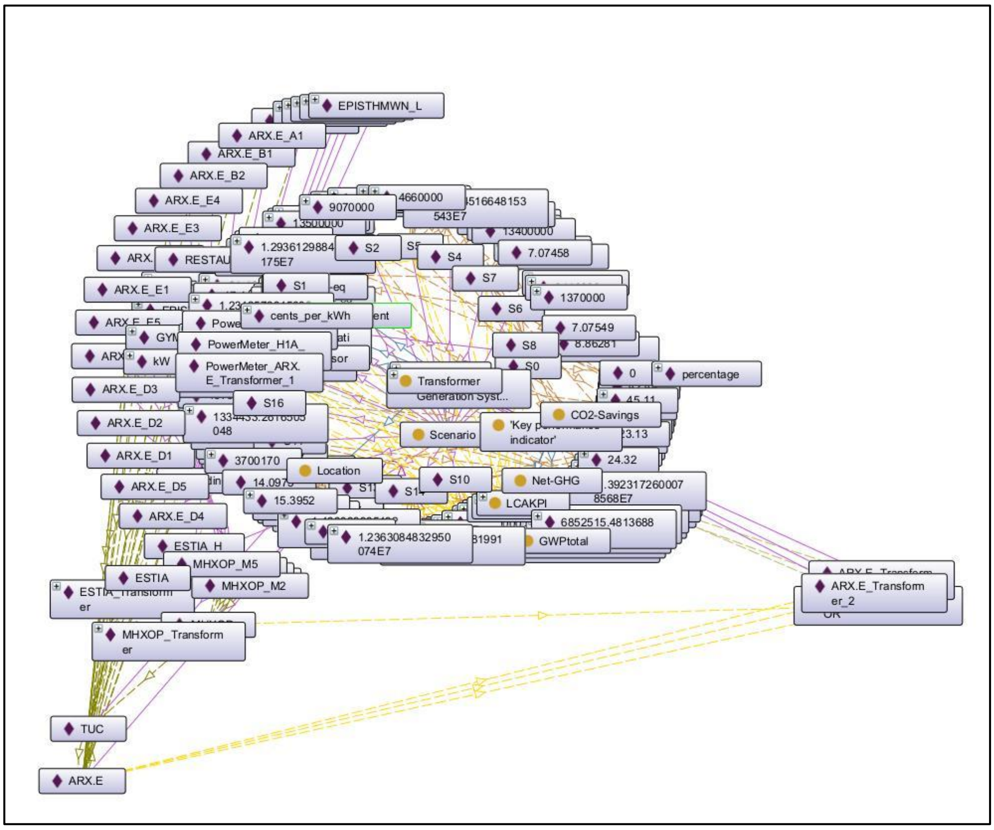


Figure 44:TUC Case Study Knowledge Graph

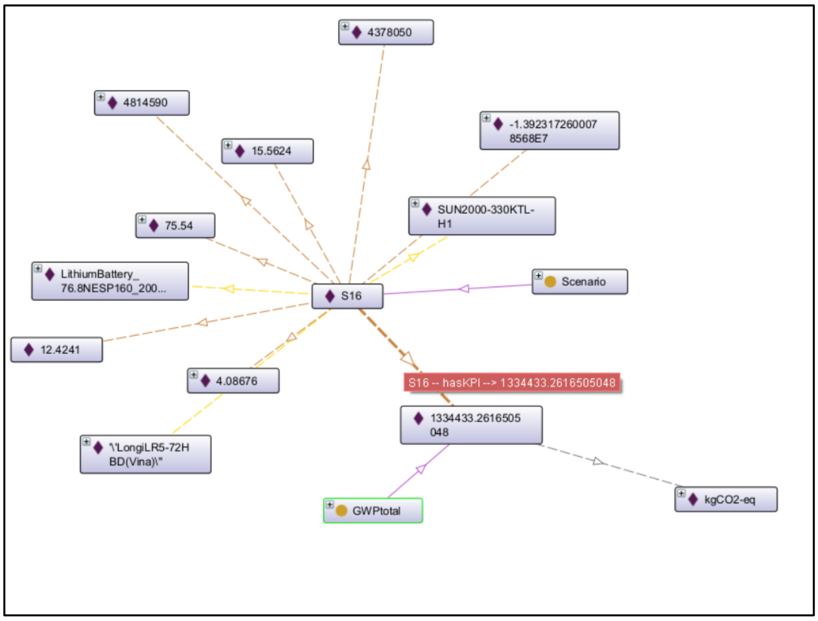


Figure 45: Part of TUC Case Study KG focused on Scenario S16 and GWPtotal; S16 hasKPI relationship shown.

6.Discussion

6.1 Discussion on Leaf House Case Study Results- Building level

The integration of PCMs into building materials such as cement and gypsum boards has demonstrated significant impacts on thermal properties and building energy consumption. This section discusses the results of DSC measurements, thermal conductivity tests, solar reflectance, and emissivity measurements, as well as the implications of these properties on the overall energy performance of buildings as determined by EnergyPlus simulations.

Figure 25-Figure 31 illustrate the enthalpy diagrams obtained from DSC measurements for cement and gypsum boards with varying percentages of PCM foam. These diagrams show that increasing the percentage of PCM foam in the boards enhances their thermal storage capacity. The enthalpy curves for higher PCM concentrations (e.g., 30% PCM foam) more closely resemble the curves of pure PCM, indicating a significant integration of PCM characteristics into the construction materials. This enhancement in thermal storage capacity is crucial for stabilizing indoor temperatures and reducing heating and cooling demands.

The thermal conductivity and specific heat measurements, presented in Table 3 and depicted in Figure 32, highlight notable differences between the samples. Cement boards with lower PCM content (10%) exhibit the lowest thermal conductivity, which is advantageous for reducing heat transfer through building envelopes. Conversely, gypsum boards with higher PCM content show increased thermal conductivity but also higher specific heat values, which can be beneficial for thermal mass and energy storage purposes. Traditional materials, such as standard gypsum boards and cement, typically exhibit thermal conductivities in the range of 0.17 to 0.25 W/mK for gypsum boards and 0.29 to 1.73 W/mK for cement. In contrast, the PCM-enhanced materials in this study demonstrated a range of thermal conductivities, from 0.063 W/mK to 0.175 W/mK, depending on the PCM content and the type of material. The lower thermal conductivity values observed in the PCM-enhanced gypsum and cement samples indicate better thermal insulation compared to their traditional counterparts. This improved insulation is crucial for reducing heat transfer through building envelopes, thereby enhancing overall energy efficiency.

Similarly, the specific heat of these materials, measured in MJ/m^3K, varied with the PCM content. The highest specific heat was observed in gypsum boards with 30% PCM, reflecting a greater capacity for thermal energy storage. This characteristic is crucial for stabilizing indoor temperatures, as it allows the materials to absorb excess heat during warmer periods and release it when temperatures drop. The enhanced specific heat, particularly in the gypsum boards, suggests that these materials could effectively contribute to the thermal mass of a building, thus improving its holistic energy management.

Reflectance measurements (Figure 33 and Figure 34) and solar reflectance data from Table 4 reveal that gypsum boards generally exhibit higher solar reflectance compared to cement boards. This characteristic makes gypsum boards more effective in reflecting solar radiation, thereby reducing cooling loads. Emissivity measurements (Figure 35 and Figure 36, Table 5) show that all samples have relatively high emissivity values, which is beneficial for releasing stored heat during cooler periods. Traditional gypsum boards generally show reflectance values around 20% to 30%, while standard gray cement typically has reflectance values between 30% and 50%. The PCM-enhanced materials in this study, however, exhibited significantly higher solar reflectance values, ranging from 42.7% to 70.31%, depending on the PCM concentration and the specific surface treatment applied. These increased solar reflectance values contribute to lower heat gain from solar radiation, reducing the cooling loads required to maintain indoor thermal comfort.

These findings highlight the dual role of PCM-enhanced materials in managing both heat gain and dissipation, making them versatile for various climatic conditions. The balance between high reflectance and high emissivity suggests that these materials can effectively reduce energy consumption by optimizing both cooling and heating needs. Further research should focus on the long-term stability of these properties in real-world conditions to confirm their practical benefits and explore the potential for further material optimization.

In summary, regarding the measurements, PCM-enhanced materials not only offer better thermal insulation by lowering thermal conductivity but also enhance solar reflectance, making them more effective in reducing energy consumption compared to traditional building materials. This dual benefit underlines the potential of PCM-enhanced materials to contribute significantly to the thermal management of buildings, leading to improved energy efficiency and sustainability in building design.

Measuring the thermal conductivity and solar reflectance of PCM-enhanced materials using the Hot Disc TPS1500 and UV-Vis-NIR spectrophotometer presents specific challenges that must be carefully managed to ensure accurate results. One primary challenge in measuring thermal conductivity is ensuring the uniform dispersion of PCM within the material matrix, as any inhomogeneity can lead to inconsistent results due to the PCM's phase change behavior, which can cause localized variations in thermal conductivity. Additionally, the phase change nature of the PCM, which involves latent heat absorption and release, complicates the measurement process, particularly if the material's temperature nears the PCM's phase transition point. To address these issues, it is crucial to thoroughly prepare the samples to ensure uniform PCM distribution and to maintain a stable measurement temperature, avoiding the PCM's phase change region. For solar reflectance measurements, challenges arise due to the PCM's optical properties, which can vary with temperature, and surface irregularities caused by PCM integration that might influence the reflectance readings. To mitigate these challenges, measurements should be conducted under controlled temperature conditions to keep the PCM in a single phase and ensure a smooth, uniform surface finish to reduce the impact of surface irregularities. These strategies help ensure that the measurements of thermal conductivity and solar reflectance accurately reflect the properties of PCM-enhanced materials. Both measurement equipments used are high-end and comply with standards that minimize the errors and result in accurate results.

The EnergyPlus simulations provide a comprehensive analysis of the energy performance of buildings utilizing PCM-enhanced materials. Scenarios with hysteresis models consistently outperform those without hysteresis, as evidenced by the greater energy savings (Table 6 and Table 7). Specifically, Scenario S14, involving gypsum board with 30% PCM foam, demonstrates the highest energy savings of 12.8% compared to the baseline scenario at standard setpoints (20 °C for heating and 26 °C for cooling). This scenario also shows substantial net annual energy consumption savings, 22.3% (Table 12 and Table 13), indicating the significant potential of PCM-enhanced materials in reducing energy usage. The increase in the savings percentage from annual energy consumption to the net annual energy consumption indicates the compatibility of RES like PV panels with the PCMs as TES. The scenarios running on PCMs melting and freezing points as cooling and heating setpoints did not reach high percentages of savings.

Table 12: EnergyPlus simulation annual net energy consumption results for all samples at 20 °C and 26 °C cooling and heating setpoints, respectively.

