

Document Version

Final published version

Citation (APA)

Zhilyaev, D. (2026). *Latent Potential, Set in Cement: Developing a Novel Thermal Performance Material Based on PCM-Embedded Cementitious Foam from an Idea to a Market-Ready Product*. [Dissertation (TU Delft), Delft University of Technology]. <https://doi.org/10.4233/uuid:0c40091f-d6b7-4b95-bfee-b44275203c93>

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LATENT POTENTIAL, SET IN CEMENT

**Developing a Novel Thermal
Performance Material Based on
PCM-Embedded Cementitious Foam
from an Idea to a Market-Ready Product**

Dmitry Zhilyaev

LATENT POTENTIAL, SET IN CEMENT

DEVELOPING A NOVEL THERMAL PERFORMANCE
MATERIAL BASED ON PCM-EMBEDDED CEMENTITIOUS
FOAM FROM AN IDEA TO A MARKET-READY PRODUCT

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**DEVELOPING A NOVEL THERMAL PERFORMANCE
MATERIAL BASED ON PCM-EMBEDDED CEMENTITIOUS
FOAM FROM AN IDEA TO A MARKET-READY PRODUCT**

Dissertation

for the purpose of obtaining the degree of doctor
at Delft University of Technology
by the authority of the Rector Magnificus, Prof. dr. ir. H. Bijl,
chair of the Board for Doctorates
to be defended publicly on
Thursday 26 March 2026 at 15:00 o'clock

by

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Horizon2020
European Union Funding
for Research & Innovation

This work was supported by the European Commission, project no. GA870114.

Keywords: Thermal insulation, phase change materials, material design optimisation, building energy simulation, life cycle assessment, thermal resilience, multi-stakeholder decision-making

Printed by: ProefschriftMaken

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ISBN 978-94-6518-269-8

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What if I just go back to sleep for a little while and forget all this foolishness

Franz Kafka, The Metamorphosis

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SUMMARY

Improving the sustainability of the built environment is one of the essential steps to meet the Paris Climate Goals and ensure a liveable future. While many approaches to improving building sustainability exist, the primary focus should be on sufficiency actions that aim to avoid the demand for energy and materials in the first place. Among the sufficiency measures, improvement in thermal performance of a building envelope for reduced energy demand is one of the most efficient and promising approaches for improved building sustainability. This thesis aims to further the research and deepen the understanding of thermal materials by focusing on the development of NRG-Foam, a novel dual-purpose material combining insulating and energy-storing properties. Using a multi-disciplinary approach, this work follows the development of the material from a laboratory sample to a market-ready product.

As the first step, this thesis introduces NRG-Foam material and provides a detailed look into the functional, environmental and economic performance of the material as well as its constituents. After modelling the overall production process of NRG-Foam, life cycle assessment (LCA) and life cycle costing assessment (LCCA) are performed. The results of the assessments indicate that the production of microencapsulated phase change material (MPCM) particles is by far the main contributor to the overall impacts. The high impacts of MPCM production, in turn, are tracked down to the high energy intensity of the manufacturing process, setting it aside as the main hotspot within the overall NRG-Foam production process. Between the two analysed MPCM types, MPCM with inorganic coacervate (IC) shell show significantly higher environmental impacts but considerably lower production costs compared to MPCM with melamine-formaldehyde (MF) shell. As an extension of the static assessments, a multi-objective optimisation of NRG-Foam has also been performed. The analysis of the obtained Pareto frontiers uncovered the presence of multiple trade-offs between functional, environmental and economic performance of the material, highlighting the inevitability of compromises in future material development.

After in-depth material-level analysis of NRG-Foam, the research shifts to the building-level, starting with the exploration of the current state of the art in PCM modelling in the context of full-building energy simulations. From the thorough comparison and testing of the existing comprehensive PCM models, it becomes evident that they currently have a number of limitations, rendering them not reliable enough for widespread practical applications. Moreover, the comparison between different PCM models and their outputs highlights that in the context of a decision-making case, they often provide contradicting results. From a broad perspective, the results of this part of the thesis raise serious questions about relying on computational simulations for PCM research. In the context of this work, the observed issues lead to the

conclusion that for the remainder of the research, simplified but more reliable PCM models should be utilised.

As the next step, the research focuses its attention on NRG-Panels (a product of casting NRG-Foam) and their performance in the context of a demonstrator building. Using LCA and LCCA extended with an *ex ante* approach and a number of up-scaling scenarios, the environmental and economic performance of NRG-Panels is evaluated and then compared with conventional insulation materials. Based on up-scaled assessments, LCA/LCCA of two demonstrator buildings are developed: one including NRG-Panels and another including EPS insulation. The obtained results show that when it comes to environmental and economic impacts, NRG-Panels are comparable to conventional insulation materials. However, when comparing building-level performance of NRG-Panels and EPS, it was observed that a building with EPS had both lower economic and environmental costs. Nevertheless, those results are only representative of a single analysed configuration of NRG-Panels that might not have been optimal for the given case. Consequently, it was concluded that to have a better understanding of NRG-Panels' performance in comparison with regular materials, an optimisation of their configuration is required.

Acting upon the suboptimality hypothesis, the research continues with a case-specific optimisation of NRG-Panels where their configuration is optimised for three different objectives: lifecycle environmental costs, economic costs of electricity for heating and cooling, and construction and demolition costs. The optimised configurations were found to outperform EPS for all objectives. However, it was also observed that the optimal configurations of NRG-Panels acted essentially as a conventional insulation material and had very limited heat storage capacity. It has thus been concluded that Sofia (the location of the demonstrator buildings) might not have been best suited for NRG-Panels' application due to the local climatic conditions.

Continuing the line of reasoning, the research proceeds with analysing and optimising NRG-Panels' performance in the context of different climatic conditions. Using multi-objective optimisation, NRG-Panels' configuration has been optimised for the current climate in 53 locations around Europe, and for 10 of those locations, for the future climate projections. The thermal performance of NRG-Panels has also been compared with EPS in all climatic contexts. The results of optimisations showed that the optimal configuration of NRG-Panels can be very different depending on the geographical location and whether the effects of climate change are taken into account or not. Across all analysed locations, the most promising ones from the standpoint of NRG-Panels' applicability were found to be located in the areas characterised by Mediterranean climate, where the heat-storing properties of NRG-Panels become an advantage compared to regular insulation materials.

The final part of the research in this PhD dissertation focused on the analysis of NRG-Panels in the context of a construction project and, more specifically, on the inclusion of subjective preferences of stakeholders into the decision-making process, as well as the effect of this inclusion. To this

end, two new decision-making approaches were developed. The first approach provided a conceptual basis and was operationalised, but its further testing revealed a number of limitations critical for its practical application. More specifically, it was prone to generating skewed results with a large disparity between satisfaction levels of involved stakeholders and relied on black-box software for operation. To address those limitations, another approach was developed called Preference-Based Goal Attainment that allowed for finding an equitable compromise solution, while also being straightforward and transparent. This new approach was then applied to a decision-making case where the most suitable thermal material was selected from a number of options, including various NRG-Panels' configurations as well as different conventional insulation materials. The decision-making case highlighted that NRG-Panels can be a competitive option compared to regular insulation materials, especially if their configuration is fine-tuned for a specific case at hand.

This thesis contributes to a wide range of topics related to thermal materials and thermal building performance. Its main focus is the in-depth analysis and optimisation of NRG-Foam and NRG-Panels, and on this front, it provides an array of valuable insights and data necessary for the further development of the material. Overarching this, it adds to the knowledge across more fundamental and far-reaching themes such as building energy modelling, PCM modelling, material and building design optimisation, thermal resilience, sustainable construction, and decision-making in construction.

SAMENVATTING

Het verbeteren van de duurzaamheid van de gebouwde omgeving is een van de essentiële stappen om de klimaatdoelstellingen van Parijs te behalen en een leefbare toekomst te waarborgen. Hoewel er vele benaderingen bestaan om de duurzaamheid van gebouwen te verbeteren, zou de primaire focus moeten liggen op maatregelen die erop gericht zijn de vraag naar energie en materialen in de eerste plaats te vermijden. Onder deze maatregelen is het verbeteren van de thermische prestaties van de gebouwschil, met als doel een lagere energievraag, een van de meest efficiënte en veelbelovende strategieën voor verduurzaming van gebouwen. Dit proefschrift heeft tot doel het onderzoek naar thermische materialen verder te ontwikkelen en te verdiepen door zich te richten op de ontwikkeling van NRG-Foam, een nieuw materiaal dat isolerende en energieopslagcapaciteiten combineert. Met een multidisciplinaire aanpak wordt in dit werk de ontwikkeling van het materiaal gevolgd van laboratoriummonster tot een marktrijp product.

Als eerste stap introduceert dit proefschrift het NRG-Foam-materiaal en geeft het een gedetailleerde analyse van de functionele, milieutechnische en economische prestaties van het materiaal en zijn componenten. Na het modelleren van het volledige productieproces van NRG-Foam zijn er een levenscyclusanalyse (LCA) en levenscycluskostenanalyse (LCCA) uitgevoerd. De resultaten tonen aan dat de productie van microgeïncapsuleerde faseveranderingsmateriaal (MPCM)-deeltjes veruit de grootste bijdrage levert aan de totale impact. Deze hoge impact is voornamelijk te herleiden tot de hoge energie-intensiteit van het productieproces van MPCM, waardoor dit onderdeel als zwaartepunt in het gehele NRG-Foam-productieproces naar voren komt. Van de twee onderzochte typen MPCM vertoont MPCM met een anorganische coacervaschil (IC) aanzienlijk hogere milieu-impact, maar beduidend lagere productiekosten in vergelijking met MPCM met een melamine-formaldehyde (MF)-schil. Als uitbreiding op de statische analyses is ook een multi-objectieve optimalisatie van NRG-Foam uitgevoerd. De analyse van de verkregen Pareto-fronten onthulde de aanwezigheid van meerdere afwegingen tussen functionele, milieutechnische en economische prestaties van het materiaal, wat de onvermijdelijkheid van compromissen bij toekomstige materiaalontwikkeling benadrukt.

Na de diepgaande analyse op materiaalniveau verschuift het onderzoek naar het gebouwniveau, beginnend met een verkenning van de huidige stand van zaken in PCM-modellering binnen het kader van volledige gebouwenergiesimulaties. Uit de grondige vergelijking en toetsing van bestaande uitgebreide PCM-modellen blijkt dat deze momenteel meerdere beperkingen kennen, waardoor zij nog niet betrouwbaar genoeg zijn voor grootschalige praktische toepassing. Bovendien toont de vergelijking van verschillende PCM-modellen en hun resultaten aan dat zij in besluitvormingscontext vaak tegenstrijdige uitkomsten opleveren. Vanuit een breder perspectief roepen de resultaten van dit deel van het proefschrift

serieuze vragen op over de geldigheid van PCM-onderzoek dat uitsluitend op computersimulaties vertrouwt. In de context van dit onderzoek leidde dit tot de conclusie dat voor de resterende analyses in dit proefschrift vereenvoudigde, maar betrouwbaardere PCM-modellen gebruikt dienen te worden.

Vervolgens richt het onderzoek zich op NRG-Panels (een product verkregen door het gieten van NRG-Foam) en hun prestaties binnen de context van een demonstratiegebouw. Met behulp van LCA en LCCA, uitgebreid met een ex ante-benadering en diverse opschalingsscenario's, zijn de milieu- en economische prestaties van NRG-Panels geëvalueerd en vergeleken met conventionele isolatiematerialen. Op basis van opgeschaalde analyses zijn LCA's en LCCA's opgesteld voor twee demonstratiegebouwen: één met NRG-Panels en één met EPS-isolatie. De resultaten tonen aan dat de milieu- en economische prestaties van NRG-Panels vergelijkbaar zijn met die van conventionele isolatiematerialen. Echter, in de specifieke gebouwconfiguratie die werd geanalyseerd, vertoonde EPS zowel lagere economische als lagere milieu-impact. Aangezien deze resultaten slechts betrekking hadden op één, mogelijk suboptimale configuratie van NRG-Panels, werd geconcludeerd dat een optimalisatie van de configuratie noodzakelijk is om een volledig beeld te krijgen.

Op basis van deze hypothese is vervolgens een casusspecifieke optimalisatie van NRG-Panels uitgevoerd, waarbij de configuratie werd geoptimaliseerd voor drie doelstellingen: de levenscyclusgerelateerde milieukosten, de economische kosten van elektriciteit voor verwarming en koeling, en de bouw- en sloopkosten. De geoptimaliseerde configuraties bleken EPS op alle doelstellingen te overtreffen. Er werd echter ook vastgesteld dat de optimale configuraties in essentie als conventioneel isolatiemateriaal functioneerden en slechts een beperkte warmtecapaciteit hadden. Hieruit werd geconcludeerd dat Sofia (de locatie van de demonstratiegebouwen) mogelijk niet de meest geschikte plaats was voor de toepassing van NRG-Panels, gezien de lokale klimatologische omstandigheden.

Voortbouwend op deze redenering is de prestatie van NRG-Panels vervolgens geanalyseerd en geoptimaliseerd voor uiteenlopende klimatologische omstandigheden. Met behulp van multi-objectieve optimalisatie werd de configuratie van NRG-Panels geoptimaliseerd voor het huidige klimaat in 53 locaties in Europa, en voor 10 van deze locaties ook voor toekomstige klimaatprojecties. De thermische prestaties van NRG-Panels zijn in alle klimatologische contexten vergeleken met EPS. De resultaten tonen aan dat de optimale configuratie van NRG-Panels sterk kan variëren afhankelijk van de geografische locatie en het al dan niet meenemen van klimaatveranderingseffecten. De meest veelbelovende locaties voor toepassing van NRG-Panels bleken zich te bevinden in gebieden met een mediterraan klimaat, waar de warmteopslagcapaciteit van NRG-Panels een voordeel oplevert ten opzichte van reguliere isolatiematerialen.

Het laatste deel van dit onderzoek richt zich op de analyse van NRG-Panels in de context van een bouwproject, met specifieke aandacht voor subjectieve

voorkeuren van belanghebbenden in het besluitvormingsproces en de effecten daarvan. Daartoe zijn twee nieuwe besluitvormingsmethoden ontwikkeld. De eerste methode bood een conceptuele basis en werd operationeel gemaakt, maar verdere tests toonden aan dat zij kritieke beperkingen had voor praktische toepassing, waaronder de neiging om onevenwichtige resultaten te genereren met grote verschillen in tevredenheid tussen belanghebbenden, en de afhankelijkheid van black-boxsoftware.

Om deze beperkingen te verhelpen werd een tweede methode ontwikkeld: Preference-Based Goal Attainment. Deze methode maakt het mogelijk een meer rechtvaardige compromis te vinden en is bovendien eenvoudig en transparant. De methode werd toegepast op een besluitvormingscasus waarbij het meest geschikte thermische materiaal werd gekozen uit diverse opties, waaronder verschillende configuraties van NRG-Panels en conventionele isolatiematerialen. De casus toonde aan dat NRG-Panels een concurrerend alternatief kunnen vormen voor reguliere isolatiematerialen, vooral indien hun configuratie wordt afgestemd op de specifieke omstandigheden.

Dit proefschrift levert een bijdrage aan een breed scala aan onderwerpen gerelateerd aan thermische materialen en thermische gebouwprestaties. De kern ligt in de diepgaande analyse en optimalisatie van NRG-Foam en NRG-Panels, waarbij waardevolle inzichten en gegevens worden verstrekt voor de verdere ontwikkeling van het materiaal. Daarnaast draagt het bij aan de kennis over meer fundamentele en brede thema's, zoals gebouwenergiemodellering, PCM-modellering, materiaal- en gebouwtwerptoptimalisatie, thermische veerkracht, duurzaam bouwen en besluitvorming in de bouwsector.

1

INTRODUCTION



1.1 Background

Buildings are essential to our lives, yet they are also responsible for a major share of global resource consumption and emissions [1], [2]. With the expanding global population and intensifying urbanisation, the demand for housing is expected to continue to grow [3], [4], thus requiring even more materials and causing larger negative environmental impacts. To meet the goals of the Paris Agreement [5] and ensure a liveable future, a decoupling of the global building stock size and overall negative emissions produced by it is urgently needed [6]. Such a decoupling is an extremely complex undertaking and can only be accomplished by a combination of measures focusing on every part of the building lifecycle. Across a building's lifecycle, it has been shown that the use stage and more specifically the operational energy use for heating and cooling is the main hotspot driving the overall negative impacts [7]. Consequently, the reduction in energy demand for heating and cooling should be one of the main priority points in enabling the emissions decoupling and reaching the Paris Agreement goals. While some fundamental steps have already been taken in this direction and new construction is generally characterised by sound energy performance enforced by various regulations [8], this is often not the case for old building stock [9], [10]. This puts even greater pressure on the countries with a high average age of building stock to promptly address this issue. This is also the case for the EU, where the vast majority of buildings currently in use were built before regulations on the thermal performance of buildings were introduced [9], [10].

When it comes to the energy demand for heating and cooling of a building, it is driven by social and technical factors. Social factors consider the impact of tenants' behaviour on the energy consumption of the building. On the other hand, technical factors are related to the physical characteristics of the building. While the contribution of the social factor is important, the research has shown that technical aspects play a significantly larger role in defining the final energy consumption of a building [11]. More specifically, heat losses through the building envelope were shown to be the main cause of high heating and cooling loads [12]. Consequently, building envelope improvements are one of the keys to reducing the overall global impacts of the built environment.

The most common way of improving the thermal performance of a building envelope is by decreasing its thermal conductivity. This is usually done by introducing a layer of insulating material that is characterised by very low thermal conductivity and the ability to decrease conduction, convection and radiation heat transfer via the building envelope. This allows to reduce the loss of heat during the heating season as well as the influx of heat into the building during the cooling season [13]. Another way of improving the thermal performance of the building envelope that is gaining momentum in recent years is the use of phase change materials (PCM) [14]. Those materials possess a unique property of being capable of absorbing

large amounts of heat without causing an increase in sensible temperature when they undergo a phase change transition. Through this property, they could perform a similar function to insulating materials and reduce the overall heat flux through the building envelope [15]. In addition to that, they might also allow for shifting the peak heating and cooling load hours [16]. Since the environmental impacts and costs of energy vary from hour to hour, load shifting might help reduce the overall environmental impacts and costs of energy used for heating and cooling [17].

While insulating materials and PCM are often studied in isolation from each other, it is also possible to combine them within the same building envelope. This can be done by introducing them as separate layers or combining them within a single material that possesses both insulating and heat-storing qualities. By doing this, it could be potentially possible to combine the positive effects of both material types and have even larger benefits compared to when the building envelope only includes insulation or PCM exclusively [18]. Such an integration, however, is a challenging task on many levels. First of all, on the material level, a trade-off between insulating and heat-storing properties might be observed: the main goal of insulation is the reduction of heat flow through the building envelope, but for a full utilisation of heat-storing properties of PCM, it is necessary to ensure an efficient heat transfer to it [19].

On the building level, PCM materials impact the building's thermal performance in a dynamic and nonlinear manner that is challenging to model [20], [21], [22]. This makes the task of balancing insulating and heat-storing properties of the building envelope for the best possible overall thermal performance particularly complex. Furthermore, on the building level, more trade-offs might come into play. For example, the introduction of PCM might result in increased material costs and embodied carbon emissions of the building and the benefits from the increased heat storage capacity of the building envelope might not be sufficient to offset the embedded impacts of added PCM [23]. Finally, the effect of insulation materials and PCM on the overall thermal performance of the building is highly sensitive to a multitude of factors such as climatic conditions, building configuration, HVAC system setup, making the holistic modelling of building performance resource-intensive and computationally demanding [20].

On the construction project level, all abovementioned challenges are still relevant, but on top of this, social aspects enter the picture. At this highest level, the final choice of the material for improved thermal performance of the building is also guided by the composition of the decision-making team, the requirements of the stakeholders involved in the decision-making process, their interaction and possible conflicts of interest, as well as the particular decision-making methodologies used in the process [24], [25], [26], [27]. All those factors should be accounted for in the modelling, analysis and optimisation of thermal materials.

The described challenges are especially critical in the case of the development of a new dual-purpose thermal material combining insulating and energy-storing properties. The market of thermal materials is already

1 saturated with a great variety of options readily available for immediate use in construction projects [28], [29]. It is thus essential to ensure that the newly developed material will be competitive and to find a market niche that it can fill. Furthermore, when it comes to new materials, the number of design parameters that can be altered during the development process is extremely high, especially for complex materials combining multiple functions. Taking into account that 80% of a new product's impacts are determined during the early design phase, the design of the material should be refined and optimised already in the very early stages of the development process [30]. This puts tremendous pressure on the material developers to thoroughly assess all the performance aspects of the new thermal material, identify bottlenecks, compare it to the existing alternatives and find the most promising and competitive design configurations as soon in the development process as possible. While some performance comparisons could be done experimentally, those are usually limited due to the difference in technology readiness level (TRL), experiment upscaling limitations, as well as time and budget constraints. The development of novel materials thus becomes largely computationally-guided, and comprehensive modelling of material performance coupled with a model-driven optimisation of the material design is playing a vital role in the success of the material development project as a whole.

1.2 Research objectives and scope

This dissertation takes on the complexity described in the previous section and focuses on the development of NRG-Foam – a novel thermal performance material based on cementitious foam with embedded microencapsulated PCM (MPCM) particles. NRG-Foam combines insulating properties resulting from its high porosity with heat-storing properties stemming from the inclusion of MPCM particles. Through comprehensive modelling and optimisation of NRG-Foam, this dissertation tells the story of material development from an idea to a competitive market-ready thermal material.

This work approaches the analysis of NRG-Foam using a cross-TRL progressively expanding scope. More specifically, it follows the development of NRG-Foam from the laboratory sample to prototype to market-ready product and is aligned with the TRL scale adopted by the EU based on the original method developed by NASA [31]. In the EU-adopted scale, the development of a new technology or product is divided into nine levels, starting from TRL1 (Basic principles observed) to TRL9 (Actual system proven in operational environment). From those levels, TRL1 to TRL4 relate to fundamental research, experiments and laboratory validation. TRL5 to TRL7 are focused on validation and demonstration of the technology prototype in the relevant and operational environment. The two highest levels, TRL8 and TRL9, refer to the stage when the finalised technology is complete, qualified and proven in an operational environment. Figure 1.1 illustrates the overall approach used in this dissertation and shows how the development level, TRL, analysis scope, and design space are connected and evolving over time.

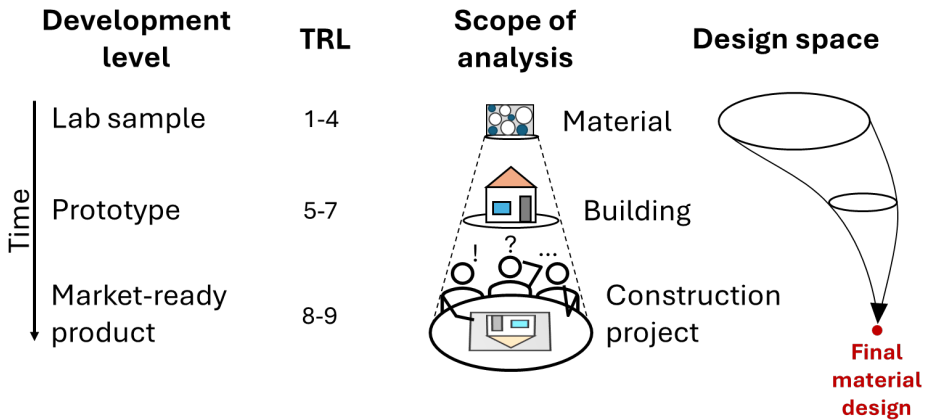


Figure 1.1: Cross-TRL expanding-scope approach to the analysis, design and optimisation of NRG-Foam.

The development of the material begins in the laboratory setting, where a number of test samples are prepared and studied. This stage is characterised by a narrow scope and revolves around detailed studies of the material and its components. At the same time, at this point of material development, the design space is as wide as it can be: the work at this stage is largely focused on exploring and testing as many possible material variations as time, resources, and budget allow.

As the material development level increases, it moves from the laboratory to the real-world setting. At this stage, functional prototypes of the material are produced and tested in the context of a building. Those tests can be physical, computational or a combination thereof. The scope widens, and instead of being analysed in isolation, the material is now viewed as a part of a larger interconnected system and as one of multiple factors impacting the overall performance of a building. Compared to the lab stage, the design space narrows down: the analysis and tests performed allow to filter out less promising design configurations, while some other configurations turn out to be unfeasible due to various constraints.

Finally, after the prototype stage, the material is entering the market. After solely technically guided development, this stage introduces the human factor into the equation. The scope expands even further from a building to a construction project, and now the material is viewed as just one of multiple variables in the project. The newly developed material is competing against other alternatives, and decision-makers involved in the construction project have to decide what material to use. The design space is reduced further and, after all the parameters of the construction project are set and agreed upon, narrows down to a single final material configuration that is the best suited for the given project.

The main objectives of this work associated with each scope and TRL described above are summarised as follows:

1

Material level

- Assess the material-level environmental, economic and functional performance of NRG-Foam and its constituents.
- Identify the hotspots within the production process of NRG-Foam and its components.
- Explore the trade-offs between different performance characteristics of NRG-Foam.

Building level

- Investigate the current state of the art and the associated challenges in modelling the dynamic behaviour of PCM within the building envelope.
- Assess the material-level and building-level environmental, economic, and functional performance of NRG-Foam and optimise its configuration in the context of a demonstrator building.
- Identify the geographical areas favourable for NRG-Foam application.

Construction project level

- Develop a new multi-stakeholder decision-making and conflict resolution approach that more closely resembles the real-world decision-making dynamics and accounts for the preferences of stakeholders.
- Assess the competitiveness of NRG-Panels in the construction project setting.

1.3 Dissertation outline

The dissertation consists of nine chapters, including Introduction and Conclusions. The main body of the dissertation is divided into three themes aligned with the expanding scope approach introduced in the previous section. Figure 1.2 provides an overview of the dissertation structure.

Chapter 1: Introduction	
Material level	2 Early-stage analysis of a novel insulation material based on MPCM-doped cementitious foam: Modelling of properties, identification of production process hotspots and exploration of performance trade-offs
Building level	3 A shot in the dark: The current state of PCM hysteresis modelling in building energy simulation software
	4 Prototype-level assessment of NRG-Foam and NRG-Panels in the context of a demonstrator building
	5 Case-specific optimisation of NRG-Foam for improved building-level performance
	6 Climate-dependent design of NRG-Panels and identification of favorable locations for NRG-Panels application
Construction project level	7 Best fit for common purpose: A multi-stakeholder design optimisation methodology for construction management
	8 Preference-based goal attainment approach for equitable decision-making
Chapter 9: Conclusions and Recommendations	

Figure 1.2: The outline of the dissertation.

A short summary for each chapter is provided below.

- **Chapter 1** introduces the motivation for the dissertation, outlines the overall study approach and summarises the main research and development goals.
- **Chapter 2** presents an in-depth laboratory-scale analysis of NRG-Foam and its components. This chapter builds an overall production system of NRG-Foam from cradle to gate and focuses on assessing the environmental, economic and functional performance of the material as well as the trade-offs between those characteristics. Furthermore, it identifies main production process hotspots, paving the way for improving and upscaling the production process – an essential step for moving to the prototype development stage.
- **Chapter 3** marks the transition from the material-level to building-level analysis of NRG-Foam and assesses the current state of the art

in computational modelling of energy performance of buildings that include PCM in their envelope. As the use stage of a building can account for more than 80% of the overall lifetime environmental impacts [7], for PCM-embedded buildings, it is of great importance to ensure that the models correctly simulate the dynamic nature of PCM. The chapter uncovers a number of limitations and issues with the currently existing models and concludes that, at the moment, it might be advisable to use simplified but more reliable models instead of comprehensive ones. Guided by those findings, the following chapters resort to using a simplified approach to PCM modelling.

- In **Chapter 4**, the analysis moves from studying NRG-Foam to the analysis of NRG-Panels – a thermal material produced by casting and curing of NRG-Foam. NRG-Panels in this chapter are studied in the context of demonstrator buildings that have been physically built in Sofia, Bulgaria. The assessments in this chapter built upon the foundation presented in Chapter 2, and the hotspots identified in that chapter are used to develop the upscaling scenarios as a part of the ex-ante assessment approach. Such an upscaling allows for bringing the assessments to the level necessary for comparing NRG-Panels with the conventional thermal materials already available on the market. The results of the chapter highlighted that while the performance of NRG-Panels was comparable to EPS, the analysed configuration of NRG-Panels that has been applied to the demonstrator buildings in Sofia may have been suboptimal for the given case.
- **Chapter 5** continues the line of reasoning started in Chapter 4 and focuses on finding an optimised configuration of NRG-Panels that is better suited for the given demonstrator building and climatic conditions of Sofia. From the optimisations performed in this chapter, it becomes evident that while NRG-Panels could outperform existing insulation materials in the context of the demonstrator building, the energy-storing properties of PCM have very limited or no positive effect on the overall performance of the building. This, however, to a large degree, is an effect of the climatic conditions in Sofia, resulting in a long heating season. In such climatic conditions, the improved insulating properties of the material are significantly more beneficial for the overall thermal performance of the building compared to increased heat capacity. Consequently, this chapter suggests that different, warmer climatic conditions might be more suitable for the NRG-Panels application.
- **Chapter 6** explores the effect of different climatic conditions on the building-level performance of NRG-Panels. Using a multi-objective optimisation approach, the material configuration is optimised for a number of locations across Europe for the present as well as for the

projected future climatic conditions. Furthermore, the energy performance of NRG-Panels is also compared to EPS. The results of this chapter indicate that NRG-Panels are most suitable for locations with warmer climates, and especially the Csa climate under the Köppen-Geiger climate classification. Compared to colder climates like in Sofia, in the Csa climate, the heat storage capacity of material becomes more advantageous compared to its insulating properties. Those findings highlight that in warmer climates, as well as in future climates impacted by climate change, there might be a larger market for NRG-Panels compared to conventional insulation materials. The final choice of thermal material for a given construction project, however, is guided not only by the thermal performance of the material but also by other performance characteristics (economic, environmental, etc.) as well as the socio-technical aspects of decision making.

- With **Chapter 7** the thesis enters the level of a construction project and presents a novel stakeholder-focused optimisation-based decision-making approach. This new approach aims to accurately reflect the dynamics of the real-world decision-making rooms and is relying on a priori integration of stakeholders' requirements and preferences into the process. The application of the new approach is further demonstrated using an example construction project.
- **Chapter 8** continues the work started in Chapter 7 and addresses the limitations of the decision-making approach presented there. The newly developed approach, called preference-based goal attainment (PBGA), aims to minimise conflicting situations by finding a more equitable solution while also moving away from using proprietary black-box software for improved transparency and verifiability. The presented approach is then applied to a decision-making case of thermal material selection for the same demonstrator building as analysed in previous chapters, under the climatic conditions of Barcelona. In addition to providing a clear demonstration of the PBGA approach, the decision-making case also highlighted that NRG-Panels could compete with conventional insulation materials and provide a balanced compromise solution satisfying the requirements of multiple stakeholders.
- **Chapter 9** summarises the findings and outlines possible directions for future research and development.

1



EARLY-STAGE ANALYSIS AND OPTIMISATION OF A NOVEL THERMAL PERFORMANCE MATERIAL BASED ON MPCM-DOPED CEMENTITIOUS FOAM

This chapter introduces NRG-Foam – a novel thermal material combining insulating and energy-storing functions – and provides an in-depth look into its properties. The analysis of NRG-Foam presented in this chapter is divided into two parts: static and dynamic. The static presents a model of the overall NRG-Foam's production process and utilises life cycle assessment and life cycle costing assessment to gain insight into the environmental and economic impacts of the NRG-Foam production. The dynamic part identifies the trade-offs between performance characteristics of NRG-Foam using multi-objective optimisation techniques. The results obtained in this chapter highlight that the production of microencapsulated phase change material (MPCM) particles is a major contributor to environmental impacts, while the addition of small amounts of reduced graphene oxide amplifies the impacts even further. On the process level, the hot spot analysis pinpointed high electricity consumption as the main driver of the environmental impacts. A multi-objective optimisation and the analysis of the Pareto frontier revealed the presence of unavoidable trade-offs between performance characteristics of NRG-Foam, emphasising the necessity of compromises during material development. From the bird's-eye view, the results of this chapter lay the foundation for the next steps in the research and development of NRG-Foam.

This chapter has been published in *Developments in the Built Environment* [32].

2.1 Introduction

Buildings are responsible for a major share of global energy consumption as well as negative environmental impacts and improving their performance is an essential task in addressing the challenges posed by global warming [33]. When it comes to the structure of the building's energy consumption, heating and cooling demand could account for up to 73% of the total, depending on the region [34]. While the occupants' behaviour has a significant impact on the energy use of a building, the main influencing factor is by far the configuration and technical properties of the building with envelope-related characteristics having the highest impact [11]. Specifically, heat losses through the building envelope have a major effect on the total energy demand [12]. The improvements in the performance of the building envelope are thus of the utmost importance. On this front, a lot of attention in the academic, industrial and legislative fields has been dedicated to building insulation and insulation materials, especially in countries with colder climates. Many countries now have requirements for insulation performance for new construction [35]. For existing building stock, improvements in the insulation performance are even more important and retrofitting old buildings using new insulation materials is one of the main priorities of the EU's "renovation wave" [36], [37].

While of primary importance for colder climates, the impact of improving envelope insulation can be much less pronounced when it comes to warmer regions [38] and could increase the risk of overheating [39]. Further, due to the effects of global warming, more and more places are starting to experience heatwaves and generally higher temperatures during the summer months and insulation can potentially worsen the indoor climate in such situations [40]. For such conditions, the incorporation of phase change materials (PCMs) within the building envelope has shown to be a promising solution. Due to the high energy storage capacity, PCMs can provide multiple benefits: they can reduce energy consumption, improve the indoor climate and provide a delay in the daytime peak cooling load [41], [42].

Traditional thermal insulation materials and PCMs are currently on different levels of technological and commercial development. When it comes to insulation materials, a multitude of commercial products of different types is readily-available on the market and the history of insulation material application in buildings goes hundreds or even thousands of years back [43]. PCMs on the other hand, have been researched actively over the last couple of decades and have found their way into some commercial construction materials [44] but are not yet applied as broadly as regular insulation materials within real-world construction projects [45].

Nonetheless, there is still room for the development of new materials and technologies in both directions. For insulation materials, while a multitude of materials exists, there is no single do-it-all material. There are multiple performance characteristics that define insulation materials such as thermal insulation, costs, environmental impacts, sound insulation, fire resistance and water vapour permeability [46]. Different insulation materials perform

differently across those characteristics and since there are inevitably some trade-offs between them, the final choice of the material depends on the context and specifics of the project [46]. For example, polystyrene-based insulation has very good insulation properties but has flammability issues and embodied environmental impacts; bio-based insulations have low environmental impacts but often have relatively high thermal conductivity, might have issues with fire safety and have high moisture absorption; mineral wool is quite good when it comes to flammability and low environmental impacts (yet generally higher than such of bio-based solutions) but performs slightly worse compared to the best polystyrene-based materials [47], [48]. As for PCM-based construction materials (such as, for example, bricks or concrete panels with PCM materials embedded), they still need more research and development to prove their environmental and economic feasibility and long-term durability before they can become commonplace in the construction sector [23], [49]. Thus, there is a large field for the development of new insulation and PCM-based construction materials as well as solutions combining those.

Developing and bringing a new construction material to the market is, however, a complex task [50]. It was estimated that 80% of a new product's impacts are determined during the design phase [30]. Consequently, early-stage design decisions play a key role in the design process: as the project moves to later stages, the design flexibility decreases and changes are getting harder and more costly to implement [51]. Early-stage design decisions are, thus, crucial for the further development of the material and its overall success. Each design decision (a design decision can be viewed as a modification to a material design variable), in turn, impacts different performance characteristics of the material and in most cases, there are also some trade-offs between those characteristics involved [52]. Therefore, in order for material designers to make informed decisions, it is important to start building a holistic overview of the material's characteristics, trade-offs between them, possible design constraints as well as the connection between those and design variables as early as possible in the development cycle of the new material.

While the experimental characterisation of the new materials is important, due to a large number of adjustable design parameters (design variables), it can often be impractical or infeasible to create all possible variants of the material in the lab and analyse their properties. The number of possible experimental measurements can further be limited by time and budget limitations. Consequently, analytical and numerical models play a key role in the development of new materials, including in the early development stages [53]. For example, finite element models can be used to model thermal (e.g., [54]), electrical (e.g., [55]) and mechanical properties of a material (e.g., [56]). Analytical models such as, e.g., the Lewis-Nielsen model could be used to obtain thermal and electrical conductivity of multi-phase materials [57]. Environmental, economic and social sustainability performance can be assessed using life cycle assessment (LCA), life cycle costing assessment (LCCA) and social life cycle assessment (S-LCA) [58]. And while life cycle

assessments are better suited for technologies with high technology readiness levels (TRL) [59], even at early stages they can provide some very important information such as hotspots within the production process [60]. Within the current material design process, numerical and analytical models accompany the experimental ones and together guide the further development of new materials [53].

In this study, we focus on an early-stage design, characterisation and modelling of a novel insulation material – NRG-Foam – that is currently being developed within the Horizon 2020 NRG-STORAGE project [61]. The material is based on a cementitious foam doped with microencapsulated PCMs (MPCMs). Being a porous material, it provides good insulation properties while the addition of MPCMs adds energy storage capabilities. Due to its dual function – insulation and energy-storing – and a large number of design variables (compared to regular insulation materials), NRG-Foam provides a challenge when it comes to its modelling, characterisation and optimisation.

This study has two main objectives:

- To model the environmental and cost performance of the NRG-Foam material and identify the hot-spots within the production process
- Explore the trade-offs between environmental, cost, thermal and electrical performance characteristics of NRG-Foam

The study is the first one to fully document and model the production process of a new-generation cement-based insulation material with energy storage capabilities and provides an in-depth look into its environmental, cost and functional performance. At the project level, the results of this study will inform the design decision-making process and guide the further development of NRG-Foam. Furthermore, this study lays the foundation for the future research of NRG-Foam on component-, building- and construction project levels. From a broader perspective, this work provides academics and practitioners within built environment and construction materials fields with a new and valuable insight into the design, development and manufacturing of a novel construction material. The study demonstrates the importance of hotspot and trade-off analysis in the early stages of material development and provides a reference point for similar projects aiming to develop a new construction material.

2.2 Materials and methods

2.2.1 NRG-Foam material description

NRG-Foam is a novel insulation material currently under development within the EU Horizon 2020 project called NRG-STORAGE [29]. It is a cementitious foam with high levels of porosity (and low density) with embedded MPCMs to enable energy storage capabilities. Within the project, two different foam configurations are being considered: passive application NRG-Foam and active application NRG-Foam. Active application foam also includes conductive fillers (reduced graphene oxide or rGO) in addition to MPCMs. The

addition of rGO makes the material electrically conductive which, in turn, makes it possible to melt embedded PCM material on demand by running electrical current through NRG-Foam.

2.2.2 General overview of the methodology

Figure 2.1 shows an overview of the methodological approach used in this study. The study consists of two parts: static and dynamic. Within the static part, a traditional LCA and LCCA have been performed to obtain the impacts of NRG-Foam production and to identify hot-spots within the lab-scale production process. Lab-scale LCA and LCCA models were developed in OpenLCA software [62] based on the input data collected from the project partners. For the static part, five base configurations of the foam have been considered differing in the type of MPCMs and presence of rGO. Based on the results of the analysis, hotspots within the lab-scale production process have been identified.

For the dynamic part, the LCA and LCCA models have been parametrised making it possible to connect them to thermal and electrical properties models and integrate them within optimisation algorithms. Thermal properties of NRG-Foam were estimated based on literature, theoretical models and computational models created by the project partner Centro de Investigación en Métodos Computacionales (CIMEC). The electrical conductivity of the material has been modelled partly based on the experimental data obtained by the project partner Agencia Estatal Consejo Superior De Investigaciones Científicas (CSIC) as well as mathematical models and the abovementioned computational models created by CIMEC. All models were either implemented in or connected to Matlab where a multi-objective genetic algorithm has been used to build a Pareto frontier and explore the trade-offs between the performance characteristics of NRG-Foam. Further, constraints reducing the feasible design space were added to the model based on the experimentally-obtained data by the project partner TU Darmstadt (TUDa). The sections below describe the methodology in more detail.

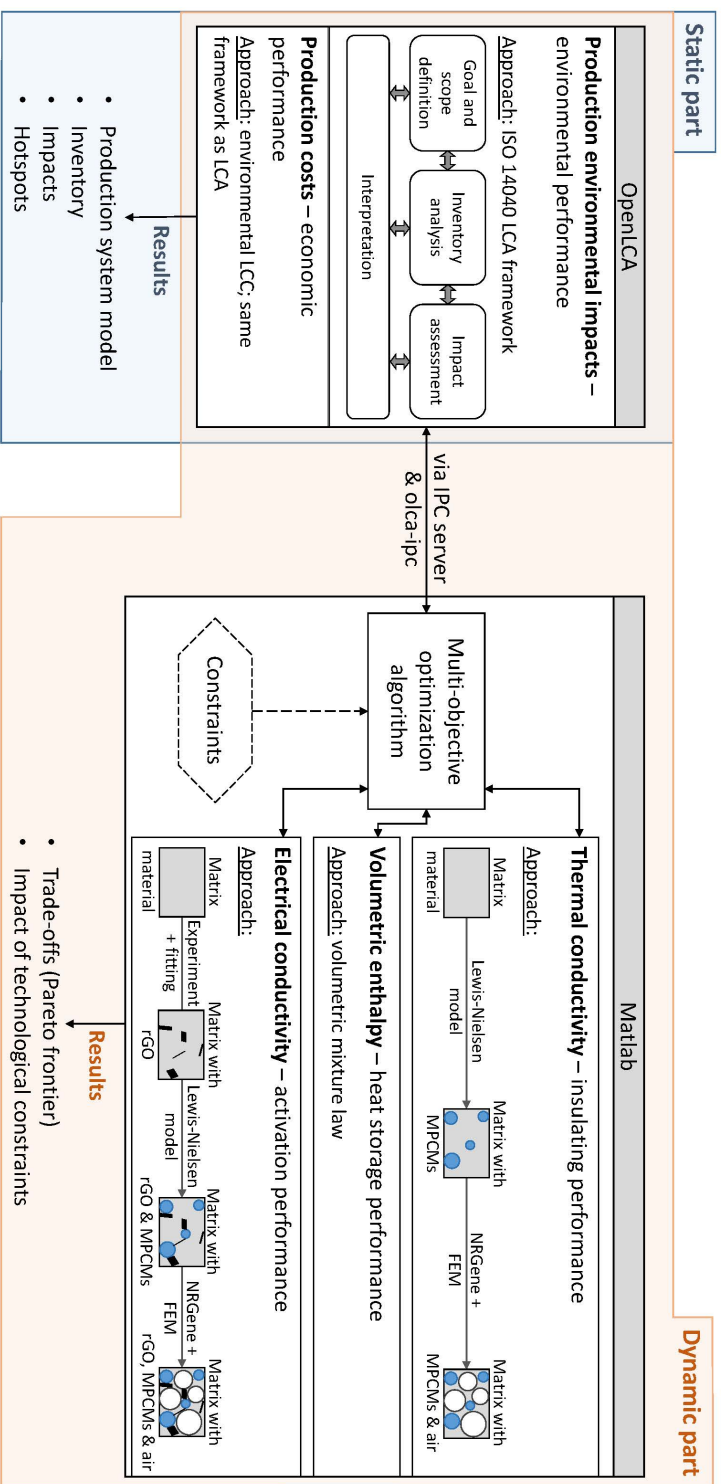


Figure 2.1: Overview of the methodological approach used in this study.

2.2.3 Static part: LCA and LCCA

Overview of the approach

For the assessment of environmental impacts, we follow general LCA guidelines outlined in ISO 14044 [63]. Based on the impact assessment results obtained from the lab scale LCA, the hotspots within the production process are identified. For LCCA, we are following the environmental LCC methodology that is defined within the same framework as LCA [64]. From this standpoint, costs can be considered as an elementary output flow, added to LCA and calculated together with the rest of LCA results as a separate impact category.

Goal, scope and functional unit

The goal of this LCA/LCCA is to evaluate the environmental and economic impacts of NRG-Foam production and to identify the hotspots within the production process. The scope of the study is cradle-to-gate (from the production of raw materials and energy to the final product - NRG-Foam). The functional unit is the production of 1 m³ NRG-Foam and all the results shown in the chapter are provided for 1 m³ NRG-Foam. We used OpenLCA software [62] to develop the model and perform calculations.

Product system and system boundaries

The production system model has been developed in cooperation with project partners and describes the actual manufacturing processes and geography: Sphera Encapsulation S.r.L. (Italy, shortly named SE) produces MPCMs, Graphenea S.A. (Spain, shortly named GR) produces rGO while the mixing and casting of the final material are done at RÖSER Ingenieurbeton GmbH (Germany, shortly named RIB).

To collect necessary data, the overall production system has been divided into small pieces called unit processes. Each unit process represents an individual process of converting inputs into outputs (Figure 2.2). Since we were performing LCCA alongside LCA, each unit process also includes economic inputs and outputs – costs and revenues.

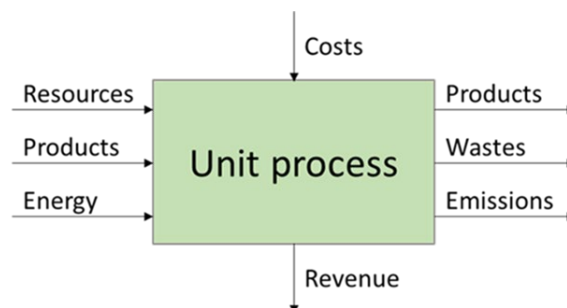


Figure 2.2: A unit process with inputs and outputs.

To compile the full inventory, project partners have been asked to provide information for each unit process separately. This information has been collected using specially developed templates. Figure 2.3 provides an example of such a template for a single unit process.

Inputs				
Input	Amount	Unit	How the value was obtained? (Measurement/Calculation/Estimation)	Cost per unit

Outputs			
Output	Amount	Unit	How the value was obtained? (Measurement/Calculation/Estimation)

Figure 2.3: An example of an inventory data collection template.

Most of the primary data provided by partners has been based on the measurements but some parts have been modelled based on estimations. In particular, the production process of MPCMs with melamine-formaldehyde (MF) shell has been based on the literature ([65], [66], [67], [68], [69]) and information from a producer and not on experimental/measured data.

The cost data have been partly based on the real purchase costs encountered by the project partners and partly collected from internet sources (e.g., Sigma-Aldrich/Merck [70]). Since the scope of the analysis is cradle-to-gate, there are no profits occurring and LCCA is thus limited to costs only.

Commercial production processes and data privacy

This study partly relies on proprietary data describing commercial production processes. Specifically, the processes involved in inorganic coacervate (IC) MPCMs and rGO production are know-how of SE and GR project partners correspondingly. Due to this, some data cannot be disclosed publicly and some of the information in this study has been black-boxed or anonymised:

- For the production of inorganic coacervate (IC) shell MPCMs, the names of the chemicals used in the production process have been anonymised. The real names have been replaced with generic ones such as Polymer 1, Polymer 2, Emulsifier, etc.
- For the production of rGO, the inventory has been black-boxed so it is not possible to see which inputs-outputs are included as well as corresponding volumes. In the figures showing relative contributions to different impact categories, the raw products used within rGO

production process have been grouped together and shown as “Chemicals – rGO” category.

- Within the cost data used for LCCA calculations, the names of the chemicals used in rGO and IC shell MPCMs production have also been anonymised.

While it is not possible to disclose detailed data on those particular production processes, the reader can refer to the patent EP3070053A1 by GR [71] for the information about rGO production process. The production process of IC shell MPCMs is a know-how of SE and its details cannot be disclosed but some general information on the process of IC shell manufacturing can be found in publications [72], [73], [74]. The MPCM manufacturing processes described in the aforementioned publications differ from SE's process but could provide the reader with some idea for the processes of IC shell forming and coacervation.

Inventory

For the foreground system, the inventory has been collected from the project partners involved in the production. For the background system processes (production of raw materials, energy, etc.) and transportation, ecoinvent v3.8 database [75] has been used. This is one of the most sophisticated and complete LCA databases. Nonetheless, there were several materials for which there was no data available in ecoinvent. Some of those materials were cut off since the amount of those used was negligible (crosslinker and emulsifier in MPCMs production; cement stabiliser in foam production) while others were modelled separately based on the literature (Polymer 1 and Polymer 3 in MPCMs production; metakaolin in foam production).

Where possible, background processes have been modelled as market processes representing average European production (RER or Europe without Switzerland geographies in ecoinvent). If there was no data for Europe available, global market processes have been used. The average market energy mixes were used corresponding to where the production takes place: Spanish mix for rGO production, Italian mix for MPCMs production, and German mix for the final fabrication of the material. The impacts of manufacturing the equipment used in NRG-Foam production have not been considered in this study.

Impact assessment

We are using ILCD 2011 Midpoint+ impact assessment method in this study [76]. This is a method developed by the EU's Joint Research Centre and Directorate-General for Environment and is commonly used within EU projects. All impact categories available within ILCD with the exception of “Ionizing radiation E (interim)” have been considered and calculated, 15 in total:

- Acidification
- Climate change

- Freshwater ecotoxicity
- Freshwater eutrophication
- Human toxicity, cancer effects
- Human toxicity, non-cancer effects
- Ionizing radiation HH
- Land use
- Marine eutrophication
- Mineral, fossil & ren resource depletion
- Ozone depletion
- Particulate matter
- Photochemical ozone formation
- Terrestrial eutrophication
- Water resource depletion

The method has been further modified to include the additional impact category of costs to calculate the LCCA impacts. The costs used for calculating LCCA impacts can be found in section A1 of Appendix A.

Base NRG-Foam configurations

The impacts within the static LCA/LCCA have been calculated for the following five foam configurations:

- Base cementitious foam - no MPCMs and rGO (short name “REF”)
- Passive application NRG-Foam, IC shell - 20% of IC shell MPCMs by volume but no rGO (short name “ICP”)
- Active application NRG-Foam, IC shell - 20% of IC shell MPCMs by volume + rGO added to NRG-Paste (circa 0.2% by weight) (short name “ICA”)
- Passive application NRG-Foam, MF shell - 20% of melamine-formaldehyde (MF) shell MPCMs by volume but no rGO (short name “MFP”)
- Active application NRG-Foam, MF shell - 20% of MF shell MPCMs by volume + rGO added to NRG-Paste (circa 0.2% by weight) (short name “MFA”)

For all configurations, the target dry density of 220 kg/m³ has been selected and rGO has been added in the form of a slurry (this differs from the dynamic part where rGO is added as a powder, more information is provided below). Those configurations can be viewed as early-stage targets for the material design.

2.2.4 Dynamic part: identification of trade-offs and effect of constraints

Optimisation problem set-up

Our case study of NRG-Foam's early-stage development is in its essence a classical multiobjective optimisation problem (MOO): there are multiple performance characteristics of the material that we want to improve (objectives) by varying a set of design parameters (variables). Normally in MOO problems, it is impossible to optimise all the objectives simultaneously and there are some trade-offs present. A common way of identifying trade-offs between objectives in a MOO problem is by finding and analysing a Pareto frontier. In this study, we find a Pareto frontier in Matlab using *gamultiobj* function (the options used for the optimisation setup can be found in section A2 of Appendix A). An additional modification has been made to the standard function and during each generation, the full population has been recorded and stored. After the optimisation terminated, the full list of all found solutions (final and intermediate) has been filtered out using *find_pareto_frontier* function [77] to extract non-dominated solutions. This has allowed us to obtain a much larger set of Pareto solutions than just the final population of the genetic algorithm.

Objectives related to thermal properties and electrical conductivity are calculated within Matlab while environmental objectives are calculated externally in OpenLCA software that is linked to Matlab via OpenLCA's IPC server. The sections below provide more detailed information on the objectives, variables and constraints used in this study.

Overview of performance objectives and design variables

Within this study, we have considered four design variables influencing the performance of NRG-Foam:

- Porosity of the foam (bounds: 0.05 – 0.95)
- Volumetric fraction of MPCMs in paste (bounds: 0 – 0.6)
- Fraction of rGO in paste by weight (bounds: 0 – 0.05)
- Type of MPCMs (categorical, 0 – IC shell MPCMs, 1 – MF shell MPCMs)

For porosity and MPCMs fraction, the upper bounds are assumed based on the maximum theoretically achievable values found in the literature: foams with porosity higher than 95% are called “dry foams” and are hardly achievable in practice since they tend to collapse [78]; the addition of MPCMs makes the material less workable and fractions higher than 60% by volume of paste are hard to achieve (in the study [79] a maximum volumetric fraction of 62% has been achieved). For rGO fraction, the upper bound has been selected to be relatively low because it is expected that due to the low electrical percolation threshold, there will be no need for adding more conductive filler in order to make NRG-Foam conductive enough. Further, the experimental observations conducted within the project have shown that at higher

fractions of rGO addition, the filler particles are starting to agglomerate and the material's workability is decreasing.

It is important to mention that only two fixed configurations of MPCMs (IC shell MPCMs and MF shell MPCMs) with sufficiently different performance characteristics have been considered. Both types have a fatty acids core but very different technological and production processes and, as a result, different fractions of PCM in MPCM particles (0.42 for IC shell MPCMs and 0.845 for MF shell MPCMs).

Five objectives have been selected to assess the performance of NRG-Foam:

- Embodied CO₂ emissions, $kg\ CO_{2\ eq}$ (environmental performance) – minimise
- Production costs, EUR (economic performance) – minimise
- Thermal conductivity, $W \cdot m^{-1} \cdot K^{-1}$ (insulation performance) – minimise
- Volumetric enthalpy, $J \cdot m^{-3}$ (heat storage performance) – maximise
- Electrical conductivity, $S \cdot m^{-1}$ (active application performance/activation performance) – maximise

The final optimisation problem has been defined as a minimisation problem. To do this, Volumetric enthalpy and Electrical conductivity objectives have been taken with the negative sign (optimisation problems of maximisation of an objective and minimisation of the objective with the negative sign are equivalent).

Not all impacts of selected variables on selected objectives have been modelled in this study. The impact of rGO fraction on thermal conductivity has not been taken into account since the thermal percolation threshold is much higher than the electrical percolation threshold [80] and within the considered bounds of rGO fraction variable (0% to 5% by rGO by weight), it is not expected that thermal conductivity would display sufficient variation. Further, the contrast between the thermal conductivities of the cementitious matrix and rGO is not as large as between their electrical conductivities further rationalising the decision of omitting the link between rGO addition and the thermal conductivity of the paste.

Modelling of environmental and economic performance

The environmental and economic performance of the material was modelled using the same general approach as described in the static model section above but the model has been parametrised with parameters corresponding to the variables used in the MOO problem set-up. This allows us to obtain LCA/LCCA dynamically while changing the input parameters (variables). In comparison to the static models where rGO has been used in a slurry form, within the dynamic modelling part, it is added in a powder form (with an additional process of drying added to the production system). The choice of

using dry rGO, in this case, is dictated by the experimental data availability (more lab measurement data is available for dry rGO addition).

As mentioned before, LCA and LCCA calculations in this study were performed in OpenLCA software. A connection between Matlab and OpenLCA has been built using OpenLCA's IPC server. The server runs in the background and listens to the incoming commands. It is possible to change model parameters, run calculations and extract the assessment results via requests to the server. The communication with the server has been set-up using *olca-ipc* Python package provided by GreenDelta [81]. A Python script based on *olca-ipc* library has been written to perform LCA and LCCA calculations in OpenLCA and extract the results. This script has been run from within Matlab using the built-in functionality of running code written in programming languages other than Matlab's own.