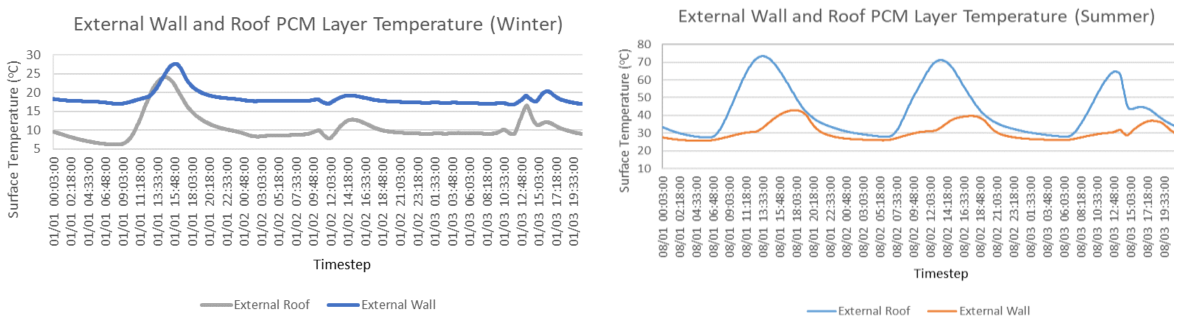
N/N	Scenario	Net Annual Energy Consumption (kWh)	kWh/m2	Savings (%)
S0	**Baseline Setpoint 20-26**	50,893	69.80	-

S1	CBF10% nonHysterisis External Wall + Roof	47,082	64.57	7.5
S2	CBF10% Hysterisis External Wall + Roof	42,784	58.68	15.9
S3	CBF20% nonHysterisis External Wall + Roof	44,412	60.91	12.7
S4	CBF20% Hysterisis External Wall + Roof	41,689	57.18	18.1
S5	CBF30% nonHysterisis External Wall + Roof	47,418	65.03	6.8
S6	CBF30% Hysterisis External Wall + Roof	42,365	58.10	16.8
S7	GBF10% nonHysterisis External Wall + Roof	48,140	66.02	5.4
S8	GBF10% Hysterisis External Wall + Roof	41,312	56.66	18.8
S9	GBF15% nonHysterisis External Wall + Roof	48,159	66.05	5.4
S10	GBF15% Hysterisis External Wall + Roof	40,959	56.18	19.5
S11	GBF20% nonHysterisis External Wall + Roof	48,093	65.96	5.5
S12	GBF20% Hysterisis External Wall + Roof	41,031	56.27	19.4
S13	GBF30% nonHysterisis External Wall + Roof	47,243	64.79	7.2
S14	**GBF30% Hysterisis External Wall + Roof**	**39,539**	**54.23**	**22.3**

Table 13: EnergyPlus simulation net annual energy consumption results for all the cement (CBF) and gypsum (GBF) board samples at materials' melting and freezing points, cooling and heating setpoints, respectively.

N/N	Scenario	Net Annual Energy Consumption (kWh)	kWh/m2	Savings (%)
S15	**Baseline Setpoint MP-FP CBF10%**	76,287	104.63	-
S16	CBF10% nonHysterisis External Wall + Roof	71,714	98.36	9.0
S17	CBF10% Hysterisis External Wall + Roof	67,733	92.90	16.8
S18	**Baseline Setpoint MP-FP CBF20%**	75,292	103.26	-
S19	CBF20% nonHysterisis External Wall + Roof	67,689	92.84	10.1
S20	CBF20% Hysterisis External Wall + Roof	66,216	90.82	12.1
S21	**Baseline Setpoint MP-FP CBF30%**	79,884	109.56	-
S22	CBF30% nonHysterisis External Wall + Roof	75,848	104.03	5.1
S23	CBF30% Hysterisis External Wall + Roof	70,972	97.34	11.2
S24	**Baseline Setpoint MP-FP GBF10%**	72,795	99.84	-
S25	GBF10% nonHysterisis External Wall + Roof	69,683	95.57	4.3
S26	GBF10% Hysterisis External Wall + Roof	64,038	87.83	12.0
S27	**Baseline Setpoint MP-FP GBF15%**	85,451	117.20	-
S28	GBF15% nonHysterisis External Wall + Roof	82,562	113.24	3.4
S29	GBF15% Hysterisis External Wall + Roof	75,873	104.06	11.2
S30	**Baseline Setpoint MP-FP GBF20%**	86,429	118.54	-
S31	GBF20% nonHysterisis External Wall + Roof	83,679	114.77	3.2
S32	GBF20% Hysterisis External Wall + Roof	76,545	104.98	11.4
S33	**Baseline Setpoint MP-FP GBF30%**	91,185	125.06	-
S34	GBF30% nonHysterisis External Wall + Roof	88,246	121.03	3.2
S35	GBF30% Hysterisis External Wall + Roof	80,870	110.92	11.3

Figure 46 illustrates the PCM layer node temperatures for the external roof and walls in Scenario 14 (Prominent GBF 30% Hysteresis) during winter (a) and summer (b). The data reveal that the PCM layers significantly moderate temperature fluctuations, maintaining more stable temperatures compared to non-PCM-enhanced materials. This stability is crucial in reducing thermal stress on building materials and maintaining indoor thermal comfort.

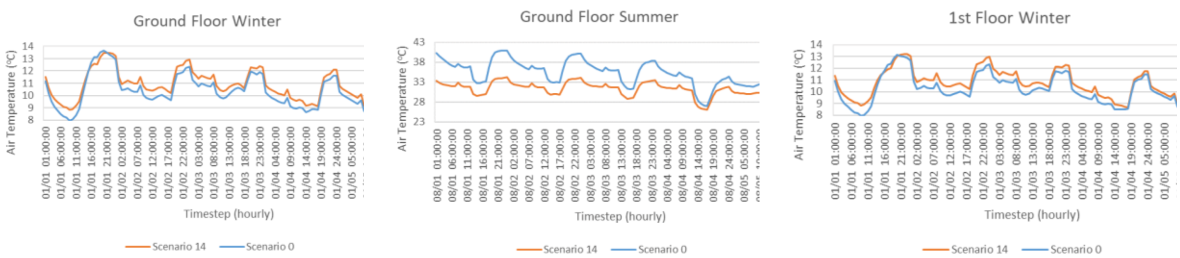


(a) (b)

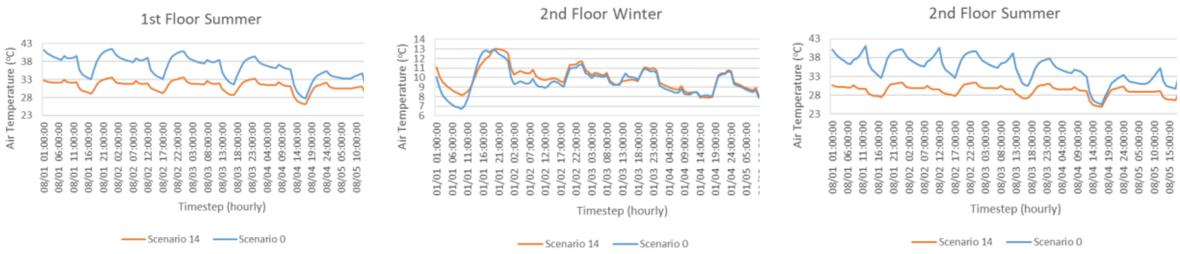
Figure 46: Scenario 14 (prominent gypsum boards GBF 30% Hysterisis PCM layer node temperatures for external roof and walls; (a) winter and (b) summer.

Figure 47 compares room air temperatures between the baseline scenario (S0) and the prominent PCM-enhanced scenario (S14) for different floors (ground, first, and second) during both winter and summer under free-running conditions (no HVAC). The results demonstrate that PCM-enhanced materials help in maintaining indoor temperatures closer to the desired comfort range without active heating or cooling. This suggests that PCMs can passively enhance thermal comfort, reducing the dependency on HVAC systems and potentially lowering energy consumption.

Figure 48 shows the temperature fluctuations within a test room equipped with PCM-enhanced materials compared to a control room for both winter (a) and summer (b), also under free-running conditions (no HVAC). The PCM-enhanced room experiences significantly dampened temperature peaks and valleys, indicating that PCMs effectively mitigate extreme indoor temperatures. This capacity for thermal regulation is particularly beneficial in maintaining occupant comfort and reducing the overall load on HVAC systems when they are in use, especially during peak heating and cooling periods.

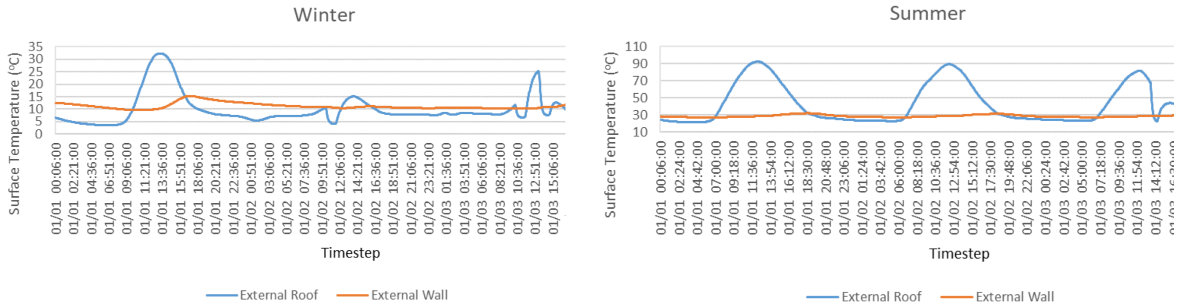


(a) (b) (c)



(d) **(e)** **(f)**

Figure 47: Free-running scenarios 0 (baseline) and 14 (prominent: GBF30% hysteresis). Room air temperature with 20-26 heating and cooling setpoints for ground (a and b), 1st (c and d) and second floor (e and f), and for winter and summer.



(**a**) (**b**)

Figure 48: Free-running scenario 14 (prominent gypsum boards GBF 30% Hysterisis) PCM layer node temperatures for external rood and walls; (a) winter and (b) summer.

Findings align with several studies that have investigated the use of PCMs in building materials. For instance, results showing up to 12.8% annual energy savings with 30% PCM-enhanced gypsum boards are comparable to the 10-46% energy efficiency improvements reported by studies in various climates ([198], [246], [247]). Additionally, the integration of PCM into walls and roofs has demonstrated similar benefits in terms of thermal regulation and energy reduction ([248], [249], [250]). However, it is noteworthy that the specific conditions under which these savings were achieved, such as the climatic context and the PCM concentrations, vary across studies. This suggests that while the trend in PCM effectiveness is consistent, the magnitude of energy savings is highly dependent on specific implementation details, such as the type of PCM, building design, and local climate conditions.

PCMs show varying performance across different climate conditions. In hot climates, they effectively absorb and release heat to reduce cooling needs, offering significant energy savings. In temperate climates, they provide year-round thermal regulation by adapting to seasonal temperature variations, ensuring frequent phase changes. In cold climates, their effectiveness is limited due to fewer phase changes, focusing more on heat retention to maintain indoor warmth. In general, the performance of paraffin-based PCMs hinges on selecting materials with appropriate melting points and optimizing thermal properties to match specific climate conditions.

Moreover, the performance of PCM-enhanced materials in this study, particularly in temperate and hot climates, supports the conclusions of Yan et al. [247] and Lee et al. [250], who demonstrated significant reductions in cooling loads when PCMs were integrated into building envelopes. The energy savings reported in this study, especially under hysteresis scenarios, are slightly higher than those reported by Lee et al. [24], which could be attributed to differences in the PCM content, the specific materials used, or the simulation settings.

In terms of thermal regulation and the maintenance of indoor comfort, the results of this work are consistent with the findings of Kuznik and Virgone [20], who also observed that PCM integration into building materials helps maintain stable indoor temperatures and reduces reliance on HVAC systems. However, while this study focuses on cement and gypsum boards, Kuznik and Virgone [20] primarily examined PCM-impregnated concrete walls, which may offer different thermal dynamics due to the inherent properties of concrete compared to gypsum and cement.

It is also important to address the trade-offs observed in our study between thermal benefits and other material properties, such as mechanical strength. Rostami et al. [251] and Miccoli et al. [252] have similarly reported that while PCMs improve thermal performance, they may compromise other material characteristics, highlighting the need for balanced material design. Our findings corroborate these observations, suggesting that while PCM-enhanced materials offer substantial energy savings, careful consideration of their mechanical properties is essential, particularly in load-bearing applications.