More details on the modelling of environmental and cost performance as well as the physical parameters of individual materials necessary for the calculations can be found in section A2 of the Appendix A.

Metamaterial and thermal properties modelling

The modelling of thermal conductivity has been done in two steps. First, the change in thermal conductivity of the paste with the addition of MPCMs has been modelled using the Lewis-Nielsen model [82], [83]. Lewis-Nielsen model describes the thermal and electrical conductivity of a two-phase material (matrix + filler) and is defined by the following equations:

$$\frac{k}{k_1} = \frac{1 + AB\phi_2}{1 - B\psi\phi_2} \quad (2.1)$$

$$B = \frac{\frac{k_2}{k_1} - 1}{\frac{k_2}{k_1} + A} \quad (2.2)$$

$$\psi = 1 + \left(\frac{1 - \phi_m}{\phi_m^2} \right) \phi_2 \quad (2.3)$$

where k is the resulting conductivity of the two-phase system, k_1 and k_2 are conductivities of the matrix and dispersed material correspondingly, ϕ_2 is the volumetric fraction of the dispersed material, A is the shape constant for the filler particles, ϕ_m is the maximum packing fraction of filler particles. For the modelling of MPCMs dispersion in the cementitious material matrix, we assumed the shape coefficient $A = 1.5$ (representing spherical particles) and maximum packing fraction $\phi_m = 0.601$ (random loose packing).

In the second step, the addition of air bubbles has been simulated using a numerical model developed by CIMEC [84]. The model utilises a newly developed representative volume element (RVE) generator called NRGene that allows the generation of representative volume elements of a studied material with given properties (porosity and pore size distribution). The generated RVE can then be used further to calculate the effective thermal conductivity of the material using the finite element modelling (FEM)

approach. Describing this method in detail is beyond the scope of this study and the reader is referred to reference [84] providing all the specifics.

The volumetric enthalpy of NRG-Foam has been selected as a measure of the heat storage performance. Volumetric enthalpy is a function of temperature and is calculated using the following equation:

$$H_{eff}(T) = \int_{T_{ref}}^T \rho c_{eff}(t) dt \quad (2.4)$$

where T_{ref} is an arbitrary reference temperature (we set T_{ref} at 0 °C in this study) and $\rho c_{eff}(t)$ is the effective volumetric heat capacity of the foam. The effective volumetric heat capacity of the material is given by the mixture law [85]:

$$\rho c_{eff} = \phi_{cem} \rho c_{cem} + \phi_{air} \rho c_{air} + \phi_{MPCM} \rho c_{MPCM} \quad (2.5)$$

where ϕ_{cem} , ϕ_{air} and ϕ_{MPCM} are the volumetric fractions of cement, air and MPCMs in; ρc_{cem} , ρc_{air} and ρc_{MPCM} are volumetric heat capacities of cement paste, air and MPCM. Since MPCM itself is a composite of shell and PCM core, its effective heat capacity is also defined by mixture law:

$$\rho c_{MPCM} = \phi_{PCM} \rho c_{PCM} + (1 - \phi_{PCM}) \rho c_{shell} \approx \phi_{PCM} \rho c_{PCM} \quad (2.6)$$

where ϕ_{PCM} is the volumetric fraction of PCM material in MPCM, ρc_{PCM} is the (latent+sensible) volumetric heat capacity of the PCM core and ρc_{shell} is the volumetric heat capacity of the shell. Here, we have considered ρc_{shell} (only sensible) negligible with respect to ρc_{PCM} (mainly latent). Regarding ϕ_{PCM} , as previously mentioned in Section 2.2.4., it is equal to 0.42 for IC-shell MPCM and 0.845 for MF-shell MPCM.

For cement paste and air, we only consider sensible heat. The final equation for volumetric enthalpy can be written as:

$$H_{eff}(T) = \phi_{air} \rho c_{air} T + (1 - \phi_{air}) * (1 - \phi_{MPCM}) \rho c_{cem} T + (1 - \phi_{air}) \phi_{MPCM} \phi_{PCM} \int_0^T \rho c_{PCM}(t) dt \quad (2.7)$$

The volumetric heat capacity of PCM material (ρc_{PCM}) includes sensible and latent heat and has been calculated based on the data sheets provided by the producer (we were using the data for PureTemp 25 PCM [86]). In this study, we have calculated volumetric enthalpy at the interval of temperatures between $T_{ref} = 0$ to $T = 30$ °C. Section A2 of the Appendix A provides the data for the heat capacities of components used in the calculations.

Electrical conductivity modelling

Electrical conductivity has been modelled in three steps. First, the change in conductivity of cementitious paste with the addition of rGO has been modelled based on experimental data collected by using impedance

spectroscopy. The measurements have been fitted using the generalised percolation model [87]. More detailed information on the experimental setup as well as the measured and fitted data can be found in section A2 of Appendix A. In the following step, the addition of MPCMs to the paste with rGO has been modelled using the Lewis-Nielsen theory [82], [83]. Finally, at the last step, the electrical conductivity of NRG-Foam has been modelled based on the same RVE/FEM model as used for thermal properties [84] (see previous section). The only difference between the Lewis-Nielsen and RVE/FEM models compared to the thermal conductivity modelling described in the previous section is that instead of the thermal conductivities of the matrix material and the filler, electrical conductivities were used.

Constraints and design space reduction

After running the optimisation model with the variable bounds specified in the sections above and obtaining a Pareto set of non-dominated solutions, constraints have been added based on the data collected by TU Darmstadt. First, a set of mix designs has been developed to test the limits of stability of NRG-Foam depending on the fraction of MPCMs added and the target porosity of the foam. Those theoretically obtained mix designs were then experimentally validated in the lab setting by producing foams with given configurations and analysing their stability. It has been observed that with the fraction of MPCMs increasing, the foam becomes less stable and the maximum achievable porosity is decreasing. At 5% by volume of paste, the maximum achievable porosity was 0.92 while at 40% - just 0.6. Between 5% and 40%, a gradual decrease in maximum achievable porosity has been observed. NRG-Foams with MPCMs fraction higher than 40% were not stable. The corresponding experimental data can be found in section A2 of Appendix A. The experimental data have been fitted using piecewise cubic Hermite interpolating polynomial (PCHIP). This fitted function and 40% limit for MPCMs fraction were further used as constraints and the Pareto solutions that are not satisfying those constraints have been filtered out.

2.3 Results and discussion

2.3.1 Results

Production system model and LCA/LCCA inventory

Figure 2.4 below shows the production system model for NRG-Foam. Note that the figure only shows the main product inputs within each unit process while water/energy inputs and waste/emissions outputs are only shown as exchanges between the foreground system and the external environment without being attributed to a particular unit process. This has been done to make the scheme more compact. More detailed information on inputs and outputs can be found in the inventories.

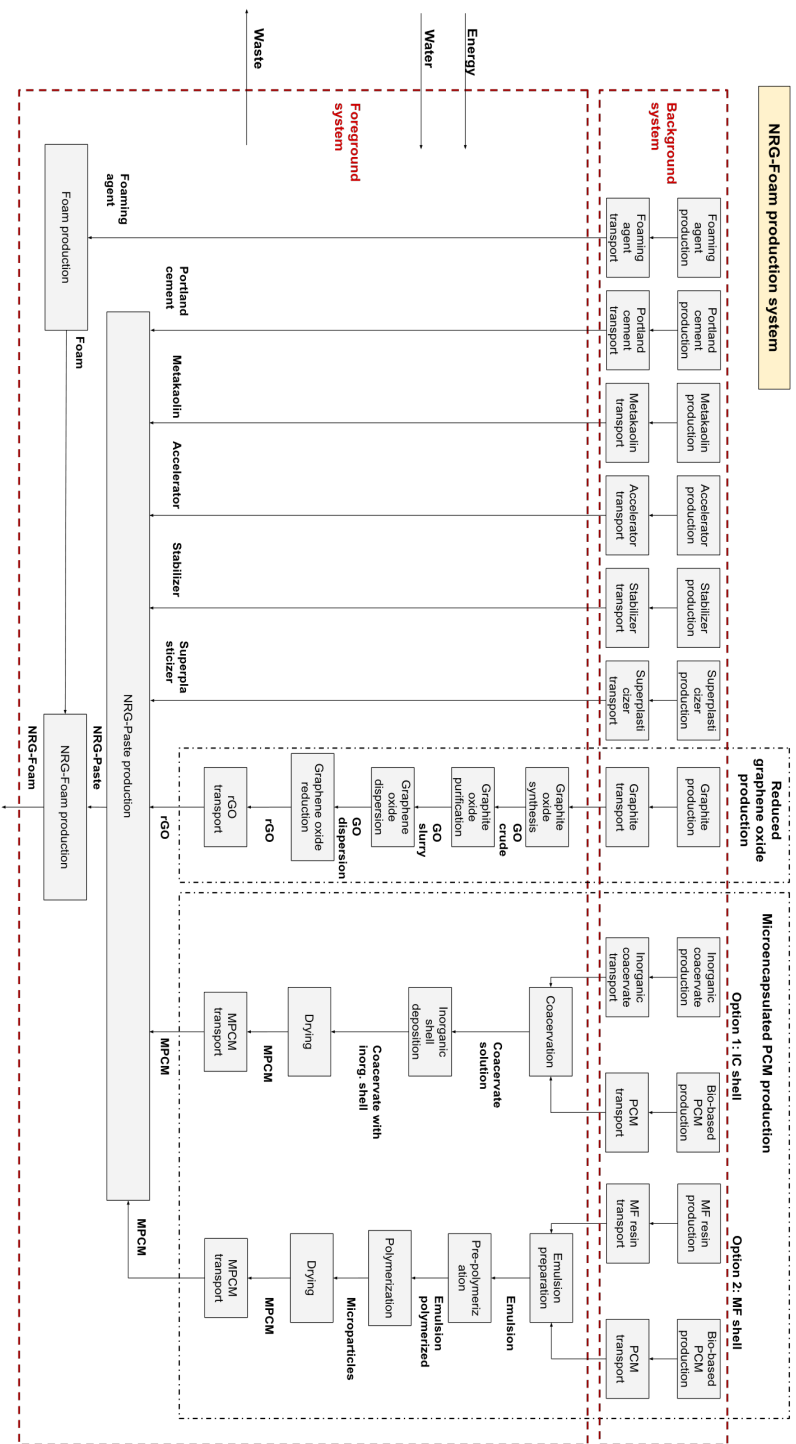


Figure 2.4: NRG-Foam production system.

Based on the developed model of the production system and the data collected from project partners, an LCA inventory has been built. As it was mentioned, five different foam configurations have been considered within the static part of this research. Table 2.1 shows the foam mix designs used for those configurations. Mix designs are the same for IC and MF shell MPCMs.

Table 2.1: NRG-Foam mix designs.

Component	Amount used to produce 1 m ³ of NRG-Foam, kg		
	Reference	20%MPCM	20%MPCM+rGO
Cement (Cem I 52,5R)	136.5	121.5	120.5
Metakaolin	22.5	20.0	19.8
Accelerator	3.2	2.8	2.8
Superplasticiser	0.8	1.5	2.8
Stabiliser	4.6	4.1	4.1
MPCM	0.0	23.4	23.3
Water (w/b)	52.5	46.7	0.0
rGO slurry	0.0	0.0	46.7
Water (foam preparation)	59.1	59.1	59.1
Foaming agent	1.2	1.2	1.2

Based on the production system model and mix designs, the inventories for all five NRG-Foam configurations have been compiled and are presented in section A3 of Appendix A. Those inventories have then been used for conducting the impact assessment. The results of the impact assessment can be found in the following section.

LCA and LCCA impact assessment and identification of hotspots

Table 2.2 presents the results of the impact assessment of NRG-Foam for all five configurations in absolute values and Figure 2.5 – a fractional increase of impacts for ICP, ICA, MFP and MFA foam configurations in comparison to the reference foam that does not contain MPCMs or rGO. As it was mentioned, costs were added as an extra impact category within the ILCD method and provided together with the environmental impacts at the last position (last row in tables, last data point in graphs).

Table 2.2: Impact assessment results for five NRG-Foam configurations.

Impact category	REF	ICP	ICA	MFP	MFA
Acidification, molc H+ eq	0.4	7.8	9.8	3.0	5.1
Climate change, kg CO2 eq	150.1	1778.4	1981.0	683.6	895.1
Freshwater ecotoxicity, CTUe	932.4	43009.7	48123.7	15258.7	20595.6
Freshwater eutrophication, kg P eq	0.03	0.42	0.48	0.17	0.22
Human toxicity, cancer effects, CTUh	4.8E-06	9.4E-05	1.1E-04	3.4E-05	4.8E-05
Human toxicity, non-cancer effects, CTUh	1.9E-05	3.1E-04	3.8E-04	1.0E-04	1.7E-04
Ionizing radiation HH, kBq U235 eq	7.9	198.5	289.0	70.2	161.7
Land use, kg C deficit	89.0	4625.3	4865.3	1963.3	2224.6
Marine eutrophication, kg N eq	0.1	1.6	1.8	0.8	1.0
Mineral, fossil & ren resource depletion, kg Sb eq	0.001	0.032	0.035	0.014	0.018
Ozone depletion, kg CFC-11 eq	5.5E-06	3.6E-04	3.7E-04	2.0E-04	2.1E-04
Particulate matter, kg PM2.5 eq	0.03	0.63	0.75	0.26	0.39
Photochemical ozone formation, kg NMVOC eq	0.3	3.8	4.5	1.6	2.3
Terrestrial eutrophication, molc N eq	1.2	14.3	16.6	6.2	8.5
Water resource depletion, m3 water eq	29.9	2887.0	3256.4	966.0	1350.8
Costs, EUR	69.3	1708.9	1992.6	3259.0	3530.3

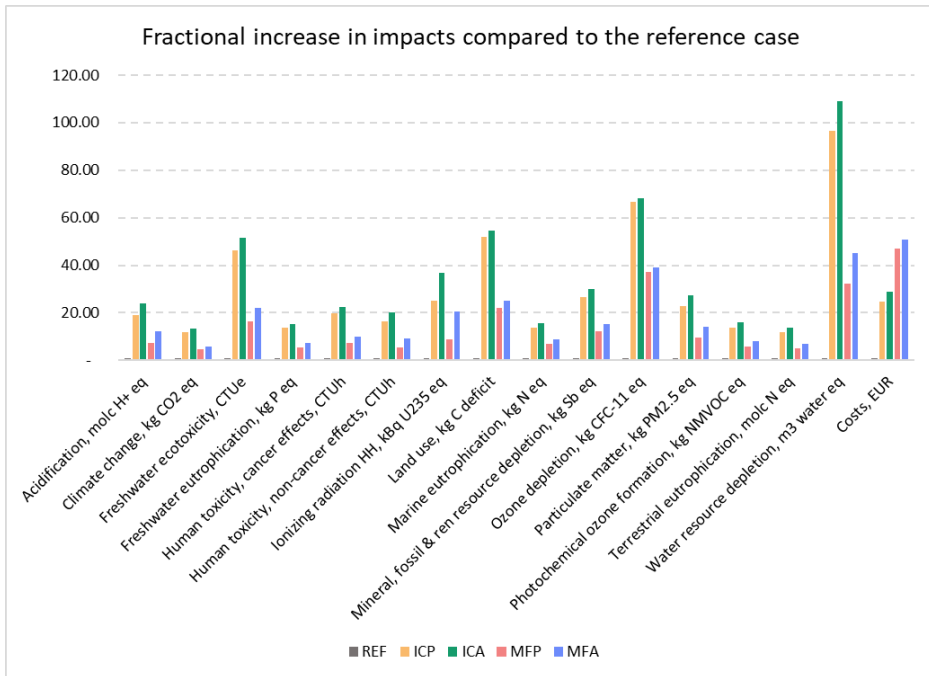


Figure 2.5: The fractional increase in impacts compared to the reference case.

As can be seen from Table 2.2 and Figure 2.5, with the addition of MPCMs, the impacts are increasing drastically. Further addition of rGO – even though the amount added is low – has a noticeable effect as well. The increase in impacts varies between 4.6 times (climate change, MFP vs. REF) and 109 times (water resource depletion, ICA vs. REF). The structure and scale of impacts' increase are different for IC-based and MF-based foams. For IC-based foam, the lowest increase compared to the reference foam is observed in the Terrestrial eutrophication impact category and the highest – in Water resource depletion. On the other hand, for MF-based foam, the lowest increase is within the Climate change impact category and the highest one – in the Ozone depletion impact category.

Another observation is that across all environmental impacts, the MF shell demonstrates better results when it comes to environmental performance (lower impacts) than the IC shell. Depending on the impact category, the impacts of ICP foam are 1.8 to 3.1 times higher than those of MFP foam. For the active application foams the difference is between 1.7 and 2.4 times. On the other hand, production costs are sufficiently higher for the foam containing MF shell MPCMs: MFP and MFA costs are 1.7 and 1.8 higher than ICP and ICA costs correspondingly.

The Ionizing radiation HH impact category is the most sensitive to the addition of rGO to the paste. When rGO is added, the impact for IC-based foam is increasing by 1.5 times and for MF-based foam by 2.3 times. On the other hand, the Ozone depletion impact category is the least influenced by

the rGO addition: it causes a 3% increase for IC-based foam and a 5% increase for MF-based foam. Such a difference in the sensitivity of the impacts to rGO addition is explained by the fact that some impact categories are dominated by electricity use (especially Ionizing radiation HH impact category) and rGO production is also an energy-demanding process. Further information on the contributions of individual processes to the total impacts can be found below.

The overall production process of NRG-Foam can be divided into three parts: production of MPCMs, production of rGO and production of the foam (final mixing of all the ingredients and forming of the foam). Figure 2.6 shows the contribution of impacts by stages for ICA foam.

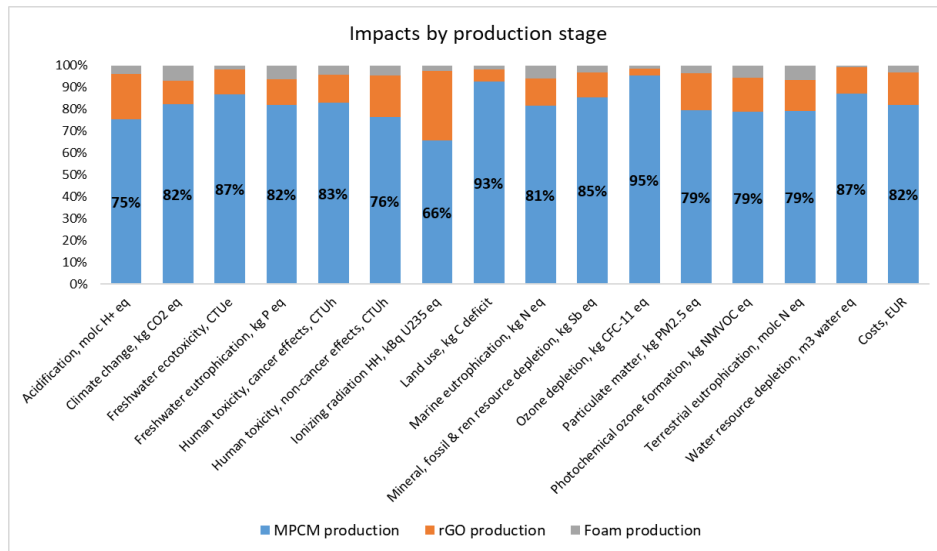


Figure 2.6: Contribution of NRG-Foam production stages for ICA foam configuration.

As can be seen from Figure 2.6, MPCM production stage is the main contributor to the overall impacts and is responsible for 66% to 95% of the total impacts. A similar situation can be observed in the case of MFA foam (see Figure 2.7) but the proportions are less skewed towards MPCM production: it is responsible for 39% to 92% of the total. Further, within the Ionizing radiation impact category, the largest impact is coming from rGO production while in the case of ICA foam, it is still MPCM production.

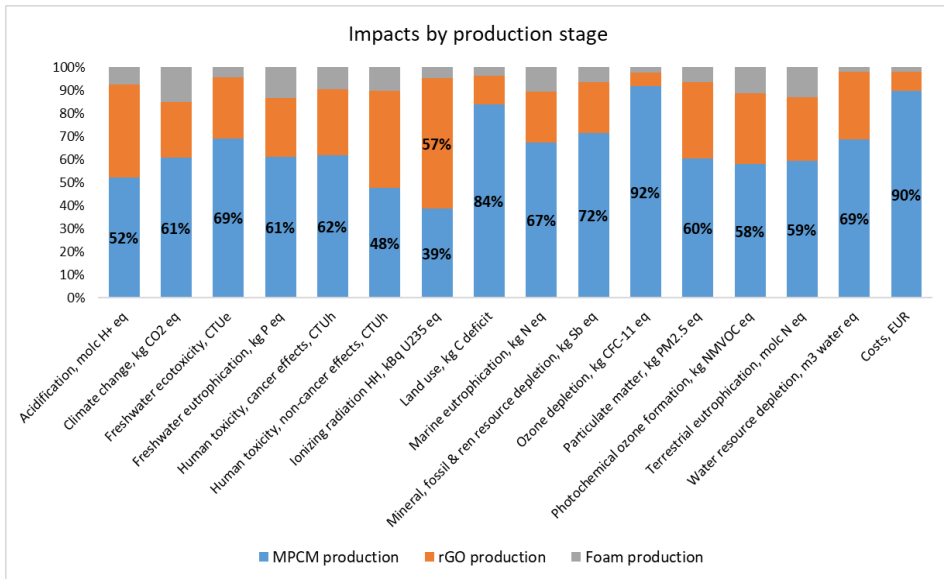


Figure 2.7: Contribution of NRG-Foam production stages for MFA foam configuration.

As the next step, the contribution of individual processes within the production chain has been analysed. This analysis has been performed for ICA and MFA foam configurations. Figure 2.8 shows contributions for the ICA configuration and Figure 2.9 – for the MFA configuration.

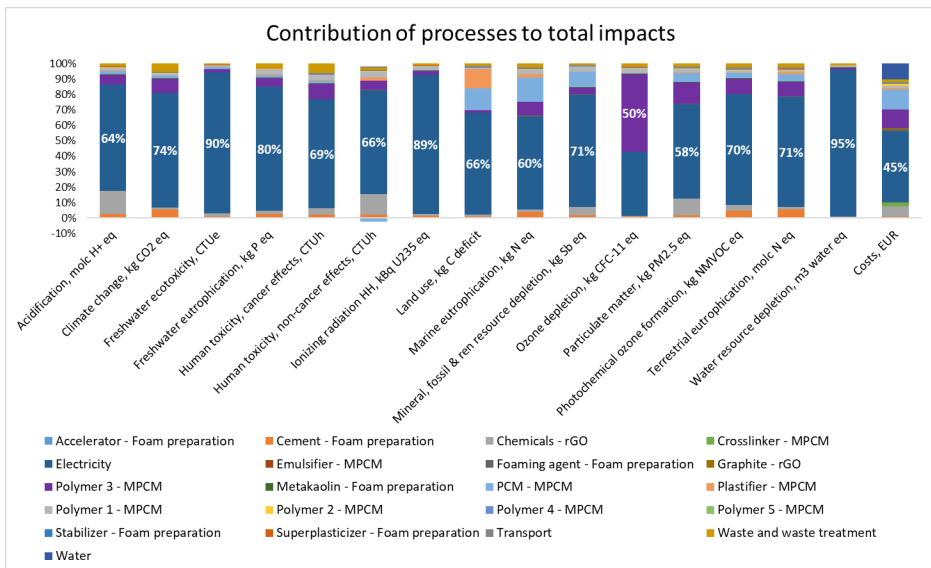


Figure 2.8: Contribution of NRG-Foam production processes for ICA foam configuration.

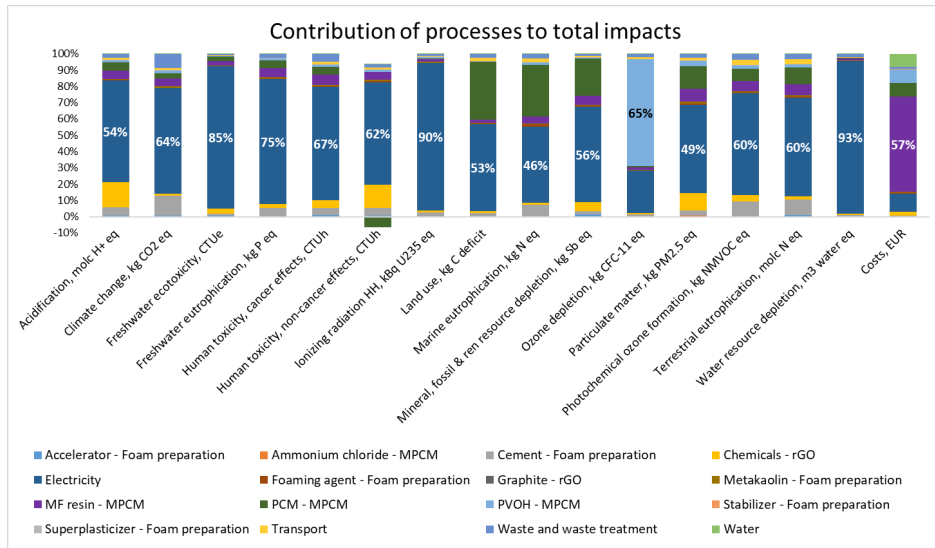


Figure 2.9: Contribution of NRG-Foam production processes for MFA foam configuration.

In Figures 2.8 and 2.9, some of the processes were merged together into larger groups. There are five groups like this:

- Electricity – combines all the electricity consumption within the production system
- Water – water consumption within the production system
- Waste and waste treatment – impacts caused by the waste created within the production chain and its treatment
- Transport – all the transport activities within the production chain
- Chemicals rGO – combines the chemicals used within the rGO production process

Within each column, a process (or process group) with the highest contribution to the total impact is highlighted by specifying its share of the total impact.

Figures 2.8 and 2.9 highlight that the NRG-Foam production process is very energy-intensive and that electricity consumption is the biggest hotspot within the production chain (it is responsible for up to 95% of impacts within an impact category). Further, as Figures 2.6 and 2.7 show, MPCM production is the most impactful stage within the production chain. Thus, the further development and upscaling of the NRG-Foam production process should focus on reducing the negative impacts caused by electricity use and MPCMs manufacturing.

In addition to a global hotspot of electricity consumption, there are also several local hotspots that influence not all but some particular impact categories. Within the Ozone depletion impact category, electricity

consumption is not the highest contributor for both, ICA and MFA foams. For ICA foam, the production of Polymer 3 has the highest impact and for MFA foam – the production of polyvinyl alcohol (PVOH). Further, MF resin has the highest impact on costs. Those hotspots are harder to address compared to electricity consumption. While it might be theoretically possible to replace those polymers with some other alternatives, it is not given that the impacts will be reduced. Further, it is hard to reduce the total amount of high-impact polymers used since they are essential to achieve the required physical properties of MPCMs. From the cost perspective, however, it might be possible to find suppliers with lower MF resin costs, especially as the production volumes increase.

Optimisation results and trade-offs between objectives

To obtain the Pareto set of solutions, genetic algorithm has been run until a termination criterion has been reached. In our case, 134 generations were evaluated before the algorithm terminated with the exit flag of 1 (termination due to the relative change of spread over the number of stall generations becoming lower than the predefined tolerance of $1e-4$). Since in our case we are dealing with a multidimensional Pareto frontier with the number of dimensions higher than three, it is not possible to show it fully. However, it is possible to depict individual two-dimensional projections of the five-dimensional Pareto surface. Those projections could provide sufficient information necessary for the identification of trade-offs between the objectives. Figure 2.10 shows all possible projections of the five-dimension Pareto frontier obtained.

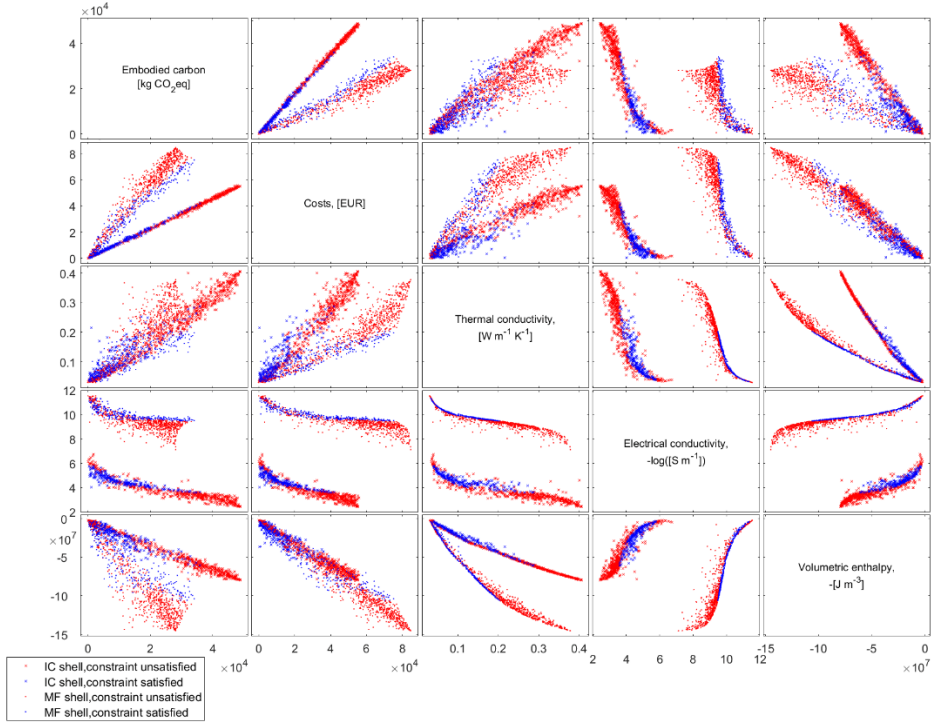


Figure 2.10: Two-dimensional projections of five-dimension Pareto frontier. The data points in blue represent the points on the Pareto frontier that satisfy the functional constraint described in Section 2.2.4 and points in red that do not satisfy this constraint. Solutions with MF shell MPCMs are represented by dots while those with IC shell MPCMs – by crosses. The electrical conductivity axis shows the logarithm of electrical conductivity with the negative sign. Volumetric enthalpy is taken with the negative sign.

The optimisation problem has been set up as a minimisation problem. Two maximisation objectives – Electrical conductivity and Volumetric enthalpy – were converted into minimisation objectives by adding the negative sign to them. Thus, the utopia point in all plots within Figure 2.10 is located at the intersection of axes in the bottom lower left corner. Having this in mind, it can be observed that Embodied carbon, Costs and Thermal conductivity objectives show no trade-offs between each other which means that it is possible to simultaneously reduce those. At the same time, the figure highlights trade-offs between six pairs of objectives:

- Embodied carbon and electrical conductivity
- Embodied carbon and volumetric enthalpy
- Costs and electrical conductivity
- Costs and volumetric enthalpy
- Thermal conductivity and electrical conductivity

- Thermal conductivity and volumetric enthalpy

Figure 2.10 also clearly shows the differences in functional characteristics of IC-shell and MF-shell MPCMs: in most of the graphs, Pareto solutions representing different types of MPCMs are separated and forming two distinct clusters. This is especially noticeable in the graphs with electrical conductivity as one of the objectives. In those, electrical conductivity differs by orders of magnitude (due to the much higher electrical conductivity of IC shell material compared to MF shell material). Consequently, in the case of active application NRG-Foam, IC-shell MPCMs might be a much better option. As an additional benefit, the foam configurations with IC-shell MPCMs are also generally characterised by lower costs. On the other hand, the solutions with MF-shell MPCMs can provide much higher levels of heat storage capacity due to a higher core-to-shell ratio.

Those results indicate that some compromises will be necessary when planning further development of NRG-Foam. What is especially important for NRG-Foam as an insulation material, is there will be a need to find a balance between the insulation performance and heat storage performance since the simultaneous improvement of those characteristics is not possible. Further, the improvement of volumetric enthalpy and electrical conductivity is not possible without compromises since those two objectives show trade-offs with all the other objectives (Embodied carbon emissions, Costs and Thermal conductivity). Finally, differences in the physical properties of IC-shell and MF-shell MPCMs largely define the characteristics of the final material and add to the complexity of the material optimisation. Compared to MF-shell MPCMs, IC-shell MPCMs allow to achieve much better electrical performance (making it a much better option for active application NRG-Foam) at a lower cost level but environmental and heat storage properties of the material are taking a hit. On the other hand, the solutions with MF-shell MPCMs can provide much higher levels of heat storage capacity due to a higher core-to-shell ratio. Yet, the costs will be high and the possibility of active application of NRG-Foam with MF-shell MPCMs is questionable due to the poor effective electrical conductivity.

The introduction of the functional constraints on the porosity and MPCMs fraction further limits the material development possibilities and renders more than 70% of depicted Pareto solutions infeasible. From all the objectives, electrical conductivity and volumetric enthalpy are especially sensitive to the introduction of the constraint since the solutions closest to the utopia point become infeasible.

2.3.2 Limitations

In the study, two types of MPCMs have been considered and modelled: IC MPCMs and MF MPCMs. However, the data and the modelling approach used for those two types of MPCMs were different. The production of IC MPCMs has been based on the experimental primary data while the production of MF

MPCMs has been modelled based on the literature, information from a producer and the experience of the project partners. As a result, there might be some discrepancy when it comes to the comparison of those two MPCM types.

The costs of materials used for LCCA calculations are not their intrinsic property and depend on the market situation, timeframe, supplier, purchase volumes, etc. In this study, we were mostly using the costs that were provided by the project partners and that are based on the actual costs they have paid for the materials. However, those costs are supplier-dependent and the prices of other suppliers could vary. Thus, the results of LCCA provided in this study are very case-specific and could change going forward. Nevertheless, for the purpose of this study, such an approach is justified since we are looking at early-stage material development. At the next stages, the costs will be reconsidered taking into account the increasing production scale (following the ex-ante LCA/LCCA approach to model the up-scaled production impacts).

While a wide range of design variables and material performance objectives have been considered in the dynamic part of this study, the set has not been complete. For example, such variables as, e.g., water-to-binder ratio and metakaolin fraction, can impact the performance of the material on several levels but have not been taken into account. From the objectives side, the mechanical performance, sound insulation, flammability, vapour permeability and some other characteristics have not been considered. Mechanical performance has, however, been introduced into the optimisation problem as constraints on porosity and MPCM fraction. In both of the cases – variables and objectives – the omission was due to the unavailability of required experimental or modelling data. While it is important to have a comprehensive overview, it is rarely possible to obtain all the necessary data at the early stages of material development since both, experimental measurements and the creation of models, are time-consuming tasks further limited by the available project budget. Nonetheless, we believe that the five-objective four-variable case we have presented in this study is comprehensive enough to guide the further development of the material.

2.3.3 Discussion and future work

In the presented study, we have modelled the detailed production process of NRG-Foam and holistically explored its properties. Two paths of production have been considered: foam with bio-based shell MPCMs and foam with MF-based shell MPCMs. Modelling and analysis of the production systems and inventories showed significant differences in the production process of those two different types of PCMs. Those differences have a clear impact on the final performance of the material. Somewhat counterintuitively, the environmental impacts of MPCMs with a bio-based shell were found to be higher than those with MF-shell. The reason behind that is that the environmental impact of chemicals used in MPCMs production is by a large margin outweighed by the impacts of energy use. From the two types of MPCMs, the process of IC-based MPCM production was found to be much

more energy-demanding. There are, however, two important aspects that should be noted. First of all, the production process of IC-shell MPCM is innovative and only exists on a very small scale. Further development of the production process could sufficiently reduce the overall impacts. On the other hand, the production of MF-shell MPCMs is a more refined process that has been optimised for a longer period of time. Secondly, the results of LCA are only considering the “business as usual” scenario. Or, in other words, LCA does not include potential risks of something going wrong during the life cycle of the material. MF-shell contains formaldehyde (albeit cross-linked with melamine) which is a well-known toxic chemical. If the production, use and disposal of the material containing MF-shell MPCMs happen in a correct, controlled and safe manner, there will be no side effects to human health beyond those reflected in LCA. However, in case of an unexpected event or event that has not been accounted for, some formaldehyde could be potentially released into the environment. For example, while MF-shell is made of cross-linked melamine and formaldehyde and those links are generally strong and stable, they can degrade and break under some specific conditions causing the release of formaldehyde [88], [89]. Such risks are not included in LCA but material designers should have them in mind when working on creating a new material. When it comes to the research of NRG-Foam, our future plans include the extension of LCA results with risks-based metrics.

Our analysis of five configurations of NRG-Foam highlighted that the base material (foam without MPCMs and rGO) has a relatively low environmental impact and costs. In the base configuration, the environmental impacts are – unsurprisingly – mainly driven by the impacts of cement production. The addition of MPCMs with their energy-consuming manufacturing processes, however, causes a many-fold increase across all the impact categories completely overshadowing the impacts of base foam production. As a consequence, the question arises: Do the benefits of adding MPCMs outweigh the negative environmental impacts of their production? When it comes to construction materials containing PCMs, the question seems to be especially relevant since the literature points to different conclusions regarding the advantages of such materials. While some researchers reported great energy-saving benefits of adding PCM to the building envelope (see, e.g., [90]), others concluded that the benefits are negligible (e.g., [91]). Answering this question is extremely important for the evolution of NRG-Foam since it will define the further development of the material and provide a better understanding of the target design parameters (fraction and type of MPCMs, porosity, rGO content, etc.). Yet, such a question can only be answered based on the building-level analysis. Such analysis will be the main focus of our future work.

It is necessary to note that the building-level LCA will not be representative of reality if we base it directly on the results of this study. This is due to the scale of the analysis presented in this work and the current TRL of NRG-Foam. Within building-level LCA, the materials are generally considered to be market-ready or mass-produced and have well-defined

properties. Since it is impossible to bring NRG-Foam to such a level within the scope and time frame of our research project, an intermediate step of up-scaling is necessary. Up-scaling aims to bring the lab-scale material characteristics (in our case, LCA and LCCA impacts) to the mass-production level using up-scaling scenarios. The scenarios should reflect possible foreseeable changes in the production process due to up-scaling. Those can be, for example, improved process efficiency, reduced costs, larger batch sizes and so forth. The scenarios are developed by all the parties involved in the material design and production and generally are guided by the results of hot-spot analysis. In the case of NRG-Foam, the development of scenarios is underway and, to a large extent, is driven by the results presented in this work.

The research of new materials often tends to be fragmented: a single material is studied by multiple people and research groups that are focused on different individual properties of the material in isolation from each other. Such fragmentation could potentially result in suboptimal decisions when it comes to the material design: there are links between all the properties of the material that can be lost if those properties are analysed in isolation. While not providing complete coverage (complete coverage, arguably, is impossible), the authors of this study have developed a holistic model of NRG-Foam tying together environmental, economic, thermal and electrical models. The results of this analysis clearly show the multiple trade-offs existing between the performance characteristics of the material. This stresses our earlier point on the importance of de-fragmentation in the material design. If the studies of the environmental, thermal and electrical performance of NRG-Foam were performed in isolation, the information on trade-offs would be lost. The results of such a holistic study provide material designers with a tool allowing them to answer “What if?” questions and see how their decisions impact different characteristics of the material. For example, we might be interested in designing NRG-Foam with the maximum possible heat capacity. What effect will it have on other properties? – Using the trade-off analysis we can see that our costs, environmental impacts as well thermal conductivity will increase drastically. Further, we can achieve much higher heat storage capacity if using MF-shell MPCMs but in that case, it will be not possible to reach high electrical conductivity levels which hinders the potential of active application of NRG-Foam. It is, however, important to note that the trade-offs presented in this study might be not completely aligned with the trade-offs arising on the building level. We aim to identify those building-level trade-offs in the following studies.

To summarise, the immediate focus of our future work will be on the following key tasks:

- Developing up-scaling scenarios for NRG-Foam and NRG-Panels (finished insulation panels made of NRG-Foam) production and conducting up-scaled LCA and LCCA.
- Developing a building-level LCA/LCCA that includes NRG-Panels as one of the components. That would allow us to analyse the impacts

of the material in the wider context and to compare the performance of NRG-Panels with other insulation materials. The building-level assessment would rely on the results of this study as well as the up-scaled assessments.

- Performing material design optimisation on the building level. The general approach would be similar to the dynamic part of this study but the optimisation will be performed on building-level objectives instead of material-level ones. This would allow us to optimise the material design in the context of a building, identify building-level trade-offs and provide further guidance for the material development process.

2.4 Conclusions

In this work, we have presented an early-stage assessment of NRG-Foam – a novel insulation material based on cementitious foam with embedded MPCMs. The cradle-to-gate production system model has been developed in cooperation with the project partners and is mostly based on the primary experimental data. Within the production system, two possible types of MPCMs have been considered: with bio-based shell (IC MPCMs) and with synthetic shell (MF MPCMs). Based on the production system developed, the inventories have been compiled for five different foam configurations varying by the type of MPCMs and the addition of rGO-based conductive filler. Based on the production system and inventories, LCA and LCCA of NRG-Foam have been performed. Production of MPCMs has been shown to be the largest contributor to the total impacts accounting for up to 95% depending on the foam configuration and impact category. The results of the impact assessment have also indicated that MF-shell MPCMs have lower environmental impacts while IC-shell MPCMs are characterised by lower costs. The addition of rGO has a pronounced effect on the impacts (accounting for 3% to 57% within an impact category) even though the amount added is very little (about 0.2% by foam weight). The large impacts of MPCMs and rGO production were found to be mostly caused by the high energy intensity of those production processes. Between 11% and 95% of impacts within a single category are caused by electricity consumption and it has thus been identified as the main hotspot within the overall NRG-Foam production process. In addition to electricity consumption, several smaller hotspots were found caused by some components used in the production process: one of the polymers used in IC shell MPCMs production as well as PVOH and MF resin used in MF shell MPCMs production.

Further, the trade-offs between multiple performance characteristics of NRG-Foam have been identified by building and running a multi-objective optimisation model and obtaining a Pareto frontier of non-dominated solutions. From the ten pairs of objectives analysed, clear trade-offs have been found in six of those cases. Electrical conductivity and heat storage capacity were shown to be in a state of trade-off with all the other objectives.

Furthermore, it has been highlighted that the performance of NRG-Foam is largely dependent on the choice of MPCMs: switching from one type to another can lead to a dramatic improvement in performance within one performance characteristic with a similarly sharp simultaneous decline within another. The multiple trade-offs imply that further development of the material will not be possible without finding compromises and prioritising some performance characteristics of NRG-Foam over others.

The results of this study will direct the development of NRG-Foam at the later stages of the project and act as the foundation for developing higher-level and up-scaled assessments.

THE CURRENT STATE OF PCM MODELLING IN BUILDING ENERGY SIMULATION SOFTWARE

The previous chapter focused on in-depth material-level analysis and optimisation of NRG-Foam. This chapter takes an essential next step and brings the analysis of NRG-Foam from the material level to the building level. When it comes to building-level assessments of phase change materials, precise modelling of their dynamic and nonlinear nature is crucial to ensure the accuracy of the assessments' results and, consequently, of the decisions that might be based on those results. This chapter provides an in-depth analysis of the current state of the art in PCM modelling in full-building energy simulation software. It identifies the existing limitations and issues, as well as demonstrates the effects those could have from the perspective of material designers and decision-makers. The results obtained in this chapter highlight that comprehensive and more physically realistic PCM models are not currently reliable enough to be used in real-world applications. Furthermore, it was observed that different models often provide contradicting results, bringing more uncertainty than clarity to decision-makers. Based on the results of this chapter, it was concluded that using a simplified PCM modelling approach would be a better option for the next steps in the analysis of NRG-Foam.

This chapter has been published in Energy and Buildings [92].

3.1 Introduction

Phase change materials (PCM) as construction materials are attracting growing attention in the literature as a way to reduce heating, ventilation, and air conditioning (HVAC) energy demand in buildings, with the number of related publications increasing steadily over the last decade [15], [16], [93], [94]. Due to time and budget constraints, full-scale real-world testing of PCM and PCM-embedded materials is limited, and most research relies on computational simulations. In these cases, the effect of PCM is evaluated based on full-building energy simulation results, which are then used to assess material performance and support design decisions at the material, component, and building levels.

Several tools have been developed for full-building energy simulation with EnergyPlus [95] developed and maintained by National Renewable Energy Laboratory (NREL) being by far the most widely used one. It is open source and free, making it accessible to researchers and practitioners worldwide. Beyond academic research, it is also widely adopted in industry, with tools such as DesignBuilder [96], OpenStudio [97], Revit [98], Ladybug Tools [99], TRACE 3D [100], and others relying on the EnergyPlus engine for energy simulations. It can also be used in regulatory contexts, as several countries are setting energy performance requirements for buildings, and simulation tools like EnergyPlus could be used for compliance verification [101], [102]. In addition, EnergyPlus and other simulation tools play a key role in building assessments such as Life Cycle Assessment (LCA) and Life Cycle Cost Assessment (LCCA), where they are commonly used to estimate impacts during the use stage — often the most significant phase in the building lifecycle [103], [104], [105], [106]. EnergyPlus is therefore essential in all areas where building energy simulations are required.

Compared to conventional construction materials, PCM require a different modelling approach due to their dynamic and nonlinear nature, which should also be reflected in full-building energy simulations [20], [22]. In the literature, PCM and PCM-embedded materials are often modelled in a simplified way, where melting and solidification follow the same enthalpy curve [20], [107], [108]. In reality, however, PCM exhibit more complex behaviour, including hysteresis [109], [110], [111] and supercooling [112], [113], [114] effects. To account for these, more detailed models are needed, especially in the cases of incomplete melting and solidification cycles [112], [115], [116], where simplified models fail to capture real-world PCM behaviour [117]. This is especially important in the case of materials with a high degree of hysteresis. For example, microencapsulation of PCM [118], [119] might significantly increase the observed hysteresis compared to pure PCM [120]. Consequently, construction materials with embedded microencapsulated phase change material (MPCM) particles will also exhibit high degrees of hysteresis. Furthermore, some PCM materials, such as inorganic PCM, are also characterised by intrinsically high hysteresis [111]. The effects of hysteresis should therefore be properly included in building energy

modelling tools to improve the accuracy of simulations for buildings containing such materials.

In the context of PCM and their integration in the building envelope, EnergyPlus includes built-in models that allow to simulate energy performance of buildings taking into account the nonlinear nature of PCM. In its early development, EnergyPlus featured only a simplified PCM model, but in 2017 a hysteresis model was introduced and later in 2018 fully integrated into full-building energy simulations. Since then, it has been actively used in both academia and industry for assessment and decision-making related to PCM integration in buildings. As the model has been reportedly validated [110], the practitioners were provided with confidence in the results of their simulations. Consequently, the results of building energy simulations involving PCM are often taken at face value without a thorough check of the consistency of the outputs. However, although the current hysteresis model in EnergyPlus has been validated, the results of the validation showed inconsistencies in case of partial melting and solidification cycles [110]. Those inconsistencies could potentially be explained by the fact that the hysteresis model in EnergyPlus is based on a simplified curve-switch theory and by the impossibility of taking supercooling effects into account [111], [121]. However, some researchers have pointed out that the hysteresis model in EnergyPlus may not be implemented correctly [122], [123], [124]. To address these concerns, alternative hysteresis models have been proposed. While many of these are developed at the micro-level or for different software [121], [125], some have also been implemented in EnergyPlus as replacements for the built-in model [124].

From the practitioner's perspective, the situation with PCM modelling and the validity of the models built into EnergyPlus is confusing and raises many questions. There is limited understanding of how the different models function, how they compare, and what consequences may arise from choosing one model over another. This work aims to close that gap by providing a detailed investigation of four EnergyPlus-based hysteresis models, two of which were implemented as part of this research.

The objective of this paper is three-fold: I) to present two new publicly available EnergyPlus PCM hysteresis models, II) to provide an in-depth analysis of four different PCM models, including the two newly introduced ones, and identify the inherent limitations of each, and III) to illustrate how the selection of a hysteresis model can impact the decision-making process, using the example of novel PCM-embedded material development.

This study is the first to provide such an in-depth analysis of different hysteresis models in EnergyPlus and aims to assist practitioners in making informed decisions regarding model selection. It also offers a set of guidelines on how to set up the models to obtain the most consistent results possible, along with an outlook for their future development.

3.2 Methodology

3.2.1 Overview of the approach

To demonstrate the effects of PCM model selection on decision-making as well to illustrate the limitations of the existing hysteresis models in EnergyPlus, we use an example case of novel thermal material development called NRG-Foam. The material has been developed as part of EU-funded "Integrated porous cementitious Nanocomposites in non-Residential building envelopes for Green active/passive energy STORAGE" (NRG-STORAGE) project [61]. NRG-Foam is a material based on cementitious foam with embedded MPCM particles that combines both, insulating and energy storing properties. For the purposes of real-world testing and monitoring the performance of NRG-Foam, four demonstrator buildings have been constructed in Sofia, Bulgaria. All the tests and energy simulations performed as part of this work use the same demonstrator building configuration that represents the physical buildings in Sofia with the only difference between the cases being the configuration of NRG-Foam used. The following sections introduce the demonstrator building and NRG-Foam in more detail and provide information on how the parameters of NRG-Foam are linked to the building-level energy simulations.

3.2.2 Description of the demonstrator building

The building model used for all tests and illustrations in this work is a modified version of BESTEST 900 [126]. Figure 3.1 shows the demonstrator building geometry and the main elements of the envelope, while Table 3.1 provides a detailed list of properties for each component and material.

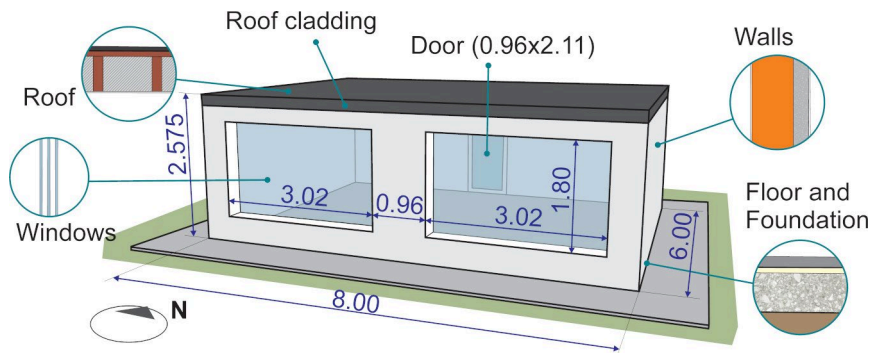


Figure 3.1: Demonstrator building configuration.

Table 3.1: Overview of the constructions and material layers of the demonstrator building with their respective properties. Those values are further used in the input files of EnergyPlus. The final properties of NRG-Panels depend on the exact material configuration and thus are not provided in the table.

Construction	Material layer	Thickness, m	Thermal conductivity, W/mK	Density, kg/m³	Specific heat, J/kgK	Roughness	Thermal absorptance	Solar absorptance	Visible absorptance
Wall	Plaster	0.01	0.47	1150	100	Rough	0.9	0.4	0.4
	NRG-Panels	Vary	Vary	Vary	Vary	Rough	0.9	0.6	0.6
	Hollow brick	0.25	0.31	500	900	Rough	0.9	0.6	0.6
	Gypsum - lime plaster	0.01	0.87	1750	1050	Rough	0.9	0.26	0.26
Roof	Bituminous sheet	0.002	0.17	600	1050	Rough	0.9	0.4	0.4
	Wooden board	0.015	0.17	550	2090	Rough	0.9	0.6	0.6
	Mineral wool	0.18	0.032	21	840	Rough	0.9	0.6	0.6
	Air buffer	Air gap with thermal resistance of 0.16 m²K/W							
	Plasterboard	0.016	0.21	900	840	Rough	0.9	0.26	0.26
Floor	Gravel	0.6	0.6	1550	900	Rough	0.9	0.6	0.6
	Bituminous sheet	0.005	0.17	1100	1050	Rough	0.98	0.98	0.98
	XPS insulation	0.1	0.033	32	1500	Rough	0.9	0.6	0.6
	Waterproof tarp	0.002	0.17	600	1050	Rough	0.9	0.6	0.6
	Reinforced concrete slab	0.2	1.63	2400	960	Rough	0.88	0.6	0.6
Windows	Triple glaze window	Simple Glazing System with U=0.7 m²K/W, solar heat gain of 0.34 and visible transmittance of 0.62							
Doors	Same as windows								

The walls of the building include NRG-Panels made of NRG-Foam, providing both insulation and energy storage. More detailed information on this material is given in the next section. The test building has an HVAC system with a dual setpoint: 20 degrees for heating and 25 degrees for cooling. The temperature is assumed to be constantly maintained within this range throughout the year. In EnergyPlus, the HVAC system is modelled as an Ideal Loads Air System.

In this study, multiple configurations of the demonstrator building presented above are used in EnergyPlus simulations for hysteresis model testing. The only difference between the models is in the parameters of the NRG-Panels layer, while the rest of the building configuration remains the same. The EnergyPlus input .idf files for each simulated configuration used in this work are available in the repository.

While the physical demonstrator buildings were constructed and monitored in Sofia, in this study we model their energy performance under

different climatic conditions. More specifically, Barcelona has been chosen as the test location. Compared to Sofia, it has a significantly warmer climate, making it more favourable for PCM utilisation. EnergyPlus simulations in this study rely on TMY weather data for Barcelona obtained from the EnergyPlus Weather Data portal [127] and can also be found in the repository.

3.2.3 NRG-Foam and NRG-Panels introduction

As it has already been introduced, NRG-Foam is a thermal material based on MPCM-embedded cementitious foam. Figure 3.2 shows the composition of NRG-Foam as well as the key properties of its constituents that were used for calculations and simulations in this study. In order to apply NRG-Foam to the demonstrator buildings, it was cast into $0.4 \times 0.6 \times 0.1$ m panels and cured. These panels are referred to as NRG-Panels throughout the text.

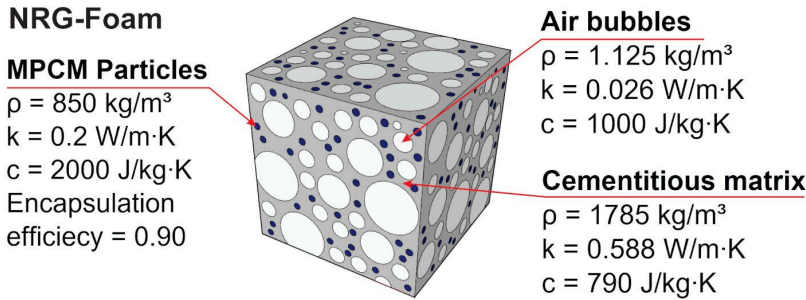


Figure 3.2: Main components of NRG-Foam and their characteristics.

Although physical demonstrator buildings were constructed in Sofia to test NRG-Panels in a real-world setting, these tests were limited in time and focused on a single panel configuration. The panels had a porosity of around 0.86, included 10% MPCM by volume in the paste, and used NEXTEK 24D MPCM produced by Microtek with a melting temperature of 24°C .

In this work, we assume that the configuration of NRG-Panels is not fixed but can be adjusted to minimise the heating and cooling demand of the demonstrator building. The following parameters are considered variable:

- Porosity
- Volumetric fraction of MPCM in the cement paste
- Panel thickness
- PCM melting temperature
- The degree of PCM hysteresis

Based on those parameters, it is possible to obtain the final properties of NRG-Panels that can be used in the input files for EnergyPlus simulations. The final thermal conductivity of NRG-Panels is obtained using Lewis-Nielsen theory that defines the effective thermal conductivity of the two-phase system using the following equations:

$$k = k_1 * (1 + AB\phi_2)/(1 - B\psi\phi_2) \quad (3.1)$$

$$B = (k_2/k_1 - 1)/(k_2/k_1 + A) \quad (3.2)$$

$$\psi = 1 + ((1 - \phi_m)/(\phi_m^2)) \phi_2 \quad (3.3)$$

where k is the resulting conductivity of the two-phase system; k_1 and k_2 are conductivities of the matrix and dispersed material correspondingly; ϕ_2 is the volumetric fraction of the dispersed material; A is the shape constant for the filler particles; ϕ_m is the maximum packing fraction of filler particles. In order to calculate the effective thermal conductivity of NRG-Panels, Lewis-Nielsen theory was applied twice. First, the effective thermal conductivity of cementitious paste is obtained using the properties of cement and MPCM particles as well as their fractions. Then, the final thermal conductivity of NRG-Panels is obtained using the above calculated conductivity of the cementitious matrix, thermal conductivity of air bubbles and their corresponding fractions.