The study's findings have significant implications for both the design and construction of new buildings and the retrofitting of existing buildings with PCM-enhanced materials. For new buildings, incorporating paraffin-based PCMs into the initial design allows for optimal placement and integration, maximizing energy efficiency and thermal performance from the outset. This proactive approach can result in substantial long-term energy savings, improved occupant comfort, and enhanced sustainability credentials, making it easier to achieve green building certifications. Conversely, retrofitting existing buildings with PCM-enhanced materials provides a viable path to improve energy efficiency without the need for major structural changes. This can be particularly beneficial for older buildings, where adding PCM-enhanced gypsum boards, walls, or roofs can significantly reduce energy consumption for heating and cooling. Both strategies demonstrate that PCM technology can be flexibly applied to improve building performance, whether in new constructions designed with energy efficiency in mind or in existing structures seeking to enhance their thermal regulation and reduce energy costs.

Overall, while paraffin-based PCMs may not have the highest thermal properties among the different PCM types, their favorable characteristics, such as chemical stability, ease of integration, and cost-effectiveness, make them a highly practical choice for building applications. The energy savings and thermal regulation achieved in this study align well with the results observed in studies using other PCM types, reaffirming the potential of PCMs in enhancing building energy efficiency.

The potential for scalability and mass adoption of paraffin-based PCM technology in the building industry is strong due to its cost-effectiveness, abundant availability, and established manufacturing processes. Paraffin-based PCMs offer significant energy savings and improved thermal regulation, making them attractive for both new constructions and retrofits. As demand for sustainable, energy-efficient building solutions grows, driven by stringent building codes and green certification requirements, the adoption of PCM technology is likely to increase. Collaborative efforts between manufacturers, builders, and policymakers can further support widespread implementation, making paraffin-based PCMs a mainstream solution in the building industry.

Future work should involve testing the replication of this methodology by subjecting the samples to stress under a weather simulation station. This approach will reveal how these materials behave and what their properties become after prolonged exposure to environmental conditions. Additionally, implementing these materials in a pilot building will be crucial to validating the findings of this study, providing also practical insights into their long-term performance and effectiveness. Furthermore, the impact of the integration of paraffin-based PCMs on the structural integrity and durability of building components over long-term use should be examined in future work. Moreover, the economic feasibility of using paraffin-based PCMs in building components should be explored in future work.

6.2 Discussion on TUC Campus Case Study Results - Neighborhood level

6.2.1 LCC Assessment

Figure 49 presents the outcomes of the LCC assessment generated by SAM through two distinct diagrams. The left diagram illustrates the NPV (€) and NCC (€) for all scenarios, while the right diagram displays the Nominal LCOE (cents/kWh), Real LCOE, and Payback Period (years). For scenarios 1-8, which involve systems comprising solely PVs with varying coverages of two bi-facial module types, an increase in the nominal power of the PV system modeled correlates with an increase in both NPV and NCC. However, for scenarios 9-16, where Li-ON batteries are added alongside the two types of PV modules, there's a decrease in NPV and a slight increase in NCC. The decrease in NPV from the PV-only scenarios to the PV+Battery scenarios are since there are added investment and operative costs, which deem the former more profitable than the latter.

LCOE is stable across scenarios 1-8 and peaks at scenarios 4 and 8 that the two PV module types are at 100% coverages. For the PV and battery scenarios 9-16, there are peaks of LCOE at S9 and S13. After that there is a decrease in its value until scenarios 12 and 16 respectively. So, for scenarios with PV only the LCOE is lower than scenarios with PV and battery, where the more the PV coverage is increased, the more the LCOE is decreased. For the PV-only scenarios (1-8), the payback period is mostly stable, and an increase is shown in the 100% coverage scenarios (S4&S8). However, for the PV+Battery scenarios (9-16), there is a decrease in the value of payback period, while the coverage of the PVs is increased. The increase in values of LCOE and payback between the PV only and the PV with battery systems is related to the increase of capital and operating costs for the added batteries. Overall, from an LCC perspective the PV only scenarios are a better choice as the NPV values has a significant increase in comparison to the PV+Battery scenarios. However, the LCA assessment results, that follow in Section 4.2, need to be compared with the LCC results.

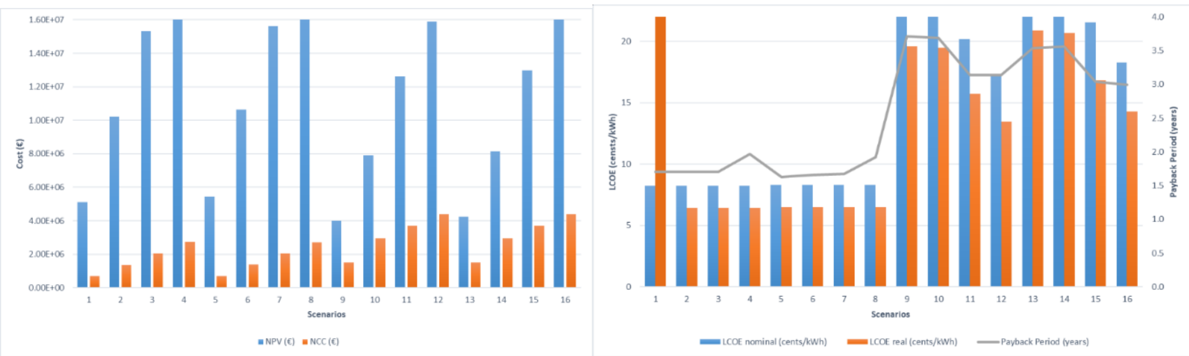


Figure 49: NPV (€) & NCC (€) (left diagram) and LCOE nominal (cents/kWh), LCOE nominal/real & Payback Period (years) (right diagram) for all scenarios

6.2.2 LCA Assessment

Figure 50 illustrates the interventions' Climate Change (GWP_{100}) alongside the CO2 emissions resulting from grid usage across various scenarios. In scenario 0, representing a baseline without any interventions, grid usage emissions reach their peak value. Across scenarios 1-8, which involve only PV interventions, there is a notable decrease in grid emissions due to varying PV coverages, albeit with an increase in the interventions' Climate Change (GWP_{100}). However, more substantial reductions in emissions are observed in scenarios 9-16, where PV installations are coupled with battery systems. Among these scenarios, 12 and 16 stand out for achieving the lowest emissions levels.

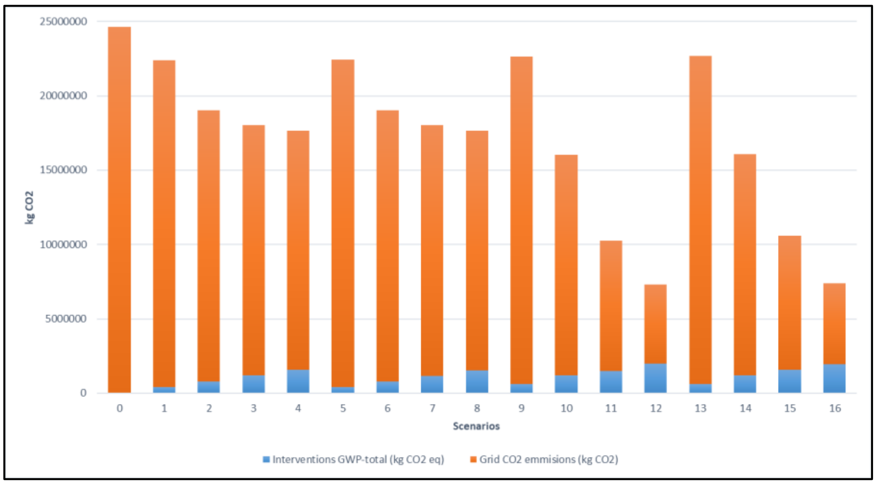


Figure 50: CO2 Emissions across all Scenarios

Figure 51 displays the percentage of CO2 savings for each scenario relative to the baseline scenario 0, along with the net GHG emissions (kg CO_2). The data clearly illustrates that as PV coverage increases, CO_2 savings also increase. Specifically, the PV-only scenarios achieve CO_2 savings of 45.11% and 44.96% in scenarios 4 and 8, respectively. Meanwhile, the PV+battery scenarios demonstrate even higher CO2 savings, reaching 76.29% and 75.54% in scenarios 12 and 16, respectively. In addition to CO_2 savings, another interesting KPI is the Net GHG emissions, as highlighted in Figure 51, the energy generated by the system lowers even more the net impact. Scenarios 1-8, which involve only varying PV coverages, show a substantial decrease in net GHG emissions attributed to energy generation. On the other hand, scenarios 9-16, where PV coverages are combined with Li-ON batteries, exhibit an even greater decrease, resulting in negative values that contribute to an overall positive impact on the neighborhood and grid system.

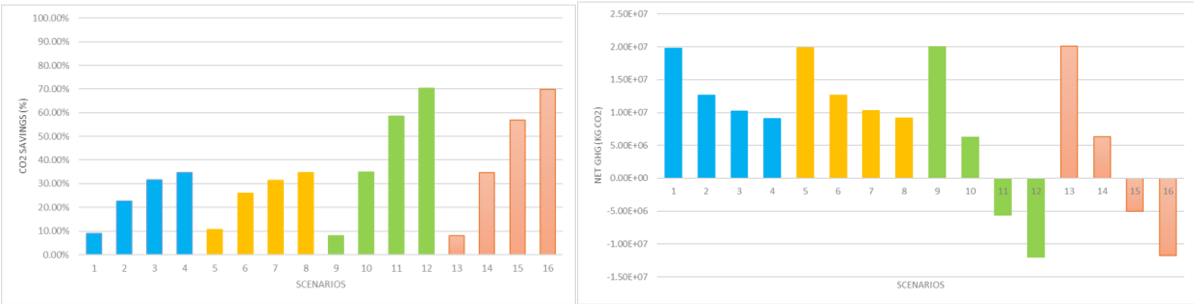


Figure 51: CO2 savings (%) (left diagram) and Net-GHG (kg CO2) (right diagram) for all scenarios

6.2.3 Prominent Scenarios

Following the LCC and LCA assessments, scenarios S12 and S16 emerge as the most prominent options. These scenarios feature 100% coverage from two types of bi-facial PV panels, alongside a Li-On battery for energy storage, operating under a self-consumption dispatch strategy. Table 10 and Table 11 present the sizing, LCC, and LCA KPIs for these scenarios. The decision to opt for PV and battery scenarios over PV-only scenarios was grounded in their superior CO2 savings and Net-GHG KPIs, despite being less financially lucrative. From a ZEN/PED perspective, prioritizing environmental and societal variables is paramount. To add on that, even though the profits of PV and battery scenarios are less profitable, they are still positive and would benefit the neighborhood.

Despite both scenarios having the same nominal power for the PV panels, S12 demonstrates higher energy production. While the LCC KPIs exhibit similarities between the two scenarios, S12 displays lower values, indicating greater financial attractiveness. Furthermore, scenario S12 boasts slightly higher CO2 savings and net GHG reductions compared to S16, rendering it more sustainable. Consequently, S12 emerges as the preferred option among the intervention scenarios, and a more thorough analysis of energy flows is given.