Density and effective specific heat of NRG-Panels are obtained using the mixture law based on the fractions of individual components and their fractions:

$$\rho_{eff} = \phi_a * \rho_a + \phi_c * \rho_c + \phi_p * \rho_p \quad (3.4)$$

$$c_{p,eff} = \frac{1}{\rho_{eff}} (\phi_a * \rho_a * c_{v,a} + \dots + \phi_c * \rho_c * c_{v,c} + \phi_p * \rho_p * c_{v,p}) \quad (3.5)$$

where ρ_{eff} and $c_{p,eff}$ are effective density and specific heat of NRG-Panels; ϕ_a , ϕ_c and ϕ_p are volumetric fractions of air, cement paste and MPCM; ρ_a , ρ_c and ρ_p – densities of air, cement paste and MPCM; $c_{v,a}$, $c_{v,c}$ and $c_{v,p}$ – volumetric heat capacities of air, cement paste and MPCM.

The overall latent heat of fusion is calculated based on the mass fraction of MPCM in panels and the encapsulation efficiency:

$$L_{eff} = \rho_p / \rho_{eff} * \phi_p * e_{MPCM} * L_{PCM} \quad (3.6)$$

where L_{eff} is the latent heat of fusion of NRG-Panels; ρ_p and ρ_{eff} are densities of MPCM and NRG-Panels; ϕ_p is the volumetric fraction of MPCM, e_{MPCM} is the encapsulation efficiency of MPCM (volume of the PCM core related to the total volume of MPCM particle); L_{PCM} is the latent heat of PCM material. Those calculations and generation of the EnergyPlus input files were performed in MATLAB using a routine written for those purposes.

3.3 Numerial Results

3.3.1 Description and examination of different EnergyPlus hysteresis models

Four different hysteresis models were analysed in this study:

- The current built-in hysteresis model in EnergyPlus.
- The modified version of the built-in EnergyPlus hysteresis model with corrected curve-switch behaviour developed as part of this work. The source code for this version is provided in the repository.
- Two-phase PCM model based on EnergyPlus v9.3 developed by Feng et al. [124].
- Two-phase PCM model by Feng et al. [124]. implemented in EnergyPlus v24.1 as part of this work. The source code for this version is provided in the repository.

The following sections provide an in-depth analysis of each model, including their working principles and identified limitations.

3.3.2 Current PCM model integrated in EnergyPlus

There are currently two ways of modelling PCM in EnergyPlus: using a single enthalpy curve without accounting for hysteresis, and a hysteresis model that uses separate curves for melting and solidification. Both approaches rely on the Conduction Finite Difference Solution Algorithm (CondFD). The hysteresis model was developed in cooperation between NREL and NRGSim and was first introduced in EnergyPlus version 8.8 (2017). Starting from version 8.9 (2018), it was fully integrated, allowing simulation of multi-layer components containing PCM layers.

The hysteresis model in EnergyPlus is reportedly based on a continuous enthalpy curve with a mushy region, as described in Egolf and Manz [128], and a constant heat capacity transition between melting and solidification curves in cases of incomplete phase change, as defined in Bony and Citherlet [129].

Identified limitations

While multiple sources (e.g. [121], [124] describe the built-in hysteresis model as based on the curve-switch method and specifically the work by Bony and Citherlet [129], it has been found that, in reality, it functions differently. Analysis of the model's source code shows that although the intention was indeed to follow the curve-switch method, the practical implementation has not been executed correctly. This can be demonstrated with a simple test: let us take an arbitrary configuration of the demonstrator building (file "model_test_1.idf" in the repository), run the energy simulation using built-in hysteresis model, and analyse the parameters of the internal nodes of the PCM layer at each time step. In particular, let us focus on the "CondFD Phase Change State" and "CondFD Phase Change Node Specific Heat" variables for

Node 4 in the south-facing wall, which output the PCM state and the modelled specific heat at that node. PCM states are encoded in EnergyPlus as follows:

- -2 - Liquid
- -1 - Melting
- 0 - Transition
- 1 - Freezing
- 2 - Crystallised

where the transition state is supposed to denote the switch between the curves during an incomplete melting or solidification cycle. Figure 3.3 shows the distribution of the PCM states throughout the whole simulation year.

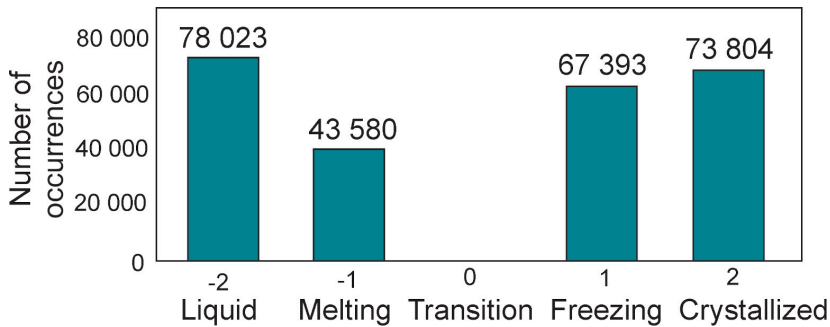


Figure 3.3: Distribution of PCM states for Node 4 of the South wall over the whole simulation year for a selected configuration of the demonstrator building and using the current hysteresis model in EnergyPlus. The simulation has been performed using the time step of 2 minutes with a total of 262800 time steps distributed across possible PCM states.

It can be observed from the model output that there is not a single time step where PCM is in the transition state. This would only be possible if the material underwent full melting–solidification cycles throughout the entire year, which is unrealistic. To explore this issue in more detail, Figure 3.4 depicts the heat capacity, node temperature, and PCM state for two full days in January (27th and 28th). Multiple inconsistencies can be observed:

- PCM is not switching to Transition state during the incomplete melting cycle (frames #2 and #4).
- PCM is going from Melting into Liquid state even though the node temperature never reaches even the peak melting temperature of 20 degrees (frames #2 and #4).
- PCM is going from Liquid to Melting state (frame #3).
- PCM is going from Crystallised to Freezing state (frame #8).

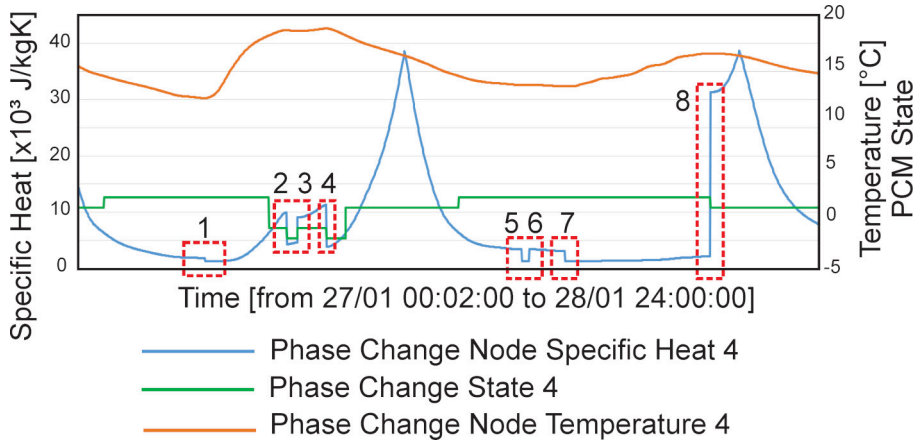


Figure 3.4: Specific heat, Temperature and Phase change state for Node 4 in the South wall of the demonstrator building during the 27th and 28th of January. Red frame lines indicate the discontinuities in the specific heat function.

All of these observations point to the fact that in its current form, the hysteresis model does not perform curve switching as intended (by PCM entering the Transition state) but instead jumps instantaneously between the melting and solidification curves. Figure 3.5 shows the temperature–enthalpy curve for the same two days in January. It can be observed that, during the two analysed days, the PCM shifted isothermally between the melting and solidification curves eight times while never entering the transition state as required by the curve-switch theory. The red frames in Figure 3.5 correspond to the same heat capacity discontinuities shown in Figure 3.4.

According to [111], the approach with the isothermal transition between the curves is also used in TRNSYS model type399. However, this is not representative of the real-world behaviour of PCM and such a modelling approach might also lead to the overestimation of PCM latent heat [111].

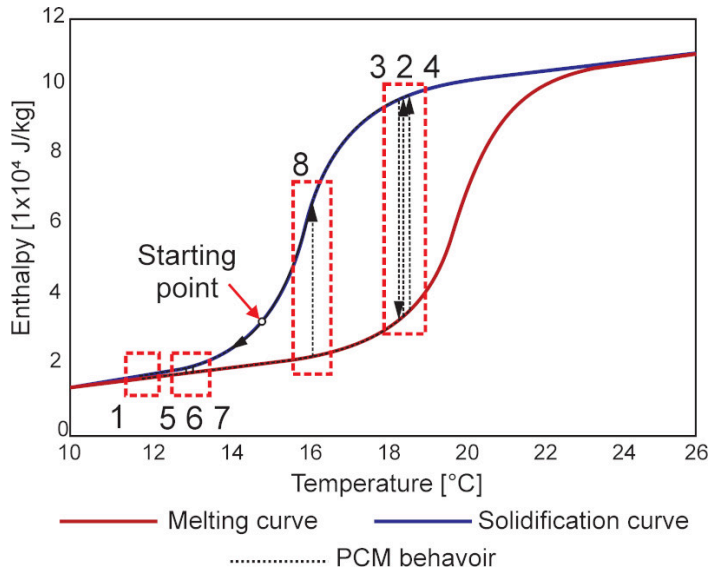


Figure 3.5: Enthalpy curve for Node 4 in the South wall of the demonstrator building. The numbered frame lines correspond to the same specific heat discontinuities shown in Figure 3.4.

3.3.3 Modified EnergyPlus PCM model with corrected curve switching

Model description

As illustrated in the previous section, the built-in EnergyPlus hysteresis model does not function as intended and is not realistically describing the real-world behaviour of PCM. To address this issue, a modified version of EnergyPlus has been developed, incorporating a functional curve-switch model along with other improvements. The following changes have been made:

- The code related to hysteresis modelling has been almost completely re-written to follow the curve switching approach as outlined in Bony and Citherlet [129].
- The boundaries where PCM is considered to be fully frozen or fully melted have been extended to prevent large jumps in enthalpy when switching between melting and freezing curves in fully melted or fully frozen states.

The mathematical modelling of PCM properties during melting and solidification cycles in EnergyPlus relies on the work by Egolf and Manz [128], where specific enthalpy and other physical properties of PCM are defined using continuous functions. Between the frozen and liquid states, a so-called mushy region exists where PCM transitions from one state to another. In EnergyPlus, this region corresponds to the melting and freezing states. Its width is finite and defined by lower and upper limits. Outside the mushy

region, PCM is considered either fully melted or fully frozen. The enthalpy curve is defined as a smooth exponential function that gradually decreases beyond the mushy region. As a result, the specific heat at the edges of the mushy region is higher than the sensible specific heat, which can cause significant discontinuities if the temperature reverses direction just outside this region, since a switch between curves will then occur.

- The part of the hysteresis algorithm that detects the reversal in PCM temperature change has been moved from the CondFD algorithm into the main hysteresis algorithm.

In the current version of EnergyPlus, this detection is handled in the CondFD code, but this causes an issue where the enthalpy and heat capacity calculations are based on data from the previous time step. In other words, not all variables are updated simultaneously, leading to synchronisation (timing) issues. In the updated version, all variables are calculated and updated at the same time.

- The transition between melting and freezing curves has been modified to happen at specific heat equal to the specific heat of fully frozen PCM.

As already mentioned, the curve-switch model implemented in this work is based on the approaches by Egolf and Manz [128] and Bony and Citherlet [129]. There is, however, a degree of incompatibility between these models. Egolf and Manz [128] describe a method for implementing a continuous enthalpy curve with a mushy region, capable of representing PCM with different specific heat in liquid and frozen states. Their work, however, does not address hysteresis and focuses only on a single enthalpy curve. In contrast, Bony and Citherlet [129] include hysteresis and implement a curve-switch mechanism for incomplete melting and solidification cycles, but assume that the specific heat of PCM is the same in solid and liquid states.

The analysis of the current hysteresis code in EnergyPlus showed that the intended way to resolve the incompatibility between the two underlying theories was to set the transition between melting and freezing curves at a heat capacity equal to the average of the fully frozen and fully melted values. However, depending on the PCM characteristics and the point where the transition begins, this can cause an issue where instead of switching from the melting to the freezing curve, the PCM loops back to the melting curve. Figure 3.6 illustrates this issue using an example where the liquid specific heat is three times the frozen specific heat (an exaggerated case chosen for the clarity of the illustration). To avoid this problem, the curve-switch model implemented in this study assumes that the transition occurs at a heat capacity equal to the fully frozen value.

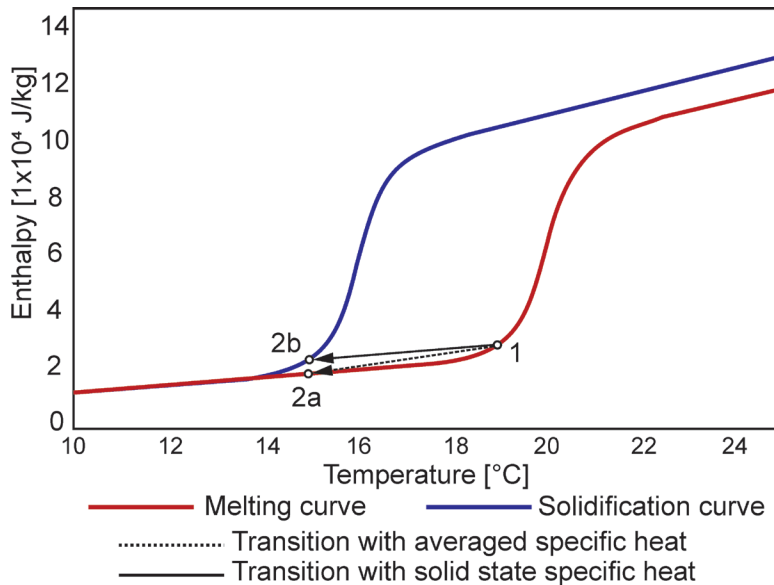


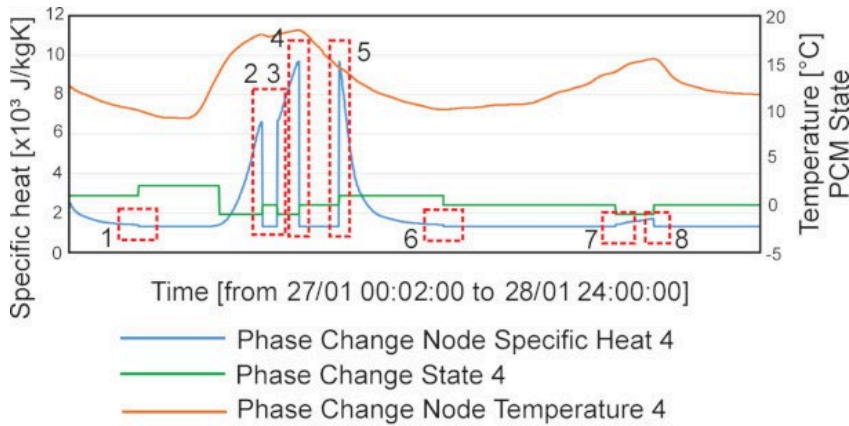
Figure 3.6: Two cases of simulating the transition between melting and solidification curves. Dotted line (1 → 2a) corresponds to the transition that happens at heat capacity equal to the average between fully melted and fully frozen heat capacities. Solid line (1 → 2b) is the transition at the fully frozen heat capacity.

- The Input Data Dictionary of EnergyPlus has been modified to allow peak melting and solidification temperatures of PCM to be negative.
- New variables have been added allowing to also output enthalpy values for each node: CondFD Phase Change EnthNew (node enthalpy for the current time step), CondFD Phase Change EnthOld (node enthalpy for the previous time step).
- The initialisation temperature that EnergyPlus is using as the starting point for all the temperatures in CondFD algorithm has been changed from 23.0°C to -33.33°C.

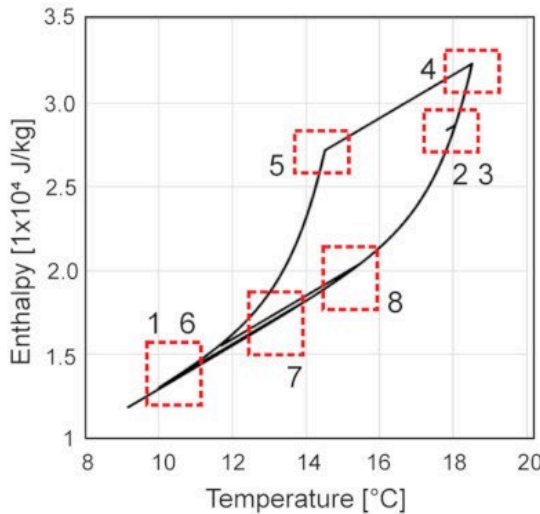
It has been observed that the modified version of EnergyPlus terminates with a fatal error if the peak melting or solidification temperature is exactly the same as the initialisation temperature. In building applications, the likelihood of a user simulating a PCM with a peak temperature of 23.0°C is much higher than, for example, -33.33°C.

- Comparison with the original model

To illustrate the difference between the original and modified models, let us consider the same building example from the previous section describing the issues with the current EnergyPlus hysteresis model (file "model_test_1.idf" in the repository). Figure 3.7 (a) shows the temperature, phase change state, specific heat, and enthalpy curve for the same Node 4 in the south wall of the demonstrator building over the period of January 27th to 28th.



(a)



(b)

Figure 3.7: Temperature, specific heat and phase change state for Node 4 in the South wall (a) and enthalpy curve for the same node (b) during the 27th and 28th of January. Red frame lines indicate the discontinuities in the specific heat function.

While discontinuities in specific heat can still be observed, they occur not due to instantaneous jumps between curves, but when PCM enters or exits the Transition state (see Figure 3.7 (b)). According to the curve-switch theory, and specifically the approach outlined by Bony and Citherlet [129], during the transition, the specific heat of PCM equals its sensible heat. As a result, depending on where the transition occurs, specific heat may show significant changes. This is thus an intrinsic feature of the curve-switch theory.

It is also possible to confirm that the modified model is stable and produces consistent results throughout the year. Figure 3.8 presents the

enthalpy curve over the full year for the same node used in the previous analysis. Figure 3.8 shows that the resulting enthalpy curve follows the theoretical one, and all transitions between the curves align with a straight line having the same slope as in the fully crystallised or fully melted states.

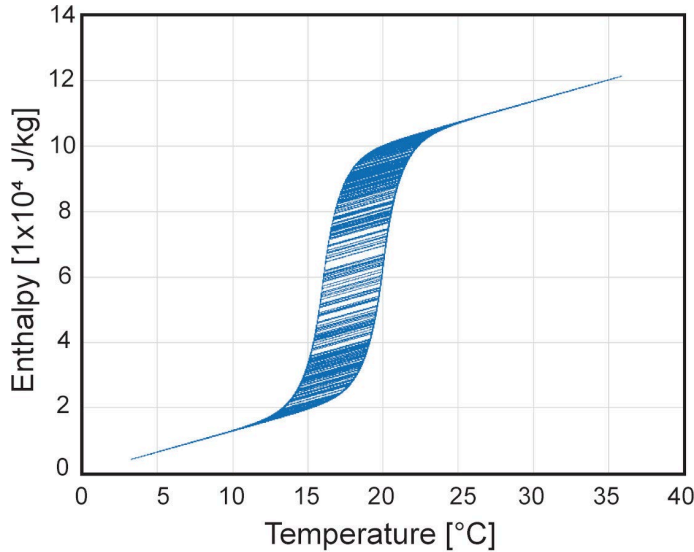


Figure 3.8: Enthalpy curve for Node 4 in the South wall of the demonstrator building over the whole simulation year.

Identified limitations

- Curve switching is a simplified model and may not be as precise as more comprehensive hysteresis approaches, such as curve scaling or the two-phase model.

According to comparison examples found in the literature, more advanced hysteresis models may produce results closer to experimentally obtained data for incomplete melting and solidification cycles [121]. Additionally, these models often show a lower degree of discontinuity in the PCM heat capacity function, making them more realistic than the curve-switch model, where heat capacity undergoes instantaneous and often significant changes not representative of real-world PCM behaviour.

- Enthalpy jumps occur when switching between melting and freezing curves in PCM with different fully frozen and fully melted specific heat.

While the model allows simulating a PCM with different heat capacities in frozen and melted states, it experiences relatively large enthalpy jumps when switching between the curves. Figure 3.9 illustrates this effect, showing the enthalpy curve over the full simulation year for a PCM with higher melted heat capacity than in the frozen state (file "model_test_2.idf" in the repository). It should be noted that the overall enthalpy across the fully

frozen–fully melted–fully frozen cycle is preserved, and the enthalpy jump does not cause a major change in heat capacity. Consequently, it should not significantly affect simulation results, as those rely on heat capacity values rather than absolute enthalpy.

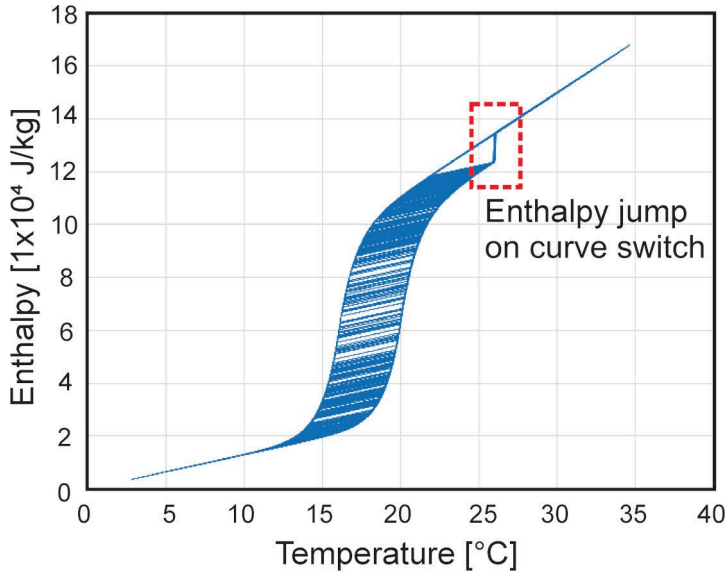


Figure 3.9: Enthalpy curve for Node 4 in the South wall over the whole simulation year in the case of unequal specific heat capacity in frozen and melted states. The highlighted area shows point where the jump between melting and solidification curves is occurring. Due to the difference in frozen and melted heat capacities, the enthalpy curve is experiencing a discontinuity and enthalpy jump is unavoidable.

- The model has not been validated on a real case.

3.3.4 Two-phase PCM model based on EnergyPlus v9.3

To address the issues with the built-in EnergyPlus hysteresis model described in the previous sections, and to enable more realistic modelling of incomplete melting and solidification cycles compared to simple curve switching, Feng et al. [124] developed the EnhancedPCM model based on EnergyPlus v9.3. EnhancedPCM relies on the two-phase PCM transition theory, specifically the static hysteresis model presented by Barz and Sommer [125].

Unlike the curve-switch EnergyPlus model described above where the state of PCM is described by five possible discrete values (frozen, melting, transition, freezing and melted), two-phase approach models PCM as consisting of two phases (liquid and solid) at any point in time. The proportion between these two phases is defined by the phase fraction parameter ξ :

$$\xi = \frac{m_l}{m_l + m_s} \quad (3.7)$$

where m_l is the mass of the liquid fraction and m_s the solid fraction. The effective properties of PCM (specific heat and enthalpy) depend on the phase fraction and can be estimated using Equation 3.8 and Equation 3.9.

$$c_{p,\xi} = \xi c_{p,l} + (1 - \xi) c_{p,s} + \frac{\Delta \xi}{\Delta T} L \quad (3.8)$$

$$h_{j+1} = h_j + c_{p,\xi} (T_{j+1} - T_j) \quad (3.9)$$

where $c_{p,\xi}$ is the effective specific heat of PCM; $c_{p,l}$ and $c_{p,s}$ are specific heat capacities of liquid and solid fractions; L is the latent heat of PCM; $\Delta T = T_{j+1} - T_j$ is the temperature change between the current and previous time step; h_{j+1} and h_j are current and previous enthalpies of PCM.

Similarly to the curve-switch method, PCM properties are defined using a continuous function. However, while in the case of curve switching the exponential function is used to define PCM enthalpy, in the work of Feng et al. [124] it is used to define the phase fraction ξ :

$$\xi(T) = \frac{1}{2} \left(e^{\frac{-2|T-T_p|}{\tau_l}} \right), \text{ for } T \leq T_p \quad (3.10)$$

$$\xi(T) = 1 - \frac{1}{2} \left(e^{\frac{-2|T-T_p|}{\tau_h}} \right), \text{ for } T > T_p \quad (3.11)$$

where T_p is the peak melting or solidification temperature of PCM depending on which curve is modelled; τ_l is the lower width of melting or solidification interval; τ_h is the upper width of melting or solidification interval. The use of exponential functions allows for seamless integration of the new model into existing functions within the EnergyPlus code.

Identified limitations

- Intermittent issue where the model fails to initialise correctly, causing the temperature at all PCM nodes to remain constant throughout the entire simulation.

It has been observed that, depending on the building configuration, PCM layer properties, weather data, and CondFD algorithm parameters, the model may fail to initialise in some cases. Figure 3.10 illustrates such a case, showing the temperature of two nodes in the south wall of the demonstrator building: one on the outside of the PCM layer (Node 1) and one on the inside (Node 4). The input EnergyPlus file "model_test_3_v93.idf" is provided in the repository.

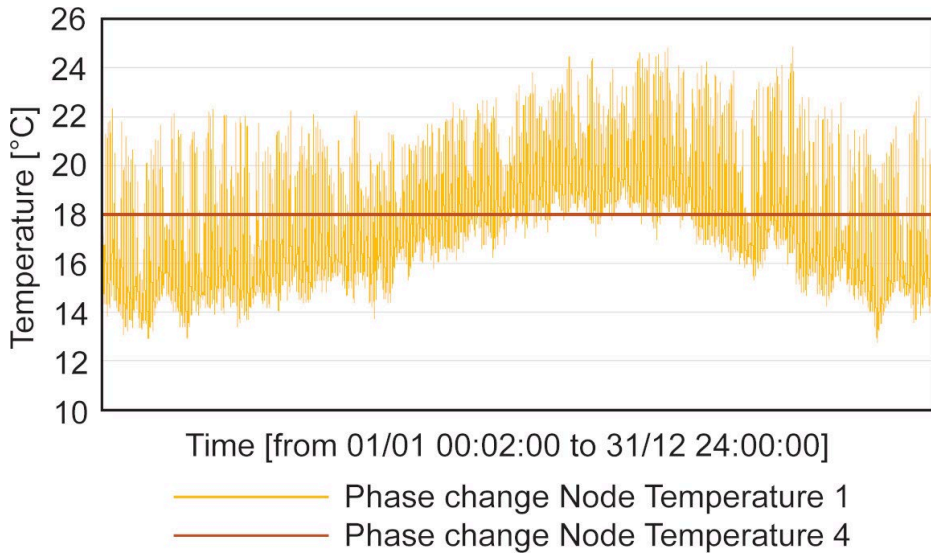


Figure 3.10: Yearly temperature variation for Node 1 (outer node) and Node 4 (inner node) in the South wall of the demonstrator building.