Recent studies conducted in the field of economy and environment focus on the issues of the utility of battery storage systems coupled with PV systems. An LCA analysis was carried out for residential solar-plus-storage systems revealed that adding battery storage can increase the life-cycle costs by 39% to 67% compared to the cost of the solar-only system[253]. Based on the different tariff structures and marginal emission factors, there was different impact on emissions, ranging from 20% decrease to a 24% increase. In another study, there was an assessment of environmental impacts of PV systems with battery storage in residential buildings, which revealed that storing excess PV generated energy in batteries can reduce GHG emissions in comparison to relying only on natural gas backup generators[254]. Although, the same study indicates that the environmental benefits are closely linked to the battery's lifecycle, which includes different factors like the charge cycles and energy density.

It is suggested by the findings that PV-plus-battery systems provide enhanced energy reliability and potential environmental benefits. However, these outcomes come along with high initial costs, as well as their environmental advantages can vary based on different system configurations and local conditions. These observations are coming in alignment with this study's results, as S12 and S16 show higher sustainability potential despite increased financial investment. In this study, the self-consumption dispatch strategy has been selected, which aims to maximize energy independence and minimize grid exchange, while it supports a continuous carbon-free energy system.

The system energy flows are shown in Figure 52, where the main nodes of this diagram are the PV, Battery, Load and Grid and where $E_{PV\text{->}B}$ is the energy from PV to Battery, $E_{PV\text{->}L}$ is the energy from PV to Load, $E_{PV\text{->}G}$ is the energy from PV to Grid, $E_{B\text{->}L}$ is the energy from Battery to Load, $E_{B\text{->}G}$ is the energy from Battery to Grid, $E_{G\text{->}L}$ is the energy from Grid to Load and $E_{G\text{->}B}$ is the energy from Grid to Battery. However, due to the self-consumption dispatch that is selected, there is no energy flow from Battery to Grid and vice versa. The concept of self-consumption dispatch aims to minimize the exchange of power with the grid, striving for a state where energy import or export is reduced to a minimum. This approach is often lauded as a pathway to achieving continuous carbon-free energy, operating around the clock.

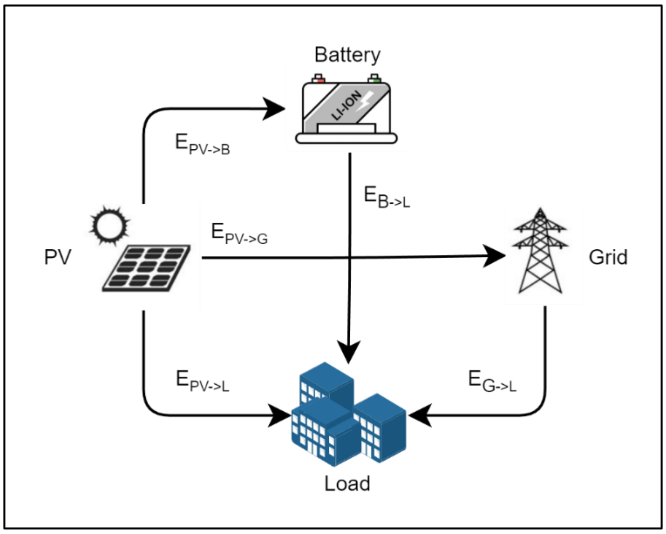


Figure 52: Energy Flows in TUC Case Study System

In Figure 53, depicting the monthly energy flows in year 1 of scenario S12, several notable patterns emerge. Firstly, the peak energy transfer from the system to the load is observed during March, June, and July, with a corresponding trough in November and December. This observation aligns logically with Crete's Mediterranean climate, although the March peak exceeds typical expectations. Additionally, energy flow from the system to the battery peaks in April, July, and October, reaching its nadir in March. Highest energy transfer from the system to the grid occurs in April and August, contrasting with minimal transfers in January, March, and December.

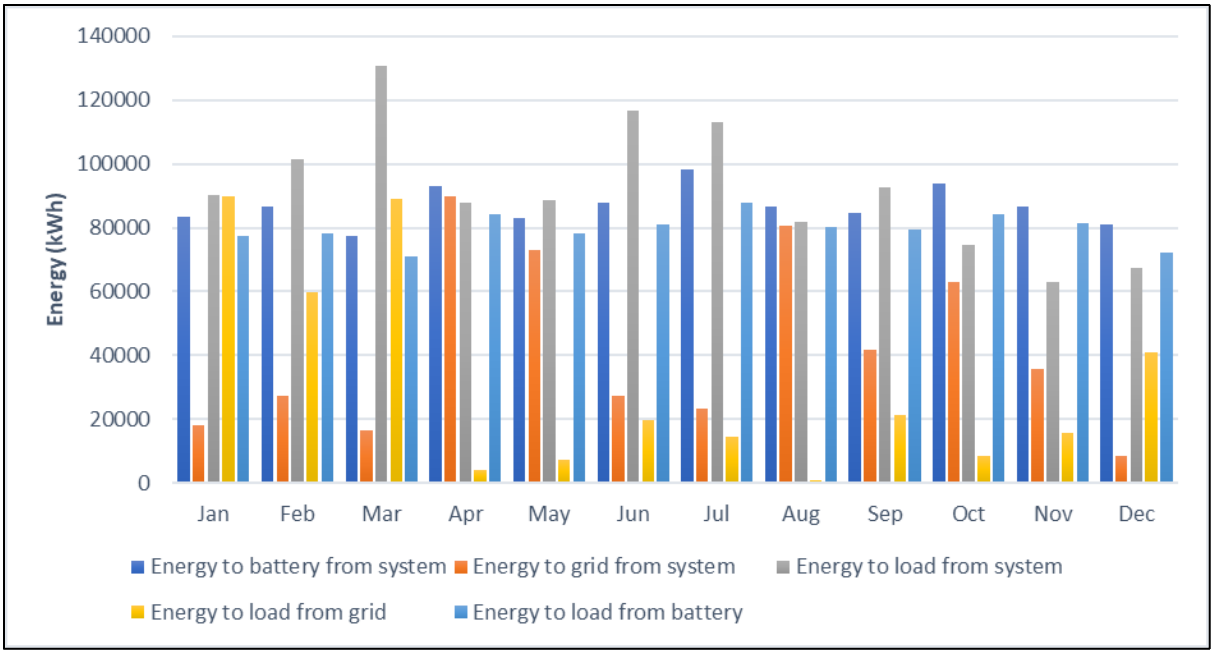
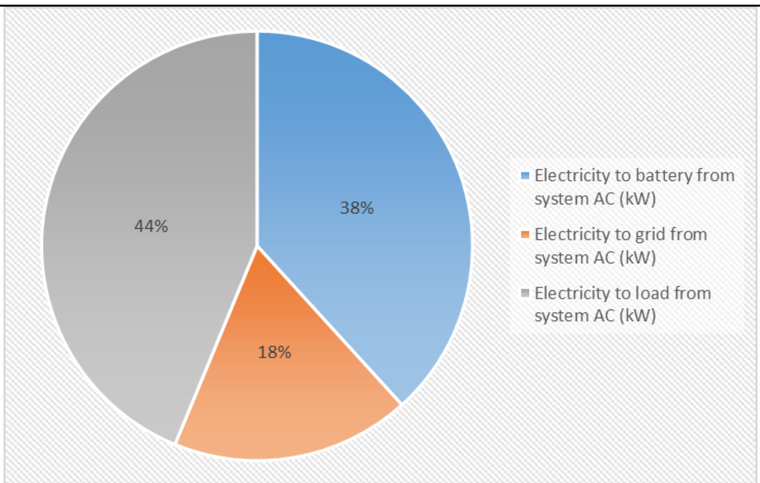


Figure 53: Monthly Energy Flows (Year 1) for Scenario S12

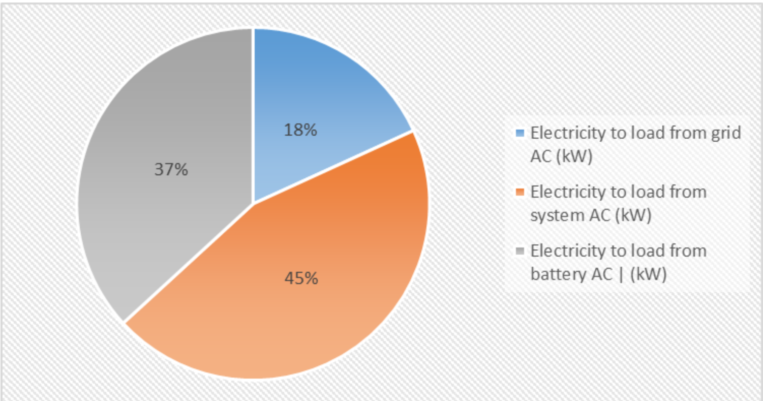
Furthermore, energy flow from the grid to the load peaks in January and March, while hitting lows in April and August. Energy transfer from the battery to the load reaches its zenith during July, June, April, October, and November, indicating diverse usage throughout the year, and is minimal during March and December.

Overall, these energy flow patterns reflect an efficient system that adapts well to Crete's Mediterranean climate, with notable increases in energy production and usage during March.

In Figure 54, the distribution of energy generated flows is depicted on the left side, revealing that 44% of the energy produced is directed towards the load, 40% towards the battery, and 16% towards the grid. On the right side, the energy flows directed specifically towards the load are illustrated, with 45% originating from the PV system, 37% from the battery, and 18% from the grid.



(a)



(b)

Figure 54: Left: Produced Electricity Flows for Scenario S12; Right: Electricity Flows to Load for Scenario S12

Moreover, Figure 55 and Figure 56 illustrate the energy flows of scenario S12 during both a typical winter day and a typical summer day respectively. In winter, energy from the grid sustains the load during early morning hours and afternoon, as the energy production from the PV system is insufficient and the battery cannot fully meet the load's demands. The peak hourly energy consumption reaches approximately 650 kWh, but the combined energy production and stored energy in the battery fall short of fully supporting the load due to limited solar radiation during this season. Conversely, in summer, the energy production from the PV system, coupled with stored energy in the battery, can cover even higher peak hourly energy consumption (around 900 kWh), given the ample solar radiation available to fuel the PV system. Excess produced energy is directed to both the battery and the grid during this period.