From Figure 3.10, it can be observed that while the temperature of the outside node (Node 1) changes, the temperature of Node 4, located inside the PCM layer, remains fixed at exactly 18°C throughout the year. This value corresponds to the initialisation temperature set within the EnergyPlus code (specifically in the CondFD algorithm) and cannot be modified by the user through input parameters in .idf file. The only way to change it is by editing the source code and recompiling EnergyPlus. Interestingly, in the original EnergyPlus code, the initialisation temperature was set at 23°C but was reduced to 18°C by Feng et al [124]. This change was not explicitly explained by the authors, but it appears that they may also have encountered stability issues during the simulations.

Based on our experiments, we were not able to identify the logic behind these intermittent initialisation errors. In some cases, when comparing two nearly identical PCM configurations that differ only in peak melting temperature by one degree, one results in an initialisation error while the other does not. Similar behaviour was observed for other PCM layer parameters as well. However, the issue may not necessarily originate from the hysteresis model itself, but rather from the CondFD algorithm or the way the new two-phase hysteresis model interacts with it.

It is also important to note that the parameters of the CondFD algorithm play a significant role in this issue. In many cases, tweaking these parameters helped resolve the problem. Specifically, decreasing the space discretisation constant and relaxation factor, as well as increasing the number of time steps per hour, had a positive effect on reducing the likelihood of initialisation errors. However, due to the intermittent nature of the issue, there is no guarantee that it will not occur with certain combinations of the building,

PCM and EnergyPlus parameters. Moreover, the parameter adjustments described above significantly increase simulation run times. Although manageable for a single case, this becomes a serious limitation for optimisation studies or situations where large numbers of configurations need to be evaluated simultaneously and it is not feasible to manually check all EnergyPlus outputs. Even more concerning is that the error does not trigger any warnings or messages in the console or error file, making it very likely to go unnoticed, potentially leading users to incorrect conclusions.

- Intermittent issue where the model initialises correctly but freezes during the simulation run.

This issue is very similar to the previous one, but in this case the simulation starts normally: node temperatures change, and all PCM parameters follow expected trends. However, at some point, the node temperatures freeze and remain unchanged for the rest of the simulation. Figure 3.11 illustrates one such case (see the "model_test_4_v93.idf" file in the repository).

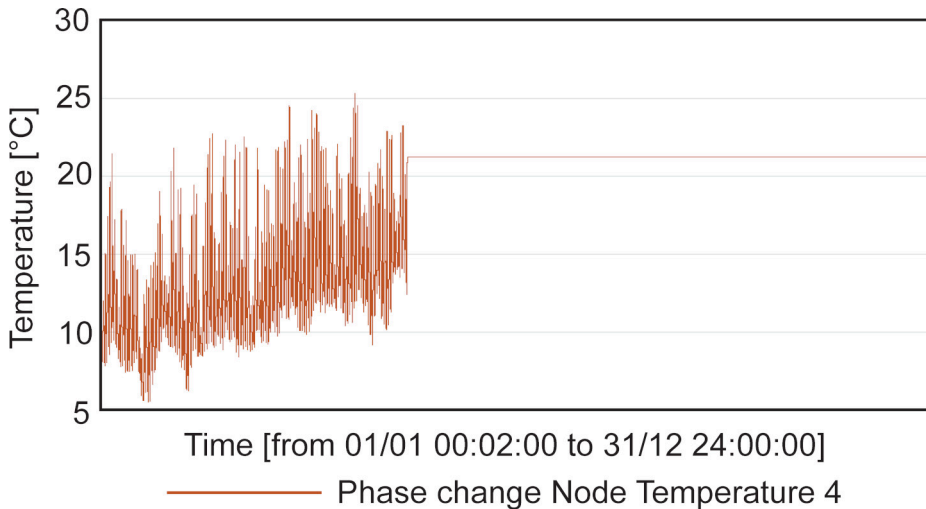


Figure 3.11: An example of the model freeze issue. The graph shows the temperature profile of Node 4 in the South wall of the demonstrator building over the whole simulation period.

As shown in Figure 3.11, the simulation appeared normal until one time step in May, after which no further changes occurred. Similarly to the initialisation issue, the model freeze is highly unpredictable and depends on the specific building case, PCM parameters, weather data, and EnergyPlus algorithm settings and especially CondFD parameters. In most cases, tweaking CondFD parameters helped resolve the issue. This issue, however, is even harder to spot since the outputs are partially correct in the beginning of the simulation run.

- Node heat capacity is taking unexpectedly high values outside of the peak melting and solidification.

Specific heat can reach very high values during peak melting and solidification. However, it has been observed that this model sometimes produces extremely high specific heat values at the far edges of the melting and solidification curves. Figure 3.12 illustrates this issue (EnergyPlus input file "model_test_1_v93.idf" provided in the repository). Since EnergyPlus 9.3 cannot directly output node-specific heat, the "CondFD Surface Heat Capacitance Inner Half Node" variable has been used instead for this illustration.

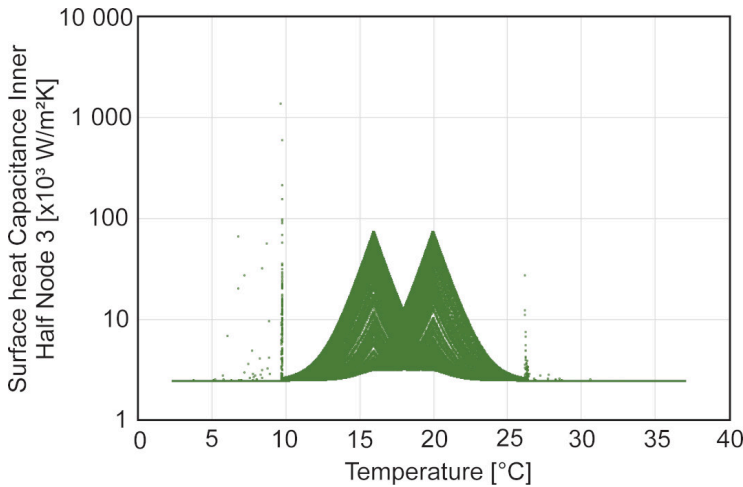


Figure 3.12: Surface Heat Capacitance (Inner Half Node) for Node 3 in the South wall of the demonstrator building over the whole simulation period. Note the logarithmic scale of the vertical axis.

Figure 3.12 clearly shows the expected melting and solidification peaks in the middle, but also two narrow abnormal spikes in heat capacity far outside the melting and solidification intervals. The heat capacitance values at those spikes are often much higher than even during peak melting and solidification.

While the outliers are significant, they are unlikely to have a major impact on overall building performance, as they occur during only a small number of time steps. However, it is possible that this issue is related to the model freeze problem described above. For example, depending on the magnitude of the heat capacity spike, the simulation may either recover or become stuck at this abnormally high value.

- If PCM has different heat capacities in frozen and melted states, enthalpy is not preserved over the full melting–solidification cycle.

As discussed earlier, EnergyPlus allows users to define different specific heat values for the liquid and solid states of PCM. However, in the hysteresis model by Feng et al. [124], assigning different heat capacities to the solid and liquid phases causes enthalpy to break the closed loop and drift away. Figure 3.13 illustrates this effect. The input file "model_test_2_v93.idf" used for this

simulation is provided in the repository. The impact of the enthalpy drift on the overall results of the simulation is, however, unclear.

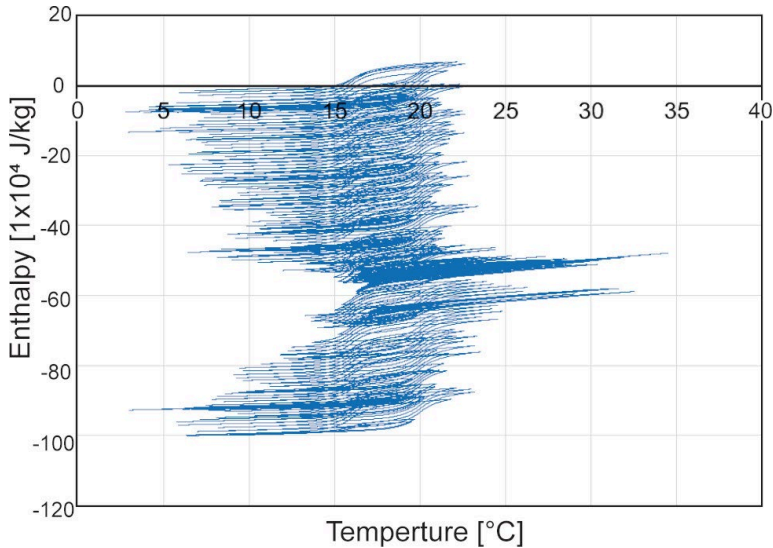


Figure 3.13: Enthalpy drift in case of PCM with different specific heat capacity in liquid and solid states.

- The model is implemented in EnergyPlus v9.3 which is an old and possibly outdated version.

3.3.5 Two-phase PCM model based on EnergyPlus v24.1

This model is an adaptation of the one by Feng et al. [124], integrated into a newer version of EnergyPlus (24.1). Additional changes that have been made:

- The initialisation temperature has been changed to -33.33°C .

Due to the observation that initialisation and model freeze issues (see Section 3.3.4) often occur when PCM melting temperature is significantly lower than the initialisation temperature, the initialisation has been changed to -33.33°C . However, since this parameter is not properly documented, it is unclear whether its modification affects other parts of the CondFD algorithm. Based on the tests performed in this work, changing the initialisation temperature did not have a major effect on the results of the building energy simulations.

- Modifications have been made to the EnergyPlus Input Data Dictionary to allow simulation of PCM with negative melting and freezing temperatures.

Identified limitations

Since this version uses Feng et al. [124] hysteresis model without modifications, it exhibits similar issues:

- There are still heat capacity outliers albeit the frequency of their occurrence is lower than in the version 9.3.
- Simulation stability might still be an issue sometimes, but the change in the initialisation temperature reduces the number of cases where model is not initialising properly or freezing during the simulation.
- Unlike the original model of Feng et al. [124] this version has not been validated using a real-world case.

3.3.6 The impacts of hysteresis model selection on decision-making

To understand the impact that the choice of hysteresis model might have on practitioners and decision-makers, let us illustrate it with an example of material design optimisation. A novel thermal material, NRG-Panels, has already been introduced in the Methodology section. For a material designer developing such a product, it is essential to identify the optimal material configuration that minimises heating and cooling loads. Because many material parameters can be adjusted, the number of possible combinations is virtually unlimited, making it physically impossible to test all of them in the lab or under real-world conditions. As a result, design decisions are highly dependent on the outcomes of full-building energy simulations.

Let us take the demonstrator building described in the Methodology section and try to find the best-performing NRG-Panels configuration for this particular case. In theory, one could define an optimisation problem to minimise building energy demand and solve it to find the optimal panel configuration. However, due to the intermittent issues described before, the optimisation algorithm may be misled and converge to a sub-optimal solution. As discussed previously, tweaking the CondFD parameters, such as reducing the time step, space discretisation constant, and temperature relaxation coefficient, can improve simulation stability, but these adjustments result in extremely long simulation times, making optimisation impractical.

Due to these limitations, a batch simulation approach was used in this study instead of optimisation. First, for each variable material parameter, a set of possible values was preselected. In our case, the parameters and their values were as follows:

- Material porosity: 0.05, 0.2, 0.4, 0.6, 0.8, 0.95.
- MPCM fraction: 0.01, 0.2, 0.4, 0.6.
- Panel thickness: 0.1 m, 0.2 m, 0.3 m.
- PCM peak melting temperature: 18°C, 19°C, 20°C, 21°C, 22°C, 23°C, 24°C, 25°C, 26°C, 27°C, 28°C, 29°C, 30°C.
- Hysteresis degree: 0.01°C, 2°C, 4°C, 6°C, 8°C, 10°C.

Other parameters, such as total latent heat and the width of the melting and solidification curves, were kept fixed. Then, a set of virtual materials was

generated using all possible combinations of the variable parameters. For each configuration, the final properties of the insulation layer were calculated and an .idf file was created. These files were then used to run EnergyPlus simulations for each material configuration.

In our case, simulations for all configurations were run using six versions of EnergyPlus: four hysteresis models discussed above, and two reference models without hysteresis (EnergyPlus v9.3 and v24.1). For the no-hysteresis models, only the melting curve of the PCM was used. To do so, the PCM parameters of each material configuration were used to build the enthalpy curve, which was then converted into the temperature–enthalpy pair format required by EnergyPlus to be provided in the MaterialProperty:PhaseChange input field of .idf file.

After obtaining the yearly HVAC energy consumption results, the best material configuration according to each model was identified. Table 3.2 provides an overview of these configurations and Figure 3.14 shows the enthalpy curves for each configuration.

Table 3.2: Overview of the analysed configurations of NRG-Panels.

Configuration	Porosity	MPCM fraction	Panel thickness (m)	PCM peak melting temp. (°C)	Melting curve width (low) (°C)	Melting curve width (high) (°C)	Degree of hysteresis (°C)	Freezing curve width (low) (°C)	Freezing curve width (high) (°C)
C1	0.05	0.6	0.2	20	2	2	6	2	2
C2	0.2	0.6	0.3	23	2	2	8	2	2
C3	0.8	0.6	0.3	25	2	2	6	2	2
C4	0.2	0.6	0.3	25	2	2	10	2	2
C5	0.95	0.6	0.3	21	2	2	2	2	2
C6	0.2	0.6	0.3	18	2	2	2	2	2

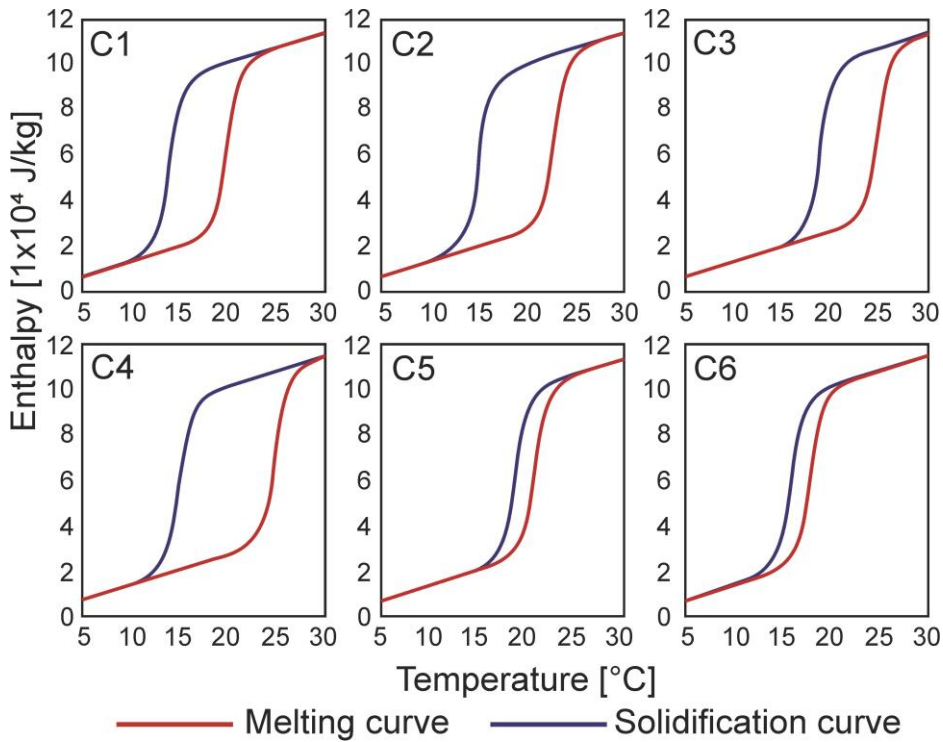


Figure 3.14: Enthalpy curves for the analysed configurations of NRG-Panels.

The resulting parameters of the layer that were used in EnergyPlus are provided in Table 3.3.

Table 3.3: Resulting calculated properties of NRG-Panels for each analysed configuration.

Conf.	Latent heat of fusion (J/kg)	Specific heat (J/kgK)	Density (kg/m ³)	Thermal conductivity (W/mK)
C1	7.50E+04	1.29E+03	1.16E+03	2.90E-01
C2	7.50E+04	1.29E+03	9.80E+02	2.29E-01
C3	7.47E+04	1.29E+03	2.46E+02	5.81E-02
C4	7.50E+04	1.29E+03	9.80E+02	2.29E-01
C5	7.36E+04	1.29E+03	6.24E+01	3.04E-02
C6	7.50E+04	1.29E+03	9.80E+02	2.29E-01

The resulting .idf files for each of the configurations can be found in the repository. For each configuration, four different .idf files are included:

- With hysteresis for EnergyPlus v9.3 (used for Feng et al. model).
- Without hysteresis for EnergyPlus v9.3 (used for no-hysteresis model v9.3).

- With hysteresis for EnergyPlus v24.1 (used for the current EnergyPlus hysteresis model, modified model with corrected curve switching and Feng et al. model integrated into EnergyPlus v24.1).
- Without hysteresis for for EnergyPlus v24.1 (used for no-hysteresis model v24.1).

The results of the simulations for each material configuration obtained using analysed PCM modelling approach are presented in Table 3.4.

Table 3.4: The final HVAC energy demand for the demonstrator building with every analysed configuration of NRG-Panels. Each building configuration has been simulated using every PCM model considered in this study. For each PCM model, the results of energy simulations were ranked and those ranks are also provided in the table. For example, for the current hysteresis model in EnergyPlus, the configuration C1 is the best ranked since it has the lowest energy consumption compared to other configurations.

Conf.	Heating and cooling demand, kWh/a						Configuration rank					
	Original	Curve-switch	Feng et al. v9.3	Feng et al. v24.1	No Hysteresis 9.3	No Hysteresis 24.1	Original	Curve-switch	Feng et al. v9.3	Feng et al. v24.1	No Hysteresis 9.3	No Hysteresis 24.1
C1	964	1667	995	1674	1008	1703	1	4	6	4	6	4
C2	1186	1545	896	1549	928	1626	2	1	4	2	4	2
C3	1770	1780	843	1781	853	1796	5	5	1	5	2	5
C4	1298	1576	892	1543	934	1638	3	2	3	1	5	3
C5	1916	1936	845	1932	844	1934	6	6	2	6	1	6
C6	1372	1601	919	1600	905	1575	4	3	5	3	3	1

As observed in Table 3.4, the models disagree on which material configuration is the most promising in terms of the optimal energy performance of the demonstrator building: every configuration is ranked as the best according to only one of the models.

The current hysteresis model clearly favours configurations with the lowest porosity, and therefore the highest MPCM content and maximum heat capacity (C1). In contrast, all other models rank this configuration as one of the least preferable. Furthermore, when comparing the energy consumption values obtained from the current model with those from the other EnergyPlus v24.1-based models, it becomes evident that the current model significantly overestimates the effect of PCM inclusion: configuration C1, which has the highest total amount of PC, shows an HVAC energy consumption of less than 1000 kWh/a according to the original model while it never drops below 1500 kWh/a according to the rest of EnergyPlus v24.1-based models.

The no-hysteresis EnergyPlus v9.3 model is at the opposite extreme, identifying the configuration with the highest porosity of 0.95 (C5) as optimal. However, this configuration is poorly ranked by all other models, including the version of the Feng et al. [124] model integrated into EnergyPlus v24.1. The only other model aligned with it is the original Feng et al. model that also favours high porosities and identifies NRG-Panels with 0.8 porosity as optimal. However, these two models do not agree on the optimal melting temperature of PCM.

It is also important to note the differences in results caused by the EnergyPlus version. The no-hysteresis models in EnergyPlus v9.3 and EnergyPlus v24.1 disagree on the optimal configuration, highlighting that the results of simulations are strongly influenced not only by the PCM hysteresis modelling but also by other changes made to EnergyPlus between the versions. This has a major impact on material design decisions, as the optimal configuration varies significantly depending on the version of EnergyPlus used. The changes between EnergyPlus versions also affect the results obtained from hysteresis models, leading to the situations where the original Feng et al. [124] model and its version implemented in EnergyPlus v24.1 produce contradictory results. For example, the two models disagree on how the porosity of NRG-Panels influences HVAC energy demand. To illustrate this disagreement, let us fix all the parameters of NRG-Panels except for porosity (0.6 MPCM fraction, 0.2 m thickness, 23°C melting temperature, 5°C hysteresis). The .idf files used for simulations are provided in the repository. Figure 3.15 compares the resulting energy consumption according to both models.

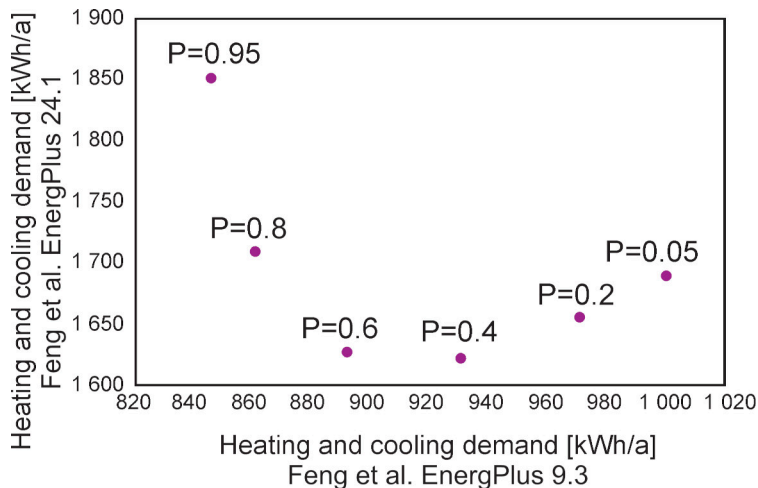


Figure 3.15: Comparison of heating and cooling energy demand according to the original Feng et al. hysteresis model in EnergyPlus 9.3 and the same model integrated into EnergyPlus 24.1 at different NRG-Panel porosities.

As depicted in Figure 3.15, a porosity of 0.95 is optimal according to the original Feng et al. model, yet it is the worst according to the Feng et al. v24.1

model, which favours a porosity of 0.4. Physically, this implies that in EnergyPlus v9.3, reduced thermal conductivity is seen as more beneficial than increased thermal storage capacity. Within the NRG-Storage project, this balance between thermal conductivity and heat storage was a key factor guiding material development. The situation where different models provide contradictory directions has a major impact on decision-making, essentially eliminating its sole foundation.

The contradictions related to the material design arise not only due to the differences in EnergyPlus version. Comparison among the models based on EnergyPlus v24.1 shows that there is also a degree of disagreement between them. The best configuration of NRG-Panels according to the no-hysteresis model v24.1 contains PCM with the melting temperature of 18°C which is significantly lower than in the case of other models. Thus, if the decision regarding the choice of PCM for NRG-Panels was to be made based on the simplified simulation without taking hysteresis into account, a PCM with a low melting temperature would be selected. However, this might be a suboptimal design decision if hysteresis is taken into account. And when it comes to the two analysed models with hysteresis based on EnergyPlus v24.1 - curve-switch and Feng et al. v24.1 - while they generally provide similar results, there are also differences in regard to how some PCM parameters impact the HVAC energy demand. One of such parameters is the degree of hysteresis and Figure 3.16 provides an illustration of one of such cases where all the parameters of NRG-Panels are fixed (0.4 porosity, 0.6 MPCM fraction, 0.3 m thickness, 20°C melting temperature) and the models are compared across different levels of PCM hysteresis. The .idf files used for simulations are provided in the repository.

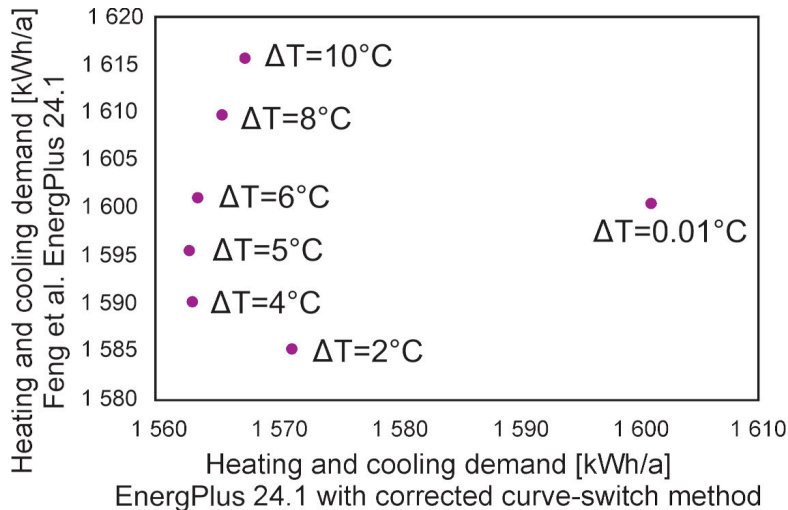


Figure 3.16: Comparison of heating and cooling energy demand between curve-switch model and Feng et al. v24.1 model at different degrees of hysteresis.

As Figure 3.16 shows, the degree of hysteresis that results in the minimum HVAC energy demand differs between the models: for the curve-switch method the optimal hysteresis is around 5°C while for Feng et al. 24.1 model - around 2°C. While the degree of hysteresis is not a design parameter that could be easily modified, it can still have influence on material design decision-making. For example, depending on what the optimal value of hysteresis is for minimised building energy consumption, a different type of PCM can be chosen (organic or inorganic, bio-based or petroleum based), a product of different producer could be prioritised (there are differences between PCM hysteresis depending on the producer and the production process), or different encapsulation techniques of MPCM particles can be selected (hysteresis degree can be influenced by the encapsulation process). Contradicting results related to the optimal degree of hysteresis could thus also be a major complication for a decision-making process and the selection of the optimal material configuration.

3.4 Discussion

The analysis of different EnergyPlus hysteresis models presented in this work highlights that there is currently no model without limitations that could be used without any reservations. The built-in EnergyPlus model is clearly not implemented correctly and cannot be recommended to be used for PCM modelling. A corrected curve-switch model presented in this study has resolved multiple issues of the original EnergyPlus hysteresis model and has been shown to be stable when it comes to simulation of a variety of PCM configurations. However, it is also based on a simplified approach to PCM modelling and has not been validated against a real-world case. The two-phase hysteresis model by Feng et al. is the most comprehensive and realistic among all the PCM models analysed in this work. Unfortunately, it is also not completely free of limitations and is susceptible to intermittent stability issues. Furthermore, the original model of Feng et al. is implemented in a relatively old version of EnergyPlus v.9.3 and switching to a newer version leads to significantly different and often contradicting results. Finally, there is currently no EnergyPlus hysteresis model that allows for modelling of supercooling effects. Practitioners should be fully aware of those limitations of the existing models when making a choice between them and be sure to not take the results of the simulations at face value, no matter which model is used. Based on a thorough analysis of the working principles and limitations of hysteresis models presented in this study, a set of practical recommendations has been compiled for the practitioners working with PCM modelling in EnergyPlus:

- Be careful with the CondFD algorithm parameters. The default values of those parameters are not suitable for PCM hysteresis modelling, especially when using the two-phase hysteresis model.
- In order to avoid the issues with model stability, decrease the space discretisation constant or the relaxation factor. Increasing the time step of the simulation is beneficial as well. In our tests, decreasing the

discretisation constant to 1, relaxation factor to 0.5 and increasing the time step to 30 or more steps per hour usually was enough to prevent model instability issues. Those values, however, vary per case and might need to be significantly different in some instances.

- Thoroughly check the energy simulation outputs at the level of nodes. Output the temperature and specific heat capacity for several nodes in the PCM layers and check the consistency of those outputs. The intermittent stability issues can often go unnoticed if only the final top-level results (e.g., building energy demand) are analysed.
- In case of optimisation study, be sure to save the results at every iteration of the optimisation algorithm. E.g., if genetic algorithm is used to minimise energy demand of the building, the population and corresponding objective functions values should be saved for each generation. After the optimisation is finished, it is often possible to spot outliers (e.g., abnormally high or low energy demand) by analysing the collected intermediate data. Those outliers should then be analysed more thoroughly since they could represent the cases where the model failed to initialise or became frozen during energy simulation.
- Be aware of the differences in results caused by EnergyPlus versions. The default assumption is that newer versions are more reliable. The results obtained previously using an older version of EnergyPlus might need to be re-evaluated using a newer version.