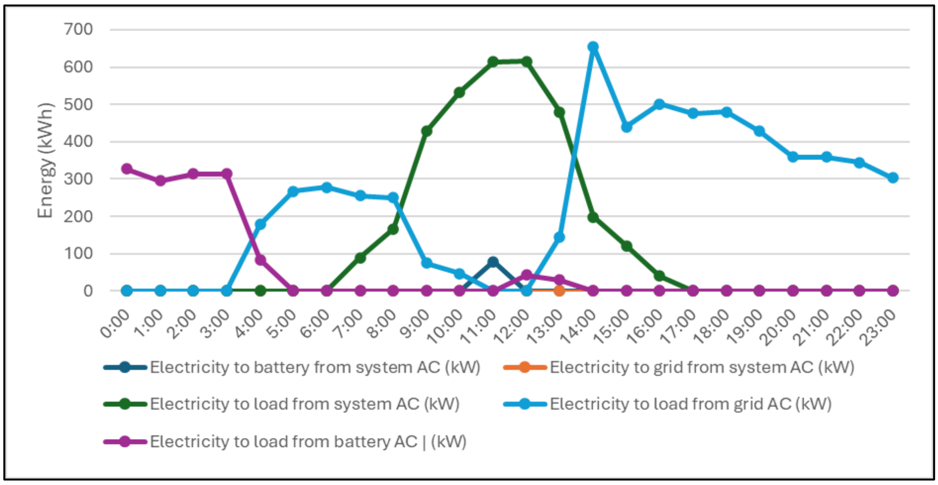


Figure 55: Energy Flows In a typical winter day for Scenario S12

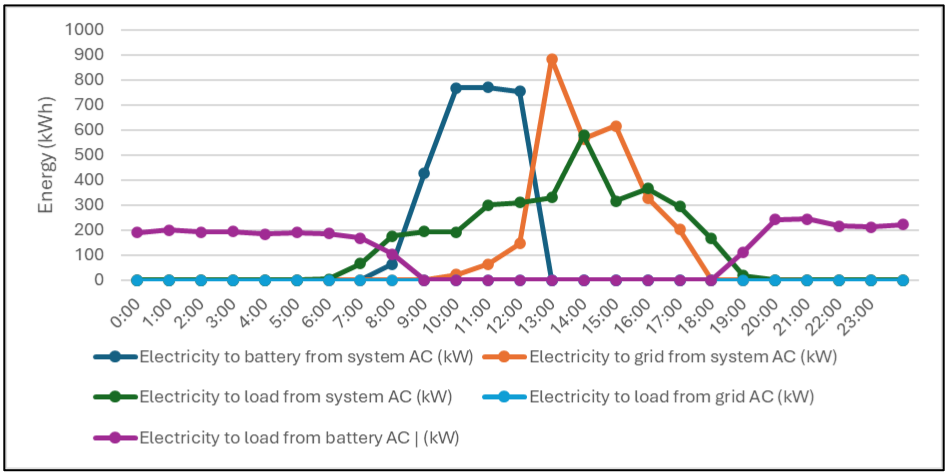


Figure 56: Energy Flows In a summer typical day for Scenario S12

6.3 Discussion on KG-based Architecture for both Case Study Results

6.3.1 KG Structure and DT Integration

Both the Leaf House and TUC case studies implemented a KG approach, but with differing scopes and ontology designs tailored to their specific needs. Leaf House focused on a single building's detailed composition and retrofit scenarios, creating a custom-tailored ontology drawn from existing building domain ontologies. This ontology emphasized building elements (e.g. walls, layers, materials) and their properties, effectively forming a "material bank" of the Leaf House's construction components. All measurement and performance data (from the building's retrofit experiments) were mapped into this ontology, producing a KG that hierarchically links the Leaf House's components to material properties and scenario outcomes. By contrast, TUC's KG encompassed a broader neighborhood-level scope: it included multiple buildings and their energy infrastructure (neighborhood grids, generators, transformers, and sensors across a campus) as the foundation. Because of this wider domain, TUC's ontology was constructed by reusing and combining several well-established ontologies, namely Brick, SAREF (with SAREF4ENER and SAREF4CITY extensions), and a KPI ontology, to cover concepts from building systems to IoT sensors and city context. This modular ontology design allowed TUC to represent physical assets, operational data, and planned renovation processes within one coherent schema.

The choice of ontologies reflects the different priorities of the two cases. Leaf House's custom ontology integrated only the classes and relationships needed for building retrofitting and performance evaluation, keeping the model lean and specific to that building. TUC, on the other hand, needed to capture a wide range of entities and their interconnections at campus scale, so it leveraged the rich schemas of Brick (for building equipment and sensors) and SAREF (for smart energy and city concepts) and then extended them where necessary. For example, the TUC ontology introduced custom subclasses like LCA-KPI and LCC-KPI to represent life-cycle assessment and life-cycle cost indicators not covered by the base ontologies. Both approaches avoided including unnecessary ontology elements beyond their use case scope, Leaf House by designing a minimal fit-for-purpose model, and TUC by selecting parts of large ontologies rather than importing them wholesale. This balance ensured that each KG remained relevant and manageable, without being bloated by classes or relationships irrelevant to the case study data. In both cases, the ontologies were developed using the

Protégé tool, allowing the teams to visually design class hierarchies and relationships and ensure alignment between the chosen schemas. Once the tailored ontologies were defined, each case study proceeded to instantiate the KG with actual data.

In Leaf House, the KG instances captured the specific materials, construction elements, and the results of various retrofit scenarios. All material information (walls, layers, insulation types, etc.) was added as interconnected instances, creating a rich graph of the building's composition. Additionally, each retrofit scenario (e.g. different material configurations or energy system upgrades simulated via EnergyPlus) was represented in the KG and linked to its corresponding outcomes, the KPIs calculated for that scenario. This means that for every scenario instance in the Leaf House KG, there were connections to the materials used, a textual description of the scenario, the affected building components, and the numerical KPIs results (such as energy savings, comfort level, cost, etc.). By structuring the data in this way, the Leaf House KG served as a centralized repository of both the building's static data and the dynamic results of retrofitting experiments, all interlinked for easy traversal.

For TUC case study, the instantiation of the KG began with the existing conditions of the campus. Instances were created for each neighborhood (or campus sector), building, energy generator, transformer, and sensor device available in the real environment. These instances were interlinked to reflect the actual topology, for example, sensors are associated with the equipment or building they monitor, and buildings are grouped under their neighborhood context. A notable implementation detail in TUC case study was how it handled timeseries sensor data: rather than storing large volumes of sensor readings in the KG, each sensor instance in the graph was annotated with a UUID corresponding to that sensor's record in an external database. This design allows the KG to remain a lightweight representation of static and metadata (what sensors exist, where, and what they measure), while still enabling retrieval of dynamic data by linking out to the timeseries source when needed. After establishing the base graph of the campus, the focus was to incorporate intervention scenario instances and their KPIs as the project's assessments progressed. In practice, this means that once a renovation or energy intervention is evaluated (through simulation or analysis tools), an instance representing that scenario (and its details) would be added to the KG, connected to relevant buildings/equipment, with properties or linked nodes for each KPI result. This approach mirrors what was done in Leaf House, albeit at a larger scale and with a more heterogeneous data set.

6.3.2 Semantic Queries for Informed Retrofit Decision-Making

Building upon the ontology structures and KG instantiations described in the previous section, this subsection focuses on how SPARQL querying enables effective scenario analysis and decision support for stakeholders. The integration of a knowledge graph within a digital twin framework allows for intuitive, semantically aligned queries across material properties, building configurations, and performance outcomes.

A major benefit of the proposed KG-DT architecture, as demonstrated in both case studies, is its ability to support informed stakeholder decision-making through native SPARQL querying. For example, an energy consultant or building designer can directly ask: “Which phase change material configuration yields the highest energy savings?” or “What are the thermal properties of the most energy-efficient PCM configuration?” These queries are not handled through spreadsheet filtering or manual simulations but through ontology-based reasoning across structured semantic data. In this way, the KG-based architecture functions not only as a structured data repository, but also as an intelligent interface for transparent, criteria-based renovation planning.

In the Leaf House case study, SPARQL queries allowed users to retrieve the PCM content and energy savings of each simulation scenario (Figure 57), or to drill into the material properties (thermal conductivity, latent heat, solar reflectance, emissivity) of the most energy-efficient configuration (Figure 58). These queries highlight how performance insights can be directly derived from structured semantic data without reprocessing raw simulation outputs.

```
SELECT ?scenario ?pcmContent ?saving
WHERE {
 ?scenario a :PCMSimulationScenario ;
        :hasMaterial ?material ;
        :hasPCMContent ?pcmContent ;
        :hasEnergySaving ?saving .
}
```

Figure 57: SPARQL query for retrieving PCM content and energy savings of each simulation scenario.

```
SELECT ?material ?thermalConductivity ?latentHeat ?solarReflectance ?emissivity
WHERE {
 ?scenario a :PCMSimulationScenario ;
        :hasMaterial ?material ;
        :hasEnergySaving ?saving .
 ?material :hasLatentHeat ?latentHeat ;
        :hasThermalConductivity ?thermalConductivity ;
        :hasSolarReflectance ?solarReflectance ;
        :hasEmissivity ?emissivity .
}
```

Figure 58:SPARQL query for retrieving material properties of the most energy-efficient scenario.

These queries support fast, repeatable evaluation of material-performance relationships, facilitating early-stage design exploration without re-running simulations. For instance, a query could identify that the 20% PCM gypsum board scenario yields the highest simulated energy savings, and then retrieve the precise thermal properties responsible for this outcome. Such insights can help architects and engineers assess trade-offs and fine-tune retrofit strategies.

In the TUC case study, semantic querying was scaled to the neighborhood level. SPARQL queries were constructed to retrieve and compare intervention scenario definitions and KPIs. For example, Figure 59 requests the scenario definitions and the results are shown in Figure 60; Figure 61 retrieves the LCC KPIs provided in Figure 62, while Figure 63retrieves environmental indicators (e.g., CO_2 savings) shown in Figure 64. These are modular, reusable, and semantically aligned queries using classes and properties such as hasProperty, NPV, CO2Savings, and PaybackPeriod.

```
SELECT DISTINCT ?scenario ?definition
WHERE {
 ?scenario skos:definition ?definition .
 ?scenario a kpi:Scenario .
}
```

Figure 59: SPARQL Query for Discovery of Available Intervention Scenarios and their definition

	Scenarios	Description
0	S0	No Interventions
1	S1	25% PV1 Coverage
2	S10	50% PV1 Coverage + Li-ON Battery Self Consumption Dispatch
3	S11	75% PV1 Coverage + Li-ON Battery Self Consumption Dispatch
4	S12	100% PV1 Coverage + Li-ON Battery Self Consumption Dispatch
5	S13	25% PV2 Coverage + Li-ON Battery Self Consumption Dispatch
6	S14	50% PV2 Coverage + Li-ON Battery Self Consumption Dispatch
7	S15	75% PV2 Coverage + Li-ON Battery Self Consumption Dispatch
8	S16	100% PV2 Coverage + Li-ON Battery Self Consumption Dispatch
9	S2	50% PV1 Coverage
10	S3	75% PV1 Coverage
11	S4	100% PV1 Coverage
12	S5	25% PV2 Coverage
13	S6	50% PV2 Coverage
14	S7	75% PV2 Coverage
15	S8	100% PV2 Coverage
16	S9	25% PV1 Coverage + Li-ON Battery Self Consumption Dispatch

Figure 60: SPARQL Query 1 Results

```
SELECT DISTINCT ?scenario ?definition ?NPV ?NCC ?LCOEnominal ?LCOEreal ?Payback
WHERE {
 ?scenario skos:definition ?definition .
 ?scenario a kpi:Scenario .
 ?NPV a <http://www.semanticweb.org/filippos/ontologies/2023/4/TUC_ONTO/NPV> .
 ?scenario s4city:hasKPI ?NPV .
 ?NCC a <http://www.semanticweb.org/filippos/ontologies/2023/4/TUC_ONTO/NCC> .
 ?scenario s4city:hasKPI ?NCC .
 ?LCOEnominal a
<http://www.semanticweb.org/filippos/ontologies/2023/4/TUC_ONTO/LCOEnominal> .
 ?scenario s4city:hasKPI ?LCOEnominal .
 ?LCOEreal a <http://www.semanticweb.org/filippos/ontologies/2023/4/TUC_ONTO/LCOEreal> .
 ?scenario s4city:hasKPI ?LCOEreal .
 ?Payback a
<http://www.semanticweb.org/filippos/ontologies/2023/4/TUC_ONTO/PaybackPeriod> .
 ?scenario s4city:hasKPI ?Payback .
}
```