The results of this work also suggest that there is still a need for the improvement of the existing hysteresis models as well as for the development of new ones. From the literature it can be observed that while the theoretical and micro-level modelling of PCM is rapidly evolving [20], [21], [111], [130], [131], [132], [133], [134], [135], the practical implementation of those models in the building energy simulation software is lagging behind. Furthermore, it is also observed that when a new practical PCM model is introduced into EnergyPlus, the validation of this model is usually limited to a very small number of cases. E.g., the performance of the model is tested against one or a couple of PCM types, usually in the laboratory setting and using small-scale cases. Such a narrow approach to the model testing and validation possesses potential risks that while the model performs well under selected conditions, it might not be the case if other PCM configurations, building case, weather conditions, etc. are considered. While it is understandable that extensive large-scale experimental testing of multiple possible PCM, buildings and weather conditions for model validation is physically unfeasible, we encourage model developers to at least perform stress-testing of their models. For that, the model is run using a wide gamut of possible PCM parameters, EnergyPlus parameters as well as using different building models and weather conditions and the output of the models is cross-checked for consistency. Such testing could generally help uncover hidden and intermittent issues that might only appear under a particular combination of input and model parameters. Beyond the necessity for the further development of hysteresis models, EnergyPlus can also benefit from

additional modifications that would allow to better integrate PCM models, improve user awareness and help uncovering possible hidden and intermittent issues when they occur. Based on the performed tests and observations resulting from this study, we identify the following possible improvements that could be implemented:

- There is a need for an automated consistency check of the simulation results. At the moment, EnergyPlus has no tools to detect the intermittent issues that were described in detail in the Results section of this work. Those intermittent issues can be identified by, for example, monitoring the temperature of the nodes inside the PCM layer. If temperature does not change over a defined number of time steps, the simulation can either be terminated with an error, or the warning can be output into the console or EnergyPlus error file.
- Introducing the uncertainty levels of the results depending on which EnergyPlus components are used. Some of the components included in EnergyPlus are more refined and thus have lower uncertainty, while others (like PCM hysteresis modelling) are more experimental and high-uncertainty. If the user is warned when using a module with high uncertainty, it might help raise their awareness and encourage a more thorough and critical evaluation of the simulation results.
- All users and especially advanced ones will benefit from a more detailed explanation of EnergyPlus parameters. This applies to both, user-definable parameters as well as built-in parameters that can only be modified by changing the source code and compiling a custom version of EnergyPlus. For the user-definable parameters, while the documentation explains their meaning, it often does not mention how the default values are selected, when they should be changed and what might be the consequences of those changes. For the built-in parameters that users cannot easily modify, and especially those that have a high impact on the simulation results and model stability (e.g., the initialisation temperature), the explanations should be provided on the reasoning behind the selection of their values. This is especially important to facilitate the integration of new advanced PCM hysteresis models into EnergyPlus.

From a broader perspective, the observed differences in the results obtained using different models have far-reaching implications for research and decision-making related to the use of PCM in construction and potential benefits of PCM for energy savings. In case we see the benefits of PCM use from energy simulations, can we be sure that those are actual benefits and not the consequences of the PCM model selection and the parameters used? And since all the studies analysing the benefits of PCM to date are not harmonised and rely on a variety of different PCM models, EnergyPlus versions and chosen simulation parameters, is it possible to make any conclusions at all about PCM applicability as an energy-saving material? In the current situation, there does not seem to be a definitive answer to these questions. It can be argued that conclusions about the benefits of PCM could be drawn from experimental studies that do not rely on computational simulations. However, as discussed before, those studies are limited and it is

hard to draw far-reaching and generalised conclusions based on them. The decision-making related to PCM use in construction is thus currently essentially a shot in the dark: the supporting information is scarce, uncertain and often contradicting yet decisions still have to be made.

3.5 Conclusions

This study highlights the critical importance of correctly modelling PCM hysteresis in full-building energy simulations. Four hysteresis models were tested and compared: the current built-in model, a corrected curve-switch model, and two implementations of a two-phase model. The analysis of the built-in hysteresis model uncovered a flawed implementation of the curve-switch logic, leading to inconsistent results during partial phase transitions. The corrected curve-switch model has fixed multiple issues of the original implementation and has been demonstrated to be stable, but remains limited by its simplified formulation and lack of experimental validation. The two-phase hysteresis model by Feng et al. provides a more realistic representation of PCM behaviour but is susceptible to intermittent stability issues and is sensitive to the conduction finite difference algorithm settings. Additionally, the same two-phase model re-implemented in a newer EnergyPlus version produces results that diverge significantly from those of its original implementation, pointing to version-related inconsistencies. Furthermore, none of the available models currently supports the modelling of supercooling effects. These limitations highlight the urgent need for the improvement of existing hysteresis models, as well as for the development and integration of new ones.

The observed limitations and issues of PCM modelling emphasise the need for a more thorough and cautious approach to simulation of buildings including PCM. It is important to check initial conditions and boundary definitions, since even minor changes can lead to significantly different results. The parameters of CondFD algorithm should be carefully adjusted, and running a few test cases with varied PCM parameters can help detect issues and physical inconsistencies. Reducing the space discretisation constant and the relaxation factor and increasing the number of time steps per hour all tend to improve stability in most cases. The output variables for PCM nodes, such as temperature and specific heat, should be carefully monitored to ensure the consistency and reliability of the results. In the case of optimisation studies, saving intermediate results and their subsequent analysis can help identify outliers that might point towards intermittent issues. Finally, the observed differences between the results obtained from the same PCM model in different EnergyPlus versions might require a reconsideration of all PCM-related results obtained using older versions of EnergyPlus.

From the perspective of decision-makers, the current situation with PCM modelling is challenging. As this work has shown, the choice of the PCM model in EnergyPlus has a major impact on the results of simulations and, consequently, on the decisions related to material, component or building

design. In some situations, when PCM is not expected to have a large degree of hysteresis (e.g., in the case of some organic PCM), it might be advisable to refrain from using hysteresis models and use a simplified but more reliable single enthalpy curve method. However, in the case of inorganic or encapsulated PCM that are characterised by higher levels of hysteresis, ignoring the associated effects might not be possible. If the number of necessary simulations is not large and the results can be manually validated for possible inconsistencies, the model by Feng et al. is the most advanced and realistic of available options. However, due to the intermittent stability issues presented in this work, when there is a need to run hundreds or thousands of simulations in an automated manner (optimisations, sensitivity analysis, etc.) curve-switch might be a better alternative due to higher stability. It might also be advisable to use multiple models and compare the results before making final decisions. And no matter which PCM model is used, we encourage practitioners and decision-makers working with PCM in EnergyPlus to be critical, thoroughly analyse the simulation outputs and take time with adjusting relevant parameters that might influence the outcomes.

EnergyPlus is an irreplaceable tool and NREL has done a commendable job developing it and keeping it open source for all of the practitioners to use and to build upon. However, like any other complex and actively developing open source project, it might have some issues and limitations. And while PCM modelling in EnergyPlus definitely requires more attention – especially since it is lagging behind the theoretical developments in the field – it is not only in hands of EnergyPlus developers but also of the academic community to advance it further and make it more comprehensive, realistic and reliable.

3.6 Data availability

The files needed to replicate this study are found in the repository: <https://doi.org/10.5281/zenodo.15320290>

PROTOTYPE-LEVEL ASSESSMENT OF NRG-FOAM AND NRG-PANELS IN THE CONTEXT OF A DEMONSTRATOR BUILDING

This chapter builds on the results of Chapter 2 and moves from the laboratory-scale life cycle assessment and life cycle costs assessment of NRG-Foam to the prototype-level assessments of NRG-Panels – the final product manufactured by casting of NRG-Foam into panels with their consequent curing. Using the ex ante approach, the production process of NRG-Panels is up-scaled using a number of scenarios aimed at reducing the impacts of their production. The up-scaling scenarios are divided into two groups: one focused specifically on the microencapsulated phase change material (MPCM) production and another on the manufacturing process of NRG-Foam and NRG-Panels. The use of the ex ante approach enables the comparison of the results of NRG-Panels' assessments with the market products that have a significantly higher technology readiness level. Furthermore, the chapter also presents building-level assessments of NRG-Panels and compares their building-level performance with EPS insulation. The comparison between the different ways of NRG-Panels manufacturing showed that when using inorganic coacervate MPCM particles, lower economic production costs can be achieved, while the use of melamine-formaldehyde MPCM particles leads to lower environmental costs of the panels. Compared to conventional insulation materials, NRG-Panels demonstrate competitive environmental and economic performance, no matter the type of MPCM used. At the building level, the total life cycle environmental and economic costs of the NRG-Panel building were found to be higher than the EPS building, mostly due to higher electricity consumption for heating. The chapter concludes that while NRG-Panels demonstrate promising results, their configuration might not have been optimal for the given case.

4.1 Introduction

A thorough analysis of the performance of new construction material and individual components that comprise this material is essential, as it lays the foundation for its further development and provides the necessary data for subsequent research. However, as the material development continues and it moves higher on the technology readiness level (TRL) scale, the assessments and optimisations of the material must also be continuously updated and upgraded along with it. The nature of those updates and upgrades is multifaceted. First of all, the analysis of the performance of the new material on the prototype scale is not possible without comparing it against the existing commercial products: we need to have a reference point to identify the possible areas for improvement and guide further development. Such a comparison, however, is not possible in a straightforward manner due to the major difference in TRL of market products and a novel material like NRG-Foam. Indeed, the environmental and cost data that can be found for those market products is representative of large-scale refined production processes, while the production of NRG-Foam only ever happened on a small scale and has not been optimised. To bring the assessment of NRG-Foam to a level where the comparison with market products will be possible, it is necessary to upscale it. This can be done by taking the lab-scale assessment and the identified hotspots and building on it using, e.g., scenario-based ex-ante life cycle assessment (LCA) methodology [136].

Furthermore, the prototype development stage generates great amounts of new data and experience. Consequently, some stages of the production process get refined and before unattainable information becomes available. Moreover, new constraints and limitations in the manufacturing process of the material, as well as in its real-world application process, come to light. Those new findings should also be reflected and taken into consideration in the prototype-level assessments.

Another important effect of moving from the lab scale to the prototype scale is the widening of the scope from the material and its constituents to the real-world prototype component that is analysed in the context of a demonstrator building. This scope widening, in turn, requires a shift from material-level assessments to assessments of a given material in the context of a building. There are several reasons for that. First of all, the sole goal of developing a new construction material is the improvement of the performance on the building level and/or higher levels, be that environmental, economic, social, circular, resilience or any other performance metric. The material-level performance, however, does not necessarily straightforwardly translate into the building-level performance since within the building system, the interplay between all the constituent parts of the system and their properties should be taken into account as well. Further, the direct material-level comparison of two materials might not be possible when their functionality is not the same. In our particular case, NRG-Foam is an insulation material, but it also incorporates phase change material (PCM) and, as such, provides an energy-storing function that regular

insulation materials do not possess. However, if NRG-Foam and an ordinary insulation material are compared in the context of a building, those two buildings will have the same functionality, and their performance (e.g., thermal) could be compared directly.

This chapter follows the transition of NRG-Foam material from the lab scale to the demonstrator scale. First, building on the LCA results presented in Chapter 2, and guided by the hotspots identified there, a set of scenarios is developed to upscale LCA and life cycle cost assessment (LCCA) of microencapsulated PCM (MPCM) production. Then, using this upscaled data as well as another set of upscaling scenarios, ex-ante LCA and LCCA of NRG-Panels production are conducted. NRG-Panels are the final product manufactured by casting NRG-Foam into panels and which are applied to a building as an insulation layer. For NRG-Panels, the results of upscaled LCA and LCCA are compared with the data for commercial products.

Finally, LCA and LCCA of two demonstrator buildings are performed: one containing NRG-Panels as an insulation layer and another containing an EPS insulation layer. Those two demonstrator buildings were physically built for the purpose of testing the performance of NRG-Panels in a real-world setting and are located in Sofia, Bulgaria. The building-level assessments use the data obtained in upscaled LCA and LCCA of NRG-Panels and allow for comparison of the performance of NRG-Panels and EPS insulation while avoiding possible issues with material-level comparisons discussed above.

4.2 Methodology and modelling approach

4.2.1 Overview

Figure 4.1 provides an overview of the overall methodology used in this chapter. Since the production of NRG-Foam is a part of the NRG-Panels manufacturing process, the assessments and scenarios for NRG-Foam are embedded in the assessments of NRG-Panels and are not presented separately. The following sections provide details for each of the depicted stages.

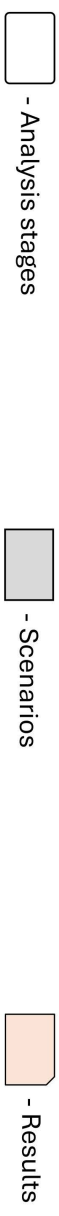
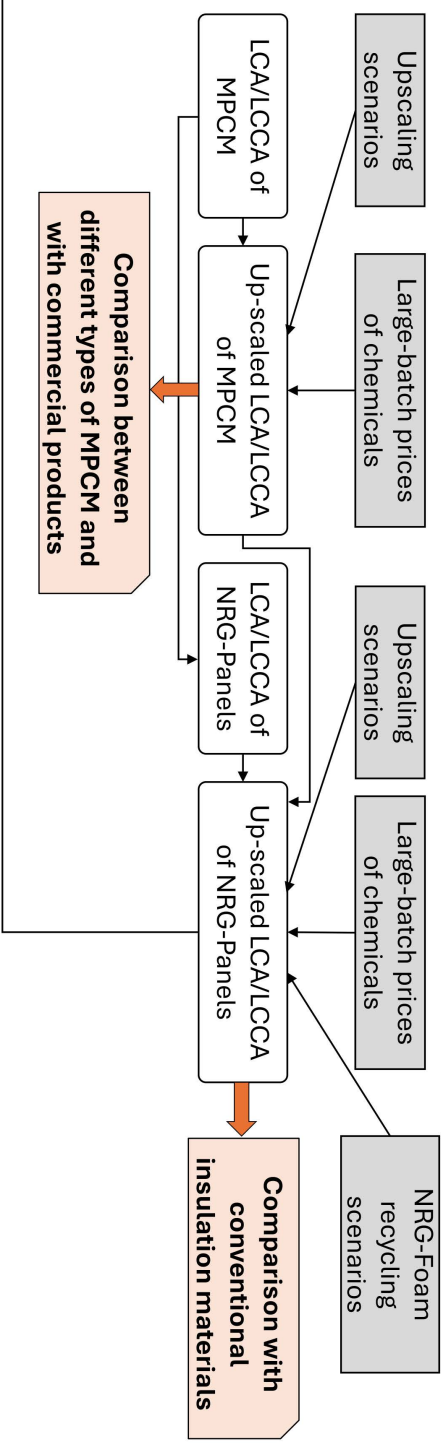


Figure 4.1: Overview of the methodology.

4.2.2 LCA/LCCA of microencapsulated phase change materials

A general approach to the data collection and modelling of the microencapsulated phase change materials production system can be found in Chapter 2 of the dissertation. The only major change in the methodological approach in this chapter is the use of a different LCA impact assessment method. In Chapter 2, the ILCD 2011 Midpoint+ impact assessment method [76] has been used, while this chapter utilises the Environmental Prices (EP) method [137], which itself is based on the ReCiPe Midpoint method [138]. There are two main reasons for switching to the EP method. First of all, the conversion of all of the different units across multiple impact categories to a single one (euro) allows for easier comparison of impacts between individual processes. Consequently, it is possible to identify the most impactful processes and prioritise between them when it comes to the development of upscaling scenarios and impact reduction measures. Secondly, the development of the material always includes multiple stakeholders and actors with different backgrounds. The native units in which environmental impacts are measured might be too complex and hard to understand for a diverse public. This, in turn, can result in problems with providing a judgment and making decisions when it comes to the development of the material. The monetary equivalent is a unit that does not require an explanation and simplifies the interpretation of the results.

4.2.3 Up-scaled LCA/LCCA of microencapsulated phase change materials

Since the production of MPCM within the NRG-STORAGE project has only been happening on a small, laboratory scale, it is not possible to straightforwardly compare the environmental and cost performance of MPCM developed during the project with the products available in the market. This is due to the fact that the cost and environmental impacts in this case will be overestimated and are not representative of large-scale production. At the same time, the products already available in the market are ahead on the development curve and are manufactured in much larger quantities, allowing for lower costs and higher production efficiency. To enable a fair comparison, it is necessary to bring the assessments of a novel product and its mass-produced counterpart to the same TRL.

Since it is not possible to make such an instantaneous jump from lab-scale production to mass production physically, this up-scaling relies on scenarios. The up-scaling scenarios are developed based on the lab-scale assessment and use environmental and economic hotspots identified within the lab-scale production process as the starting point. More specifically, all the unit processes within the overall production chain of MPCM are ranked based on their contribution to the overall impacts and the ones on top are considered to be the hotspots. Consequently, scenarios are developed that allow for the

reduction of those impacts and the elimination of the identified hotspots. For example, if some chemical is shown to have a very large contribution to the overall environmental/economic impacts, we might consider some ways of reducing the volume needed for the production or using a functional replacement with lower impacts. This process of hotspot identification and scenario development is iterative and is generally continued until the overall impacts are more homogeneously spread around all the contributors. It is worth noting that such a homogeneous distribution of impacts is not always possible since certain production processes may possess inherent qualities that prevent that. For example, some processes are energy-intensive by their physical nature and in that case, energy use will always be the largest contributor to the overall impacts. Nonetheless, a homogeneous distribution of impacts can be considered as a general target for scenario creation.

While the abovementioned approach is applicable to both LCA and LCCA, in the case of LCCA and economic impacts up-scaling is also done by collecting large-batch prices for the chemicals and products used in the production process. The up-scaled price information is mostly collected by project partners via inquiries to suppliers, as well as based on market research. In some cases, the price projection is used, which is based on communication with industry specialists and their expectations of the market development in the future.

Guided by the approach described above, the MPCM production process has been assessed, and multiple scenarios have been developed for up-scaled LCA/LCCA. Two types of MPCM have been considered and modelled: inorganic coacervate MPCM (IC MPCM) and melamine-formaldehyde MPCM (MF MPCM). Those two types differ in the encapsulation process used and, consequently, the final composition of the shell. While most of the up-scaling scenarios are applicable to both IC MPCM and MF MPCM, there are some differences in their implementation. Further, some up-scaling scenarios are impacting both, the environmental and cost performance of MPCM, while others are focused specifically on one of the aspects. Table 4.1 provides an overview of the up-scaling scenarios implemented alongside their aim and applicability scope.

Table 4.1: Up-scaling scenarios for MPCM production process.

ID	Description	Applied to IC MPCM	Applied to MF MPCM	Reduces environmental impacts	Reduces economic impacts
M1	Producing MPCM in the form of a slurry instead of a dry powder	x	x	x	x
M2	Using an industrial-grade large-scale disperser and homogeniser	x	x	x	x
M3	Using fatty acid methyl esters produced from waste cooking oil as the core material	x	x	x	x
M4	Using large-batch prices of materials	x	x		x
M5	Using gelatine produced from bone using one-step biocatalysis	x		x	
M6	Using gelatine with a lower melting temperature	x		x	x

The sections below provide more detailed information on each of the up-scaling scenarios.

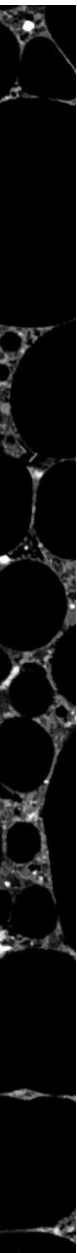
Scenario M1. Producing MPCM in the form of a slurry instead of a dry powder

The original MPCM production system (described in more detail in Chapter 2) included a spray drying step at the end of the production process. When NRG-Panels were produced by RÖSER Ingenieurbeton GmbH (further, RIB), MPCM was obtained and used as a dry powder as well. However, MPCM can also be produced and used in the form of a slurry. While storing and transporting dry powder MPCM is generally easier than MPCM slurry, the latter has much lower environmental impacts and lower production costs due to dramatically reduced electricity consumption: lab-scale assessments have shown that electricity use for the drying step of MPCM production was the largest hotspot within the production process. Furthermore, during the manufacturing of NRG-Panels, it has been observed that dry MPCM can cause



issues when it comes to mixing it into a cementitious paste. Finally, the MPCM drying step was essentially unnecessary since at the stage of cementitious paste preparation, water needed to be added again to reach the target water-to-binder ratio (w/b ratio of 0.4 has been used in the final mix design). Yet, this water demand could have been fully or partially covered by the water contained in the MPCM slurry. Due to the aforementioned observations, the production of MPCM in the form of slurry can be seen not only as an up-scaling scenario but also as a necessary next step in the development of NRG-Foam and NRG-Panels. The production system should thus be modified to remove the drying step.

4



In a modified production system without the drying step, the slurry that comes directly out of the production system has a fixed solids-to-water ratio that depends on the technological processes used in the production. In our case, the solid content of IC MPCM slurry coming out of the Inorganic shell deposition step is 12.7% while for MF MPCM slurry coming out of the Polymerisation step is 25.1%. Depending on the final application of the slurry, it might be needed to concentrate it to achieve a higher solid-to-water ratio. In our particular case, the slurry is intended to be used in the production of NRG-Foam with 10% MPCM particles by volume in the paste. Based on the final mix design (it can be found in Table 4.4 below), per 1 m³ of NRG-Foam 10.19 kg of MPCM and 57.72 kg of water should be added to the mix. This requirement can be satisfied by using 67.91 kg of slurry with 15% solid MPCM content. Having 15% of solid content as a target, it can be observed that MF MPCM slurry is concentrated enough (and some extra water will need to be added), but IC MPCM has too high a water content.

Higher solid-to-water ratios can be achieved using a variety of techniques, such as centrifuging, sieving or evaporation. For our specific application, a route that utilises IWE HP DRY industrial evaporator [139] has been chosen. Those evaporators have high efficiency, large capacity and have been proven to work well for the given application. The final production system, thus, includes an evaporation step for IC MPCM slurry where the solid content is raised from 12.7% to 15% at the evaporation rate of 40 l/h with the efficiency of 0.25 kWh/l of water evaporated (in accordance with the specifications of the chosen evaporator [139]). In the case of MF MPCM slurry, no evaporation step was necessary since its initial solid content was already higher than 15%. The final MPCM slurry production system is shown in Figure 4.2.

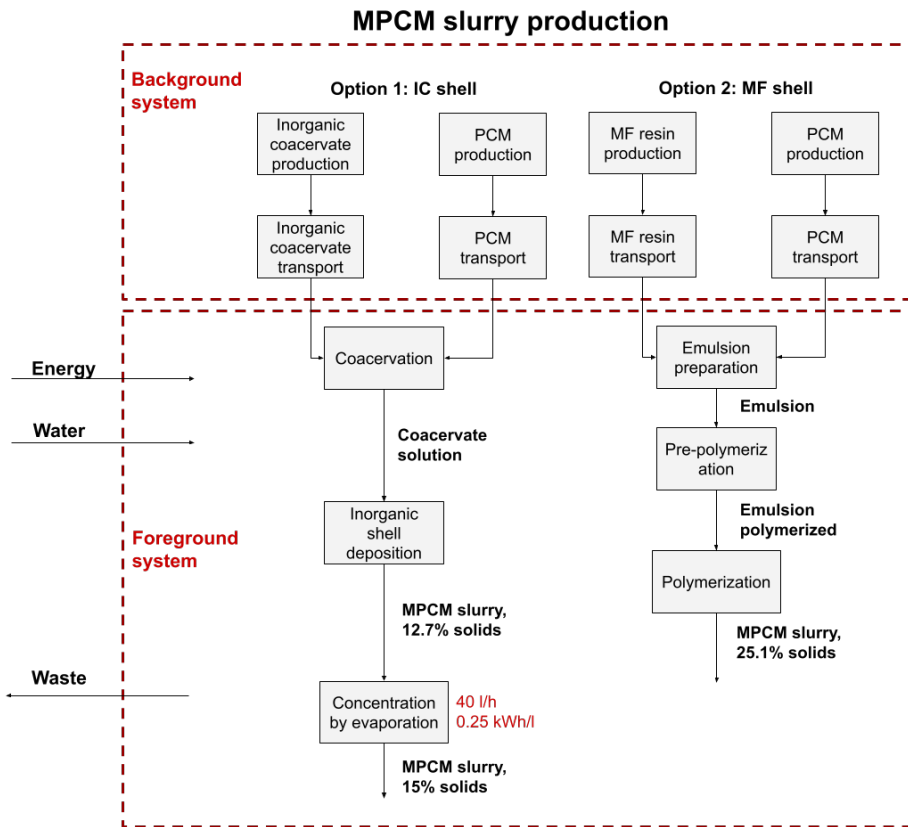


Figure 4.2 Final MPCM slurry production system.

Scenario M2. Using an industrial-grade large-scale disperser and homogeniser

The original MPCM production system was built based on lab-scale production runs by the project partner Sphera Ecapsulation (SE) and scientific literature, which, in turn, is also relying on small-volume laboratory experiments. Due to that, the size of the batches and the capacity of the equipment used in the production are very small, and, as a consequence, the efficiency of the processes per unit of output is low. More specifically, the production of both types of MPCM requires intensive dispersion and/or homogenisation of chemical components during all the steps of the production chain. Lab-scale dispersers and homogenisers have much lower capacity than industrial-grade ones, but their energy consumption is not proportionally lower. Therefore, switching the production from lab-scale dispersers and homogenisers to large-scale ones could result in greatly reduced energy consumption per kg of MPCM output. This switch would lead to reduced environmental impacts as well as lower production costs.

In this scenario, the model of the production system has been up-scaled by assuming that the production of MPCM happens in large batches using

ELE EBJ/XD-500 disperser [140] and GEA Ariete 5400 homogeniser [141]. The choice of equipment has been made based on the experience of SE and the fact that this equipment has already been successfully used for similar applications. Based on the specifications of the abovementioned equipment as well as the process requirements for dispersion and homogenisation, up-scaled energy consumption has been calculated for every step of the production process. This energy consumption has been assumed to consist of the following components:

- The energy needed for heating the chemicals from room temperature to the operating temperature (in case of the first production step) or from one operating temperature to the next operating temperature (in case the next step in the production requires needs higher temperature)
- The energy needed to keep the temperature at a constant value, compensating for heat losses
- Energy for dispersion
- Energy for homogenisation

All of those energy requirements were calculated and added together for each of the production process steps. Table 4.2 below provides an overview of the final scenario values that were used in the model. The energy requirement is provided per litre of working solution.

Table 4.2: Overview of the final parameters of Scenario M2.

Step	Operating temperature, °C	Dispersion time, h	Energy required, Wh/l	Homogenisation required?
IC MPCM				
Coacervation	35	3	156.6	Yes
Inorganic shell deposition	35	2	91.8	No
MF MPCM				
Emulsion preparation	50	0	44.9	Yes
Pre-polymerisation	70	1	79.1	No
Polymerisation	80	4	233.9	No

Scenario M3. Using fatty acid methyl esters produced from waste cooking oil as the core material

Initially, one of the aims of the NRG-STORAGE project was to use bio-based MPCM in the manufacturing of NRG-Foam. Such MPCM would have a core made of bio-based PCM (e.g., fatty acids) and a shell made of inorganic coacervate. However, due to technical difficulties, the final foam and the panels used in the demonstrator buildings in Sofia were produced based on MF MPCM with the paraffin-based core. Nevertheless, in both cases, the production of PCM would require raw materials and inevitably have quite

significant environmental impacts, which has also been observed in the initial lab-scale LCA. One of the prospective ways of reducing those impacts is using PCM produced from waste. In this scenario, PCM produced from raw materials has been substituted with PCM based on fatty acid methyl esters (FAME) produced from waste cooking oil [142], [143], [144].