Figure 61: SPARQL Query for Discovery of LCC KPIs of the Intervention Scenarios

	Scenarios	Description	NPV(€)	NCC(€)	LCOEnominal(€/kWh)	LCOEreal(€/kWh)	Payback(years)
0	S1	25% PV1 Coverage	4640000	680568	8.78302	7.01157	1.7
1	S10	50% PV1 Coverage + Li-ON Battery Self Consumption Dispatch	1953450	2940340	21.2986	16.9999	5.2947
2	S11	75% PV1 Coverage + Li-ON Battery Self Consumption Dispatch	3280820	3700170	17.6606	14.0973	4.60026
3	S12	100% PV1 Coverage + Li-ON Battery Self Consumption Dispatch	4763300	4380740	15.3952	12.2903	4.11672
4	S13	25% PV2 Coverage + Li-ON Battery Self Consumption Dispatch	784709	1512930	21.5346	17.1901	5.90069
5	S14	50% PV2 Coverage + Li-ON Battery Self Consumption Dispatch	1545420	2943850	21.3527	17.0431	5.85415
6	S15	75% PV2 Coverage + Li-ON Battery Self Consumption Dispatch	3370630	3692490	17.8774	14.2709	4.51979
7	S16	100% PV2 Coverage + Li-ON Battery Self Consumption Dispatch	4814590	4378050	15.5624	12.4241	4.08676
8	S2	50% PV1 Coverage	9070000	1360000	8.78302	7.01157	1.7
9	S3	75% PV1 Coverage	13500000	2040000	8.78302	7.01157	1.7
10	S4	100% PV1 Coverage	15800000	2720000	8.78302	7.01157	2
11	S5	25% PV2 Coverage	4660000	685566	8.86684	7.07847	1.7
12	S6	50% PV2 Coverage	9110000	1370000	8.86684	7.07847	1.7
13	S7	75% PV2 Coverage	13400000	2030000	8.86158	7.07458	1.7
14	S8	100% PV2 Coverage	15800000	2720000	8.86281	7.07549	2
15	S9	25% PV1 Coverage + Li-ON Battery Self Consumption Dispatch	1009130	1508860	21.4393	17.1141	5.28596

Figure 62: SPARQL Query 2 Results

```sparql
SELECT DISTINCT ?scenario ?definition ?GWPtotal ?CO2Savings ?NetGHG
WHERE {
 ?scenario skos:definition ?definition .
 ?scenario a kpi:Scenario .
 ?GWPtotal a <http://www.semanticweb.org/filippos/ontologies/2023/4/TUC_ONTO/GWPtotal> .
 ?scenario s4city:hasKPI ?GWPtotal .
 ?CO2Savings a <http://www.semanticweb.org/filippos/ontologies/2023/4/TUC_ONTO/CO2-Savings> .
 ?scenario s4city:hasKPI ?CO2Savings .
 ?NetGHG a <http://www.semanticweb.org/filippos/ontologies/2023/4/TUC_ONTO/CO2-Savings/Net-GHG> .
 ?scenario s4city:hasKPI ?NetGHG .
}
```

Figure 63: SPARQL Query for Discovery of LCA KPIs of the Intervention Scenarios

	Scenarios	Description	GWPtotal(kg CO2)	CO2 Savings(%)	Net GHG(kg CO2)
0	S1	25% PV1 Coverage	306692.67	23.13	1.2936129884189175E7
1	S10	50% PV1 Coverage + Li-ON Battery Self Consumption Dispatch	753051.0597	47.28	586480.0544300172
2	S11	75% PV1 Coverage + Li-ON Battery Self Consumption Dispatch	1065869.3307	66.3	-9099388.914549321
3	S12	100% PV1 Coverage + Li-ON Battery Self Consumption Dispatch	1371692.2017	76.29	-1.4330399854928743E7
4	S13	25% PV2 Coverage + Li-ON Battery Self Consumption Dispatch	371562.5715473096	24.16	1.2363084832950074E7
5	S14	50% PV2 Coverage + Li-ON Battery Self Consumption Dispatch	738633.1408199186	47.22	633364.3813366257
6	S15	75% PV2 Coverage + Li-ON Battery Self Consumption Dispatch	1035471.2821325745	65.54	-8695836.311849697
7	S16	100% PV2 Coverage + Li-ON Battery Self Consumption Dispatch	1334433.2616505048	75.54	-1.392317260078568E7
8	S2	50% PV1 Coverage	611555.34	34.9	6830140.028333474
9	S3	75% PV1 Coverage	918248.01	42.44	4643914.336289534
10	S4	100% PV1 Coverage	1223110.68	45.11	3633019.773135133
11	S5	25% PV2 Coverage	298622.67	24.32	1.2954516648153543E7
12	S6	50% PV2 Coverage	597245.34	37.31	6852515.48136881
13	S7	75% PV2 Coverage	886918.01	42.24	4710704.99501626
14	S8	100% PV2 Coverage	1185540.68	44.96	3668054.812285006
15	S9	25% PV1 Coverage + Li-ON Battery Self Consumption Dispatch	378481.8114	24.19	1.234257894568293E7

Figure 64: SPARQL Query 3 Results

These queries allow stakeholders to run "what-if" analyses at scale, such as identifying the scenario with the shortest payback period or comparing the environmental benefits across multiple interventions. Rather than relying on static spreadsheets or isolated reports, users interact with a dynamic, semantically rich interface that enables transparent exploration of retrofit trade-offs.

Beyond static querying, the system is designed for extensibility. Real-time ingestion pipelines and AI-enhanced analytics could further support design updates or post-occupancy monitoring. As the authors in [255] illustrate, the integration of KGs with visual analytics platforms is increasingly feasible.

In summary, both case studies demonstrate how semantically structured knowledge graphs can power stakeholder-driven queries that link design choices, material properties, and performance outcomes, delivering a practical, extensible digital twin framework for renovation planning.

6.3.3 Limitations and Challenges

Implementing KGs for both case studies revealed several technical and practical challenges and limitations that warrant consideration. A notable initial challenge was determining the appropriate scope of ontology reuse versus customization. Identifying the optimal balance required careful decision-making, particularly in the TUC case study, where integrating multiple existing ontologies was necessary. To maintain manageability and relevance, segments of existing ontologies were selectively extracted rather than importing entire ontologies, thus avoiding unnecessary complexity. Nevertheless, specific new classes, particularly for domain-specific KPIs such as LCA and LCC, had to be created. This balance between reuse and customization highlighted the importance of careful ontology design to ensure both extensibility and stability as new requirements emerged.

Data integration and quality presented further significant challenges. Populating the KG involved considerable effort, particularly in ensuring data accuracy and availability. In the Leaf House case, previously measured data and simulation outputs required careful mapping and transformation into RDF triples. Although this process was partially automated using scripts, manual transformations remained necessary and error-prone. Conversely, the TUC case managed varied data sources through semi-automated approaches, employing Protégé for manual entries and Python scripts for batch insertions. Even with these automated processes, substantial initial effort was required for data collection, formatting, and cleaning to comprehensively capture necessary sensor details.

Handling real-time data posed distinct considerations, particularly in the TUC case. Given the complexity and volume of time-series data, the approach taken involved storing only references (UUIDs) within the KG, with actual readings maintained externally. While this strategy effectively managed the KG's complexity, it introduced practical considerations, requiring additional steps for stakeholders when querying current sensor data. Although the Leaf House case did not immediately require real-time data handling due to its reliance on simulated data, similar considerations would become relevant in scenarios involving live data integration.

Performance and scalability emerged as further considerations, particularly as the KG expanded. Complex queries demonstrated decreased performance without optimized infrastructure, necessitating strategies such as limiting ontology scope to manage performance efficiently. However, scalability issues could arise if future expansions include additional scenarios or buildings, potentially requiring more robust infrastructure beyond initial implementations.

Finally, stakeholder accessibility and usability emerged as subtle yet essential considerations. The inherent technical complexity of KG interfaces, such as SPARQL endpoints or Protégé editors, and limited direct stakeholder engagement. Consequently, researchers or technical specialists often mediated interactions, conveying results through reports or specialized tools. To enhance KGs as effective decision-making tools for broader stakeholders, the proposed architecture integrates a human-machine interface within the DT, ensuring intuitive, user-friendly access to the KG data. This approach aims to facilitate stakeholder engagement and usability, promoting effective decision-making and practical application of the KG.

6.3.4 Future Improvements and Optimizations

Looking ahead, several key improvements and optimizations can significantly enhance the KG-based approach for decision support, informed by insights from both case studies.

A unified and extensible ontology framework is a primary goal for future development. Reconciling and unifying the ontologies from both case studies into a more generic, flexible structure capable of handling both building-level and neighborhood-level concepts would streamline processes. Aligning the material-focused ontology from Leaf House with broader standards like Brick/SAREF utilized by TUC would facilitate interoperability and simplify ontology engineering for future deployments. Standardizing common classes, such as KPI definitions related to energy, cost, LCA, and others, would enhance reuse and maintainability. Contributions from these customized ontologies could be returned to public domain repositories, benefiting broader communities tackling similar issues.

To address the challenges of labor-intensive data integration, automation and streamlined data integration processes should be prioritized. Developing adapters capable of converting common data sources, such as BIM files or building energy models, directly into KG-compatible triples would significantly reduce manual input. Implementing automatic exports from platforms like EnergyPlus or integrating IoT platforms directly into the KG would further streamline data collection and maintenance, enhancing accuracy and consistency. Standards like Brick schema tagging or Project Haystack conventions could further simplify sensor data integration.

Improving the integration of time-series data and enabling real-time analytics is another crucial optimization. Future work could explore federated querying, allowing seamless retrieval of time-series data alongside static KG information through unified SPARQL queries. Alternatively, adopting RDF triple stores with native time-series support or leveraging RDF Data Cube Vocabulary would simplify querying historical and real-time performance metrics. Such integration would facilitate dynamic, real-time decision support systems, such as dashboards displaying current KPIs for energy consumption or other critical metrics.

Enhancing stakeholder accessibility and usability through user-friendly decision support tools is essential for maximizing KG effectiveness. Designing intuitive graphical interfaces or conversational interfaces, which translate stakeholder queries into SPARQL automatically, would bridge the technical gap. Graphical dashboards driven by simple stakeholder interactions, or conversational interfaces translating natural language queries into SPARQL queries, would substantially improve stakeholder engagement and usability. Additionally, presenting query results visually and clearly would further support informed decision-making and build stakeholder trust in the system.

Investing in robust scalability and maintenance practices will become increasingly crucial as KG deployments expand. Transitioning from file-based ontologies to enterprise-grade graph databases or triple stores will enhance performance and scalability. Adopting scalable database solutions, employing efficient querying mechanisms, and establishing clear protocols for routine KG updates and data integration are essential steps. Implementing version control, change tracking, and regular consistency checks using tools such as SHACL shapes or OWL reasoning would further maintain high-quality data and facilitate easier management and updates.

Lastly, closing the loop from data to decisions by integrating KGs closely with decision-support workflows presents significant potential. Automatically triggering simulation or calculation engines based on KG inputs, and subsequently storing new KPIs and scenario outcomes back into the KG, would transform the KG into a dynamic, queryable repository. Advanced capabilities could include pattern identification or optimal scenario recommendations based on accumulated data, employing higher-level analyses and machine learning to identify successful strategies. This would transition the KG from a static data repository to an active, predictive, and recommendation-driven decision support system, fully leveraging its structured knowledge architecture.

7.Conclusions

In the current thesis, the neighborhood level data and knowledge management challenge was tackled by developing and demonstrating an innovative KG-based DT architecture for stakeholders' decision support.

The first case study demonstrates significant benefits of integrating paraffin-based PCMs into building materials like cement and gypsum boards, resulting in enhanced thermal performance and improved energy efficiency. DSC measurements revealed that increasing PCM content substantially elevates thermal storage capacity, with enthalpy values rising from 45,851 J/kg (0% PCM) to 80,042 J/kg (30% PCM). Thermal conductivity tests indicated distinct benefits based on material type: cement boards with lower PCM content (10%) exhibited minimal thermal conductivity (0.063 W/mK), effectively limiting heat transfer, while gypsum boards with higher PCM content (30%) showed increased conductivity (0.173 W/mK), beneficial for enhancing thermal mass and energy storage. Solar reflectance tests underscored the cooling potential of gypsum boards with 10% PCM content, achieving the highest reflectance at 70.31%. Additionally, emissivity values (0.78 to 0.91) confirmed effective heat release during cooler periods. EnergyPlus simulations further validated these findings, demonstrating significant energy reductions. Notably, gypsum boards enhanced with 30% PCM achieved up to 12.8% annual energy savings (reducing consumption from 121.63 to 106.05 kWh/m^2) and a 22.3% decrease in net annual energy usage compared to baseline conditions. Incorporating hysteresis models further amplified these savings, highlighting the critical role of thermal cycling effects in PCM applications.

Key insights include: a) High PCM content (30%) in gypsum boards significantly improves energy efficiency, providing substantial reductions (up to 22.3%) in net annual energy consumption. b) Incorporating PCM hysteresis effects significantly enhances the accuracy of simulations and performance outcomes. c) PCM-enhanced building materials contribute considerably to improved indoor thermal comfort by stabilizing indoor temperatures and reducing thermal stress on structural components.

These results highlight PCMs as promising materials for sustainable and energy-efficient building design. However, future research should investigate long-term performance under realistic environmental conditions, structural durability implications, and economic feasibility to encourage widespread adoption.

Moreover, in the second case study, the conducted LCC and LCA analyses provided valuable insights into the economic and environmental performance of neighborhood-scale PV systems with and without battery storage. The LCC analysis identified PV-only scenarios as economically more advantageous due to lower capital and operational costs. Conversely, the LCA demonstrated that PV-plus-battery scenarios significantly improve environmental sustainability by substantially reducing CO_2 emissions and overall GHG impact. Scenario 12 that features comprehensive coverage using bi-facial PV modules combined with lithium-ion battery storage under a self-consumption dispatch strategy, emerged as optimal, balancing economic viability with environmental benefits. Despite higher initial investments, Scenario 12 delivered the highest CO_2 savings, lowest net GHG emissions, and maintained attractive financial returns.

A distinctive feature of the proposed architecture in both case studies is its integration of SPARQL querying for decision support. By representing material configurations, performance results, and scenario metadata as semantic triples, stakeholders can retrieve insights such as optimal PCM concentrations or intervention strategies directly through ontology-based queries. For example, users can ask: *"Which material setup yielded the highest energy savings?"* or *"What are the thermal properties of the top-performing PCM scenario?"*, eliminating the need for manual filtering or simulation reruns and enhancing transparency and repeatability.

Throughout both implementations, a core challenge was striking the right balance between ontology reuse and customization. The Leaf House case developed a lean, material-focused ontology tailored to PCM retrofitting, while the TUC case extended existing vocabularies like Brick and SAREF to accommodate neighborhood-scale energy systems and KPIs. This balance between using standard ontologies and introducing custom classes, especially for performance indicators, was critical to ensuring both interoperability and precision.

Lastly, the implemented KG-based DT architecture provided a robust methodology for integrating and managing complex neighborhood-level datasets, facilitating informed decision-making. Its flexibility, interoperability, and dynamic data-handling capabilities demonstrate high potential for scalability in broader urban applications. Nevertheless, addressing computational complexity, enhancing interoperability with existing urban systems, integrating real-time sensor data, and deploying AI-driven predictive analytics remain crucial areas for future improvement to maximize stakeholder support in sustainable urban planning.

In upcoming research, this architecture is going to be used for urban heat island assessment at neighborhood level, in a way that connects with other assessments in a concrete and holistic framework for sustainable neighborhoods. Other life cycle stages of a neighborhood are also planned to be explored. Furthermore, expanding the KG with real-time data sources, including IoT sensor networks, weather data, and dynamic energy pricing, will further enhance the architecture impact. Moreover, the KG architecture aims to connect with a GNN recommendation system to provide stakeholders with optimized scenarios and their KPIs. In order to ensure interoperability, a connection with existing BIM, GIS and digital twin platforms will be established. Another anticipated integration involves linking with a DT model focused on agent-based modelling for occupancy and mobility in sustainable neighborhoods. Other DT models will be connected with the architecture and tested. These case studies, and the applications on a real pilot, will contribute to the advancement of the tailored ontology of the TUC case study in order to go towards a complete and comprehensive neighborhood construction renovation and energy management ontology.

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Appendix I

Table 14: Reviewed Ontologies for Built Environment

Category	Name	Scope/Description	Year	Ref
Building Design Phase	Industry Foundation Classes (IFC)	Gives spatial and other properties to every building entity	2013	[256]
	ifcOWL	Descriptive OWL representation of IFC schema	2016	[257]
	simpleBIM	Simplified version of ifcOWL	2017	[258]
	Green Building XML (gbXML)	Information exchange between BIM and Models	2000	[259]
	Tubes	High-level description of building service systems	2020	[260]
	SimModel Ontology	Exchange of energy simulation data	2014	[261]
	EnergyADE	Exchange of energy simulation data	2014	[262]
Sensors	Semantic Sensor Network/Sensor, Observation, Sample, and Actuator (SSN/SOSA)	Focuses on sensors in buildings	2011	[263]
IoT	Web Thing Model (WoT)	Model to describe the virtual counterpart of physical objects in the Web of Things	2015	[264]
	oneM2M BaseOntology's	Provide syntactic and semantic interoperability between oneM2M and external systems	2016	[265]
	One Data Model (OneDM)	Model to support a common language for the Internet of Things	2018	[266]
Smart Buildings	Smart Energy Aware Systems		2016	[267]
	ThinkHome	Ontology that includes concepts needed to realize energy efficient and intelligent control mechanisms	2011	[268]
	Building Ontology for Ambient Intelligence (BOnSAI)	A smart building ontology for ambient intelligence	2012	[269]
	DogOnt	Model for all devices being part of IoT inside a smart environment	2008	[270]
	Ontology of Smart Building (SBOnto)	Smart Building Ontology	2017	[271]
	Smart Applications REFerence (SAREF)	Matches existing assets in the smart applications domain	2014	[272]
Building Automation & Monitoring	Project Haystack 3	Hierarchical representation of buildings entities and concepts utilizing tagsets	2014	[273]
	BASont	Building Automation & Monitoring	2012	[274]
	Project Haystack 4	Hierarchical representation of buildings entities and concepts utilizing tagsets	2019	[275]
	Haystack Tagging Ontology (HTO)	Streamlining Data from IoT based on Project Haystack	2016	[276]

	Brick Schema	Metadata and data points from building advancement and needs based on end-use applications	2016	[277]
	Google Digital Building Ontology	Represent structured information about buildings and building-installed equipment	2020	[278]
	Semantic BMS ontology (SBMS)	BAS-protocol-independent model of intelligent building systems	2016	[279]
	CTRLont	Model of Control Logic in Building Automation Systems	2017	[280]
	Green Button	Building Automation & Monitoring	2011	[281]
	RealEstateCore (REC)	Usage analysis & optimization and presence analysis of a building structure	2017	[282]
	Building Topology Ontology (BOT)	Representation of physical and conceptual objects of a building and the connections between them	2019	[283]
	Building Automation and Control Systems (BACS)	Supports the modeling control behavior in a BAS, physical devices of BAS and their location in the building & connection to technical equipment and appliances	2017	[284]
	Knowledge Model for City (KM4City)	Representation model for city and mobility	2014	[285]
	EM-KPI Ontology	Enhance energy management at district and building levels	2017	[286]
GEB Applications	Facility Smart Grid Information Model	An abstract information model of what the Smart Grid looks like from the perspective of a facility	2014	[287]
	RESPOND	Manage real-time optimal energy dispatching, considering all energy assets on site	2020	[288]
Occupant Behavior - Centric	DNAs Framework (obXML)	Represent the impact of the behavior of occupants on the building's energy efficiency	2015	[289]
	Occupancy Profile (OP) Ontology	Semantic model for occupancy profile	2020	[290]
	Onto-SB	Human Profile Ontology for Energy Efficiency in Smart Building	2018	[291]
	OnCom	Occupant Thermal Comfort Optimization	2019	[292]
Audits & Assets Management	Building Energy Data Exchange Specification (BEDES)	Data information gathering and storing based on building's systems	2014	[293]
	Virtual Buildings Information System (VBIS)	Classifies and connects asset data sources and systems	2020	[294]
	Ontology of Property Management (OPM)	Vocabulary for modeling complex assets in a building design environment	2018	[295]

Table 15: Reviewed Ontologies' Applications in Built Environment

Category	Scope	Ontology Used	Case Study	Year	Ref
KPI Calculation	Reduce the performance gap between the real and simulated data	ifcOWL, SimModel, SSN and custom	Use of simulated and measured KPIs to assess the thermal comfort conditions and the HVAC system performance	2015	[296]
	Gather and prepare data streaming from various sources and calculate the building performance	RDF and custom	Energy Performance assessment using real-time data streaming in a university building, assessed by building managers and engineers	2017	[297]
	Performance tracking at building and district level	ifcOWL, SimModel & SSN ontology	Nineteen solar houses microgrid	2019	[298]
Energy Performance Improvement	Building energy savings	RDF schema	Identify any energy waste in an office zone	2015	[299]
	Support of the selection for efficient and best-cost HVAC systems/the evaluation and prioritization of energy performance values (cooling/heating) consumption	InterfaceOnto	Design phase of an office building	2015	[300]
	Optimize the energy performance	SPORTE2	Building Energy Performance Optimisation of a swimming pool using ANN, Genetic Algorithms, real-time sensors and SWRL rules	2014	[301]
	Optimization problem generation on minimizing comfort dissatisfaction of building users regarding specific parameters and minimizing costs of energy consumption	Custom Ontology	Two office rooms are used to evaluate the scope of the ontology	2017	[302]
Data Injection	Creation of a BIM-based system that automatically associates and updates	gbXML	Two case studies that the method they proposed minimizes the gap between architectural information	2015	[303]

	thermal property measurements with BIM elements in a gbXML schema		in BIM and the real data for energy performance simulation		
	Use of gbXML schema to convert semantic information coming from raw point cloud data and use it into energy simulation tools	gbXML	Five existing buildings (three residential and two bank buildings)	2015	[304]
	Use of gbXML framework to store data from big buildings, like factories, in gbXML format, to make it easier to import into simulation tools	gbXML	University's manufacturing facility	2018	[305]
Facility Management	Provide modification options to facility managers	gbXML, EnergyPlus	Educational building application of real-time data in building energy simulation modifications	2017	[306]
	Creation of semantic relationships between BMS data and building spaces	SSN/SONA and BOT ontologies	Educational building support of data analysis, lacking real-time data that was found to be a challenge in HVAC system control	2018	[307]
	BIM and BMS data connected with the semantic web to assist facility managers	-	-	2018	[308]
Occupant Behavior-Centric	Targets the occupants in a building and makes suggestions to reduce building energy by their behavior	OPTIMUS, SSN/SONA, Urban Energy Ontology	Use of ontology to provide solutions in energy reduction and comfort increase based on the building's assessment/ application of ontology in a lab in Athens where the building's energy was reduced in contrary to the year before the ontology was applied	2018	[309]
	Modeling tool that takes into consideration occupant behavior	obFMU/DNAs, EnergyPlus	coupled obFMU with EnergyPlus to model occupant behavior lighting control, to model occupant behavior window action and to model HVAC control	2016	[310]
	Reduce building energy consumption by having as top priority occupant behavior changes and covering their thermal comfort needs	Onto-SB	Residential building with four people, where they apply distinctive characteristics and after they integrate the mechanism that is proposed they conclude with a 40% energy consumption reduction	2019	[311]
	Efficient control of appliances and devices in smart buildings, targeting the	Onto-SB	Reduce the energy consumption by altering distinctive characteristics in the scenario and make the simulation process quicker	2020	[312]

	occupants' comfort and energy consumption reduction				
	Combination of a wireless sensor network and an emotional state analysis from occupants to calibrate indoor thermal comfort	OnCom	Testing eleven participants with distinctive characteristics and each one responds to the system's actions in a different situation with respect to the indoor thermal comfort and the results showed that the mean of users agreed with the system's decisions	2019	[292]
Decrease of Reused Ontologies	Context-awareness architecture for managing thermal energy in nZEBs	OWL, SWRL	Showing that SPARQL and Semantic Web Rule Language were compatible with decision making in a building	2017	[313]
	Supports the modeling control behavior in a BAS, physical devices of BAS and their location in the building & connection to technical equipment and appliances	BACS, EXPRESS, OSPH, SSN/SOSA, BOT and FSM	Inclusion of a room and the automated control of the windows' shades using SPARQL queries	2017	[314]

Appendix II

Table 16: Material properties inputs in EnergyPlus for the cement (CBF) and gypsum (GBF) board samples.

Field	Units	Samples						
Name		CBF28_30	CBF28_20	CBF28_10	GBF28_30	GBF28_20	GBF28_15	GBF28_10
Roughness		Smooth	Smooth	Smooth	Smooth	Smooth	Smooth	Smooth
Thickness	m	0.2	0.2	0.2	0.2	0.2	0.2	0.2
Conductivity	W/mK	0.086	0.086	0.063	0.173	0.170	0.175	0.164
Density	Kg/m3	650	630	540	950	940	960	870
Specific Heat	J/kgK	125	160	106	118	105	101	103
Thermal Absorptance		0.94	0.98	0.91	0.91	0.88	0.9	0.87
Solar Absorptance		0.57	0.55	0.55	0.51	0.44	0.32	0.30
Visible Absorptance		0.58	0.55	0.58	0.54	0.48	0.35	0.33

Table 17: Material phase changing properties inputs in EnergyPlus for the cement (CBF) and gypsum (GBF) board samples.

Field	Units	Samples						
Name		CBF28_30	CBF28_20	CBF28_10	GBF28_30	GBF28_20	GBF28_15	GBF28_10
Temperature 1	C	10.04	10.03	10.07	10.04	10.09	10.06	10.06
Enthalpy 1	J/kg	12604	16,462	15,973	18,421	11,035	11,985	11,821
Temperature 2	C	26.54	26.53	26.31	28.29	28.09	27.06	25.57
Enthalpy 2	J/kg	45,851	53,285	50,519	68,868	41,898	37,234	33,808
Temperature 3	C	26.79	26.78	26.7	28.54	28.33	27.31	25.82
Enthalpy 3	J/kg	47,203	54,550	51,534	71,305	43,379	38,363	34,378
Temperature 4	C	30.04	30.03	35.07	30.04	30.09	30.06	30.07
Enthalpy 4	J/kg	54,085	61,478	67,477	80,042	47,978	43,248	41,169

Table 18: Material phase changing properties inputs in EnergyPlus for the cement (CBF) and gypsum (GBF) board samples.

Field	Units	Samples						
Name		CBF28_30	CBF28_20	CBF28_10	GBF28_30	GBF28_20	GBF28_15	GBF28_10
Latent Heat during the Entire Phase Change Process	J/kg	66,811	77,246	44,500	100,033	60,108	55,726	54,022
Liquid State Thermal Conductivity	W/mK	0.086	0.086	0.063	0.173	0.170	0.175	0.164
Liquid State Density	Kg/m3	650	630	540	950	940	960	870
Liquid State Specific Heat	J/kgK	125	160	106	118	105	101	103
High Temperature Difference in Melting Curve	deltaC	2.34	1.93	2.17	2.72	2.24	2.61	2.12
Peak Melting Temperature	C	26.7	26.6	26.4	28.3	28.1	27.2	25.7
Low Temperature Difference in Melting Curve	deltaC	7.4	5.57	7.58	4.01	5.26	4.39	4.63
Solid State Thermal Conductivity	W/mK	0.086	0.086	0.063	0.173	0.170	0.175	0.164
Solid State Density	Kg/m3	650	630	540	950	940	960	870
Solid State Specific Heat	J/lgK	125	160	106	118	105	101	103
High Temperature Difference in Freezing Curve	deltaC	1.84	3.9	2.3	1.52	1.71	1.70	5.03
Peak Freezing Temperature	C	23.4	22.8	22.7	24.5	24.3	24.04	22.2

Low Temperature Difference in Freezing Curve	deltaC	8.41	2.8	7.44	3.73	3.29	3.05	3.47

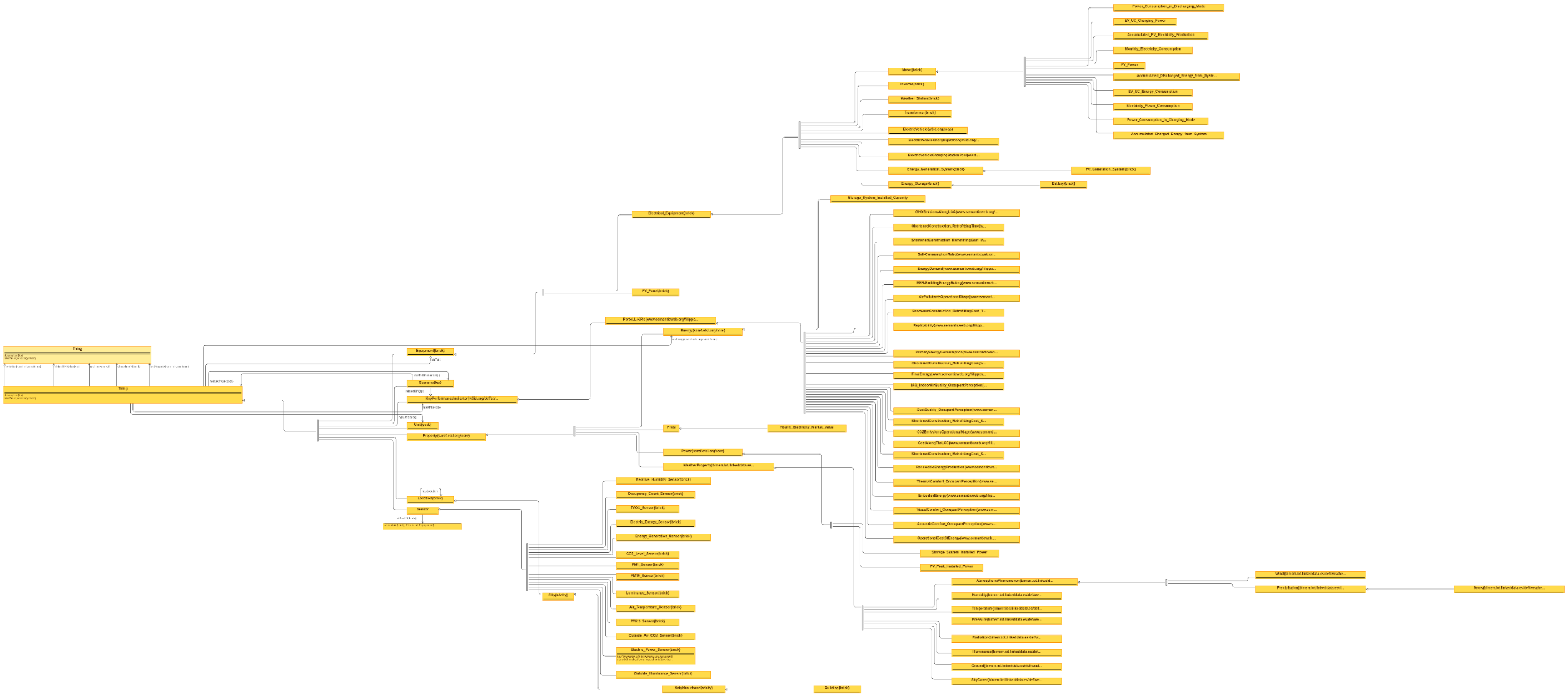

Figure 65. Current Version of NCREM Ontology

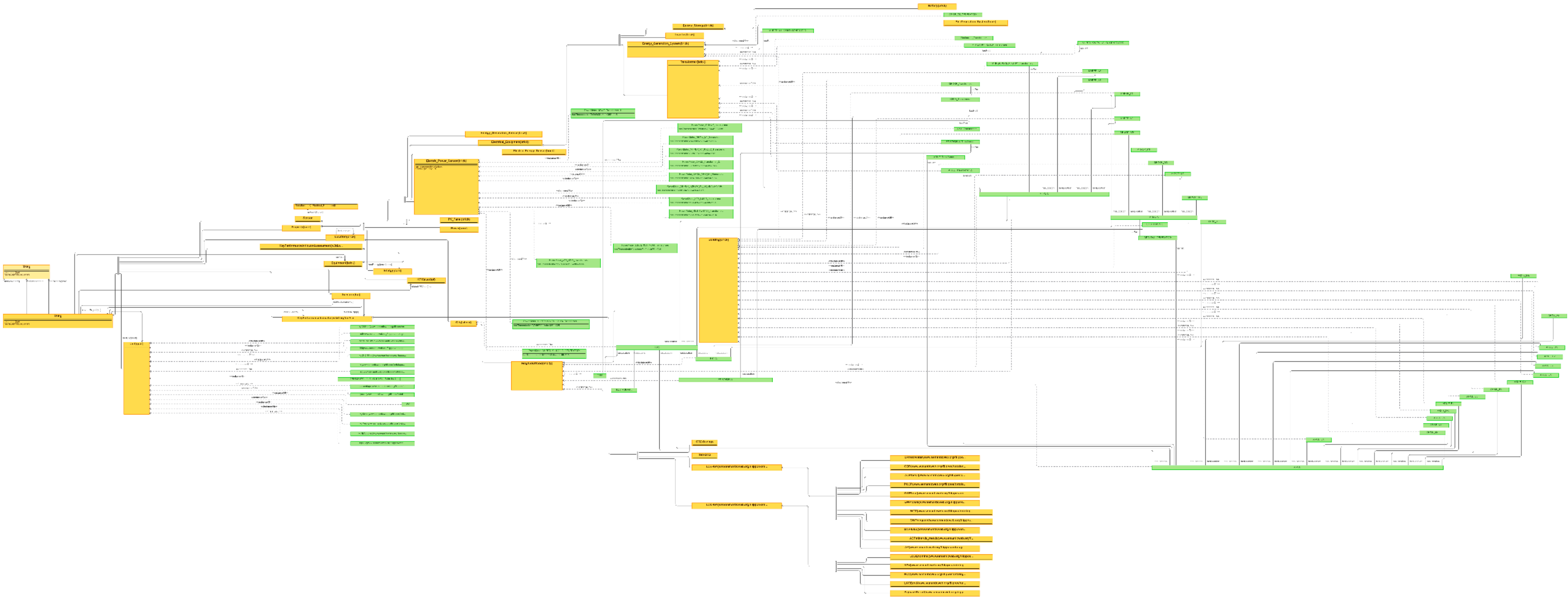

Figure 66. TUC Case Study Ontology with Instances