For the LCA model, this scenario has been implemented by using “*treatment of waste cooking oil, purified, esterification / fatty acid methyl ester / Cutoff, S*” process as a representation of PCM produced from waste cooking oil. The environmental profile of this process is available from the ecoinvent database [75]. For LCCA, the price of FAME produced from waste cooking oil has been assumed to be 2 EUR/kg. This is sufficiently lower than the current price level of PCM available on the market. The quoted large batch prices of commercial PCM that were collected by SE ranged from 4.4 to 7 EUR/kg for bio-PCM and from 6.6 to 12.2 EUR/kg for paraffin-based PCM. However, 2 EUR/kg is a prospective price that has been communicated by industry specialists as an achievable target within the next seven years.

Scenario M4. Using large-batch prices of materials

In the lab-scale LCCA, the prices of materials used in the production of MPCM have been mostly collected from the lab supplier Sigma-Aldrich/Merck [70]. While very useful for lab-scale assessment, those prices are not representative of large-scale production. It is possible to find much lower prices at the wholesale and large-batch industrial suppliers. Furthermore, the high price of chemicals at Sigma-Aldrich is also caused by the lab-grade purity of those chemicals that might be excessive for real-world large-scale production.

For this scenario, SE collected large-batch prices of all chemicals used in the manufacturing of IC and MF MPCM and those prices were then used in the up-scaled LCCA. Table 4.3 lists those prices alongside the name of the supplier.

Table 4.3: Large-batch prices of chemicals used in MF MPCM production.

Chemical	Supplier	Price, EUR/kg
MF 60% solution	Ottokemi	18.59
PVA	Tradicon GmbH	3.59
Formic acid	Perstorp Group	0.65
Ammonium chloride	RUBIN KIMYEVI MADDELER SAN TİC.LTD.ŞTİ	0.54

Scenario M5. Using gelatine produced from bone via one-step biocatalysis

When conducting lab-scale LCA of IC MPCM production, it was found that in the ecoinvent database, there is no dataset available for gelatine. The production of gelatine and its associated impacts have then been modelled based on the paper by Ma et al. [145]. In the paper, two ways are described: the conventional method and the environmentally-friendly method based on

one-step biocatalysis. In the original lab-scale LCA of MPCM, the conventional method has been used. For this up-scaling scenario, the alternative environmentally-friendly method has been modelled, integrated into the LCA model, resulting in a substantial effect on the overall environmental performance of IC MPCM. This scenario is only applied to LCA, and the price of gelatine has been considered to be the same, no matter the production route.

Scenario M6. Using gelatine with a lower melting temperature

The operating temperature at which coacervation and inorganic shell deposition are taking place is, to a large extent, determined by the melting temperature of the gelatine used. The operating temperature should not be lower than the melting temperature of the chosen gelatine. In the original lab-scale LCA, the required operating temperature was 40°C. In this up-scaled scenario, gelatine with a lower melting temperature has been used, allowing for a reduction in the operating temperature to 35°C. This leads to lower energy use and, consequently, reduced environmental impacts and costs. It is worth mentioning that energy requirement values in Scenario M2 have been calculated based on a 35°C operating temperature, thus taking this scenario into account.

4.2.4 LCA/LCCA of NRG-Panels

The initial lab-scale LCA/LCCA of NRG-Foam presented in Chapter 2 has been based on the originally envisioned NRG-Foam mix design and lab-scale LCA/LCCA of MPCM. While those initial mix designs had 20% MPCM by paste volume, for the actual production of prototype NRG-Panels for application in the demonstrator buildings in Sofia, the amount was reduced to 10%. This change was due to technical complications in the production of NRG-Foam with a higher load of MPCM. Furthermore, NRG-Panels with reduced graphene oxide (rGO) were only manufactured as test samples and late in the project. This chapter, therefore, is focused on a single mix design of NRG-Foam that is representative of the final panels installed in the demonstrator buildings in Sofia. The details of this mix design are provided in Table 4.4 below.

Table 4.4: Final NRG-Foam mix design containing 10% of MPCM by the volume of the paste and with a water-to-binder ratio of 0.4.

Mass of components to produce 1000 dm³ of NRG-Foam:		
Binder		
Portland cement CEM I 52.5 R	124.85	kg
Metakaolin	19.47	kg
Additives and Water		
MPCM	10.19	kg
Hardening accelerator	2.89	kg
Superplasticiser	0.72	kg
Stabiliser	4.17	kg
Water (for w/b)	57.72	kg
Resulting properties of NRG-Panels and components		
Paste in foam with PCM	209.81	kg
Foam (w/b) (2.0% foam agent)	60.86	kg
Aqueous foam density	70.00	kg/m ³
Calculated density (wet paste)	1684.67	kg/m ³
Calculated density (wet foam)	280.86	kg/m ³
Cured density	220.00	kg/m ³

To produce NRG-Panels from NRG-Foam, two more components are required: reinforcement mesh and moulds for casting the panels. The reinforcement mesh that has been used in the production of the panels at RIB was Caparol Gewebe 650 – glass fibre reinforced plastic mesh with a surface density of 165 g/m². The amount of reinforcement mesh required to produce 10 m² of 10 cm thick panels (corresponding to 1 m³ of NRG-Foam) is 3.3 kg. The moulds used in the production at RIB were made of plywood and could only be used five times before they needed to be replaced. Taking this into account, the required amount of wood material was estimated to be 0.0074 m³ per 10 m² of 10 cm thick panels produced. The production losses were estimated to be around 10% of the volume of NRG-Foam. Finally, the production of 1 m³ of NRG-Foam generates 1.16 kg of waste sludge and 78.36 l of waste water (water that is used for foam generation and water for cleaning the equipment). All those values were used for building the initial LCA/LCCA of NRG-Panels.

4.2.5 Up-scaled LCA/LCCA of NRG-Panels

In the up-scaling of LCA/LCCA of NRG-Panels, the same general approach as already described in Section 4.2.3 is followed. In addition to scenarios of production process up-scaling, compared to the cradle-to-gate assessment of NRG-Foam presented in Chapter 2, the assessment of NRG-Panels has also been expanded to include End of Life (EoL) and Benefits Beyond End of Life (BBEoL) stages in accordance with the framework described in the EN 15804

standard [146]. The assessment of EoL and BBEoL life cycle stages of NRG-Foam is based on the recycling experiments conducted by the project partner Silesian University of Technology (SUT) and has been included as an extra scenario below. Table 4.5 provides an overview of all the scenarios that were developed and implemented.

Table 4.5: Up-scaling and recycling scenarios for NRG-Panels production.

ID	Description	Reduces environmental impacts	Reduces economic impacts
P1	Substituting CEM I cement with CEM III/C cement having high content of blast furnace slag	x	
P2	Reduction of production losses from 10% to 5%	x	x
P3	Using reinforcement mesh with reduced environmental impact	x	
P4	Using steel moulds that can be reused at least 100 times	x	x
P5	Using large-batch prices of materials		x
P6	Recycling scenarios for NRG-Foam and NRG-Panels	-	-

Each of the scenarios is described in detail in the sections below. While not included in the table as a scenario, up-scaled LCA/LCCA of NRG-Panels uses the data from up-scaled LCA/LCCA of MPCM.

Scenario P1. Substituting CEM I cement with CEM III/C cement having a high content of blast furnace slag

The panels produced for inclusion in the demonstrator buildings in Sofia used CEM I cement as the main component of the cementitious foam. It is well known, however, that ordinary Portland cement has high environmental impacts. The effect of those high impacts has also been observed when conducting the initial LCA of NRG-Foam: cement has been one of the largest contributors to the overall environmental impacts. This scenario has been developed to tackle the abovementioned issue and replaces CEM I cement with CEM III/C cement. CEM III/C is a more environmentally-friendly alternative to ordinary Portland cement and contains around 90% of blast furnace slag. Such cement has significantly lower environmental impacts due to the greatly reduced content of clinker and lower production energy demand.

In order to implement this scenario in up-cycled LCA of NRG-Panels, “market for cement, blast furnace slag 81-95% / cement, blast furnace slag 81-95% / Cutoff, S” dataset from ecoinvent database has been used instead of “market for cement, Portland / cement, Portland / Cutoff, S”. Those datasets contain averaged environmental profiles of CEM III/C and CEM I

correspondingly. While some variations are possible, the price of CEM III/C on the market is generally similar to the price of CEM I. Consequently, this substitution does not affect LCCA.

Scenario P2. Reduction of production losses from 10% to 5%

As mentioned before, the production losses of NRG-Foam during the production of NRG-Panels were estimated to be around 10%. Those losses were mostly coming at the beginning of every manufacturing run since all the production parameters (foam consistency, paste consistency, water content, etc.) needed to be tuned in before panels could be cast. However, when producing the panels at a larger scale and with more production experience accumulated, those losses can be greatly reduced. For this scenario, it is assumed that the losses would be reduced to 5% - a realistic target based on the manufacturing experience of RIB. Improved efficiency of the production process has a positive effect on both the environmental and economic performance of NRG-Panels.

Scenario P3. Using reinforcement mesh with reduced environmental impact

The reinforcement mesh used in the production of NRG-Panels is made of polymer-coated glass fibre and can be produced in multiple ways. In the small-scale LCA of NRG-Panels, it was assumed that the reinforcement mesh is produced using injection moulding, and the corresponding dataset from the ecoinvent database has been used. Injection moulding, however, has relatively high environmental impacts.

In this scenario, reinforcement mesh has been assumed to be produced using a hand lay-up method that has lower environmental impacts. It has been done by using *“market for glass fibre reinforced plastic, polyester resin, hand lay-up | glass fibre reinforced plastic, polyester resin, hand lay-up | Cutoff, S”* dataset of the ecoinvent LCA database instead of *“market for glass fibre reinforced plastic, polyamide, injection moulded | glass fibre reinforced plastic, polyamide, injection moulded | Cutoff, S”*. The substitution is only influencing the environmental impacts of NRG-Panels and the costs of the two types of reinforcement mesh were assumed to be the same.

Scenario P4. Using steel moulds that can be reused at least 300 times

Due to the relatively short timeframe of NRG-STORAGE project and the low required production volumes of NRG-Panels for the project, RIB decided to make the moulds for casting of NRG-Panels from plywood. Such moulds are quicker and easier to manufacture, yet they have a rather short lifespan and can withstand only five castings before they need to be replaced. Such frequent replacement leads to excessive use of raw materials and, consequently, high environmental impacts and costs. As an alternative, there are other types of moulds available on the market that could be used for a much longer time. Those include steel moulds and polymer (e.g., HDPE) moulds.

In this up-scaling scenario, the wooden moulds were substituted with steel ones that are assumed to be used 300 times before they need to be

replaced (in reality, the effective number of uses can be even larger than that). With this assumption, the amount of steel needed to produce 10 m² of 10 cm thick NRG-Panels has been estimated to be 2.4 kg. The price of steel moulds has been taken at 24.5 EUR/m².

Scenario P5. Using large-batch prices of materials

Up-scaled LCCA of NRG-Panels relies on large-batch prices of components. Those prices are presented in Table 4.6 below.

Table 4.6: Large batch prices of NRG-Panel components.

Component	Price
Cement	150 €/t
Metakaolin	228 €/t
Accelerator	3.32 €/kg
Superplasticiser	1.58 €/kg
Stabiliser	2.93 €/kg
Water	5 €/m ³
Foaming agent	6,16 €/kg
Reinforcement mesh	0.25 €/m ²
Steel moulds	24.5 €/m ²
Electricity	0.3 €/kWh

As mentioned before, the price of MPCM has been taken from the up-scaled LCCA of MPCM (see Sections 4.2.2 and 4.2.3). However, for reference, the quoted large-batch price of Nextek 24D was 9.8 EUR/kg.

Scenario P6. Recycling scenarios for NRG-Foam and NRG-Panels

To cover the whole life cycle of NRG-Foam/NRG-Panels, it is important to understand how the material will be dealt with at the end of its service life. Since it is a novel material, this stage can currently only be based on scenarios. In this chapter, the LCA of NRG-Panels recycling is built based on the experiments conducted by SUT. Detailed information on those experiments and the results can be found in the publication by Klemczak et al. [147], and this section will only provide a short overview of it.

The recycling experiments were focused on producing recycled foam concrete powder (RFCP) from NRG-Foam to use it as a substitute for ordinary Portland cement (OPC) in mortars. Three different approaches to RFCP production have been investigated: Crushing, Crushing + Grinding and Crushing + Heat treatment. Those three methods differ in the size of the particles produced, process yield and required energy. Table 4.7 provides an overview of the RFCP production methods and their corresponding parameters.

Table 4.7: RFCP production methods.

Name	Particle size, mm	Yield	Energy requirement, kWh/kg
Crushing	<0.125	40%	0.086
Crushing + Grinding	<0.063	90%	0.461
Crushing + Heat treatment	<0.125	29%	4.286

It has been observed that mortars prepared with 20% of RFCP produced using any of the abovementioned methods fit the requirements defined in EN-196-1 [148] for CEM 42.5. This demonstrates the potential of using RFCP as a partial substitute for OPC in the production of CEM II/A-F 42.5. From the perspective of LCA, this means that at the end of its service life, NRG-Panels could be recycled, and the RFCP produced from those waste panels could replace some of the raw primary OPC used in construction. Consequently, if the environmental impacts of RFCP production are lower than those of OPC production, using RFCP instead of OPC in mortars will have a positive environmental impact. It is important to mention here that RFCP is not replacing OPC at a 1:1 ratio. Instead, the substitution rate is 20% according to the experiments conducted so far. Nonetheless, even at this substitution rate, it is expected that there will be some environmental benefits since the production of OPC from raw materials is very energy-intensive.

Since the recycling experiments were conducted for NRG-Foam, there are two important modifications that have to be made for conducting the upcycled LCA of NRG-Panels. First of all, the recycling experiments did not take into account the reinforcement mesh that is present in NRG-Panels but absent in the case of NRG-Foam. This reinforcement mesh also needs to be recycled. Since there is no dataset specifically for the recycling of reinforcement mesh available in ecoinvent, a generic dataset for plastics recycling has been used: *“market for waste plastic, mixture / waste plastic, mixture / Cutoff, S – BG”*. Secondly, within Scenario P1 presented above, CEM I has been replaced by CEM III/C. Due to that, it is expected that RFCP produced from such panels based on CEM III/C would not be a substitute for primary OPC but for the primary production of CEM III/C. In other words, our avoided product will be CEM III/C. As there is no experimental data available for the recycling of such foams, the same 20% substitution rate is assumed as in the case of OPC, which has been discussed above.

Since the goal is to compare the performance of NRG-Panels with conventional insulation materials, the data for the end of life and benefits beyond end of life for a conventional insulation material is also required. In our particular case, EPS is used in one of the demonstrator buildings, and it has thus been chosen for the comparison. When it comes to the recycling of EPS, it can be incinerated to produce heat and electricity, and this produced energy would substitute the energy originating from other sources. The data for assessing the impacts and benefits of EPS recycling has been taken from the ecoinvent database. According to that data, the burning of 1 kg of EPS

generates 4.08 MJ of electricity and 7.88 MJ of heat. It is assumed that this energy substitutes primary production. For the environmental impacts of primary heat and electricity production, average European data has been used.

The results of NRG-Panels' recycling modelling and comparison with EPS can be found in Section 4.3.2.

4.2.6 Demonstrator buildings description

To test the performance of NRG-Panels in the real-world environment and compare it with ordinary insulation materials, three demonstrator buildings were built by the project partner Glavbolgarstroy (further, GBS) in Sofia, Bulgaria. Figure 4.3 shows the location as well as the external view of the finished buildings.

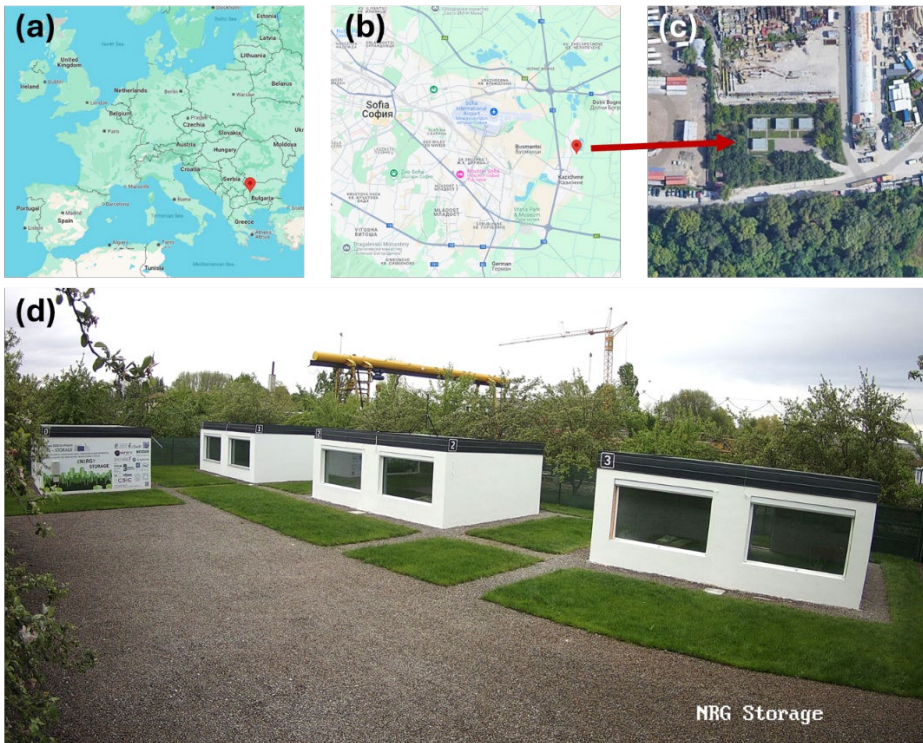


Figure 4.3: The location (a) and (b), satellite image (c) (from Google Maps [149]) and photograph (d) (from the web camera installed by GBS to document the project) of the demonstrator buildings.

As can be seen from the satellite image and the photo, there are in total four buildings at the site. Building 1 (the farthest one on the right in the photo in Figure 4.3) is a reference building that has EPS insulation in its walls. Building 2 (in the middle) is identical to Building 1 but includes NRG-Panels

instead of EPS. Building 3 (the closest in the photo) is similar to Building 2 and also has NRG-Panels as an insulation layer, but is further equipped with a rolling blind on the western wall. The rolling blind has been installed to test the performance of active application of NRG-Foam, where its performance can be dynamically altered by changing the amount of solar radiation hitting the wall. In addition to those three demonstrator buildings, there was also a technical Building 0 (on the left side in the photo) that hosted all the necessary IT equipment for the control and monitoring of buildings' performance.

The design of the demonstrator buildings is based on the BESTEST 900 building model – one of the case models of a small single-room case building with heavy walls and floor that has been originally developed by the International Energy Agency (IEA) for testing of building energy simulation software [126]. As such, BESTEST 900 is not an actual building but a digital representation of a concept building. Consequently, the actual demonstrator buildings have similar geometry and orientation but are significantly different when it comes to all other parameters. Figure 4.4 provides a schematic representation of the demonstrator buildings, including the physical dimensions as well as the material layers used within the building envelope.

More detailed information on the materials used in the demonstrator buildings, the total volumes and prices of those materials, as well as the details of the computational models of the buildings, is provided in the following sections.

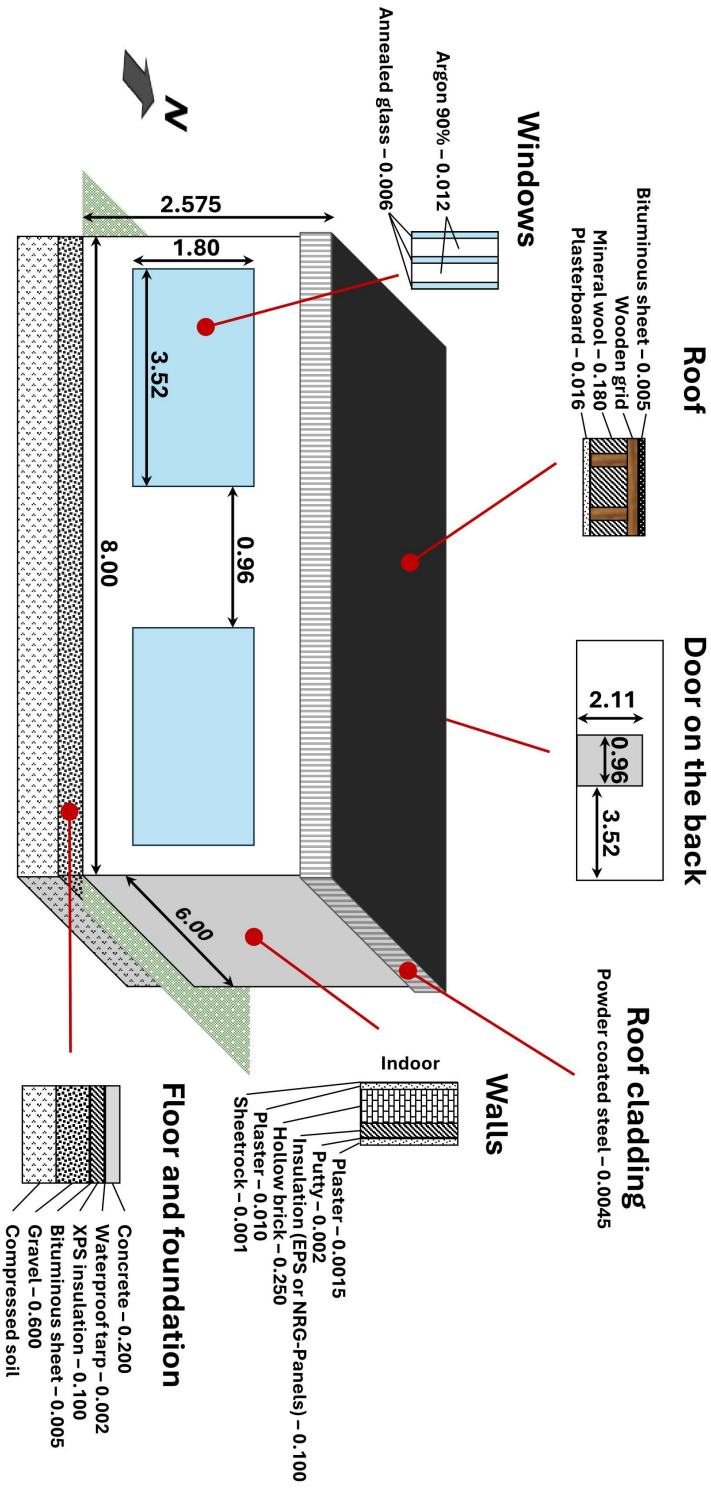


Figure 4.4: Schematic diagram of the demonstrator buildings. All of the measurements are provided in metres.

4.2.7 Building-level LCA/LCCA

The modelling of the environmental and economic performance of demonstrator buildings in Sofia follows the guidelines described in standards EN 15978 [150] and EN 15804 [146]. In the standards, the lifecycle of a building is divided into four stages: Product, Construction Process, Use, End of Life. Each stage consists of several modules. In addition to building life stages, there is also Module D that provides information on the benefits beyond the building life cycle, such as benefits from reuse, recycling or energy recovery of building materials and components. The information in Module D is provided separately from the rest of the assessment and the impacts (or benefits) calculated in Module D are not added up to those calculated for the life cycle of the building (stages A-C). Figure 4.5 below shows the overview of all the stages covered by the LCA of buildings according to EN 15978.

The building-level LCA/LCCA presented in this chapter considers all the stages of the life cycle of demonstrator buildings in Sofia. However, in the use stage, only module B6 is included. Modules B1-B5 are not included due to the uncertainty and lack of data on the direct emissions, maintenance, repair, replacement, and refurbishment of NRG-Panels. To add those modules, a prolonged testing of NRG-Panels and their real-life durability and performance is necessary. Module B7 has been omitted since the purpose of the demonstrator buildings is the comparison of EPS and NRG-Panels, and operational water use plays no role in it.

As already mentioned, LCA and LCCA were conducted for two of three demonstrator buildings: Building 1 (with EPS insulation) and Building 2 (with NRG-Panels insulation). Building 3 has not been included since the aim of the assessment is a comparison between the performance of NRG-Panels and conventional insulation materials. Buildings 1 and 2 are identical beyond the insulation material used, which makes it possible to compare them straightforwardly: the observed difference in the performance of the buildings, in this case, is a direct consequence of the differences in the performance of the corresponding insulation materials.

The sections below go over each of the stages in more detail.

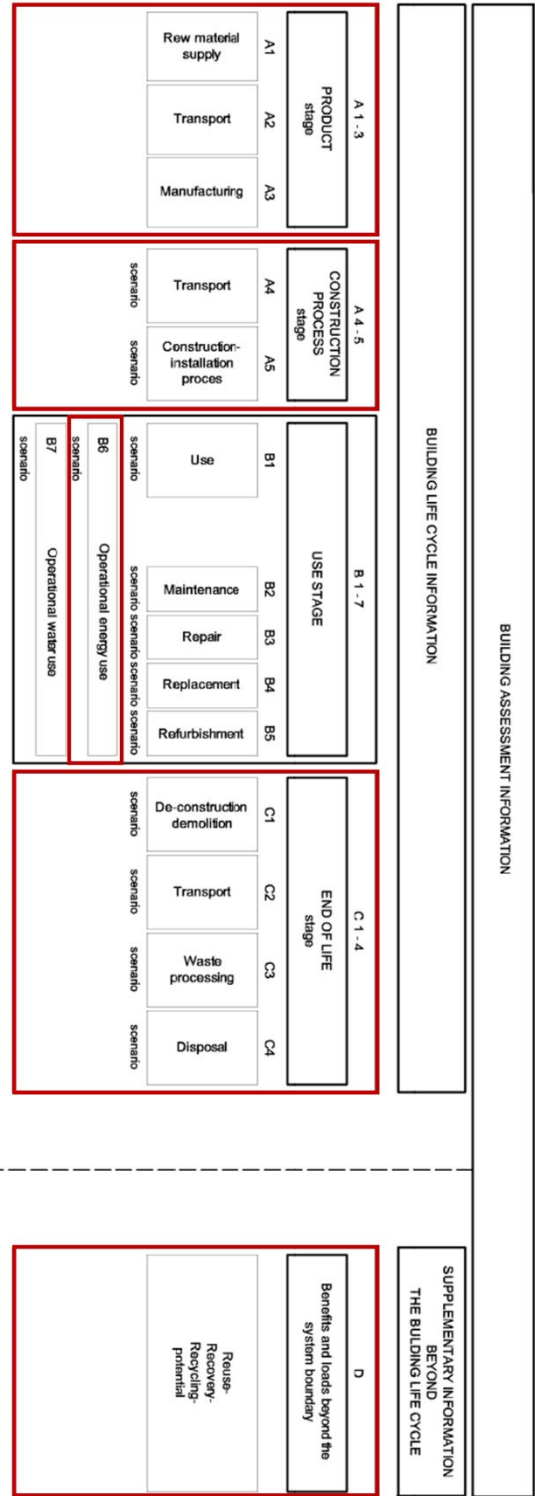


Figure 4.5: Life cycle stages of a building covered in building-level LCA [150]. Red frames highlight the stages that are covered in this work.

Product stage

The product stage of the life cycle of a building includes the environmental impacts and costs of all materials and components used in the construction of the building. From the LCA perspective, it includes the downstream environmental impacts from the manufacturing of all of the materials in the building's bill of materials (BOM). The supply chain starts with raw material supply and ends with the manufacturing of the final construction materials (to clarify, "raw materials" refers to basic materials such as wood, ore, coal, etc. and "construction materials" are final products made of those basic materials). The BOM for the demonstrator buildings has been provided by GBS and has been used as a foundation for LCA/LCCA of this stage. For LCCA, the prices of all materials were also provided by GBS. For LCA, each material in the BOM has been matched with a fitting dataset in the environmental database ecoinvent. For NRG-Panels, the cost data has been taken from the up-scaled LCCA and the environmental impacts from the up-scaled LCA, both of which were described in the preceding sections. The table with all the materials used in a single demonstrator building, as well as the volumes and prices of the materials, can be found in Table B1 of Appendix B.

Construction process stage

The construction project stage was modelled based on the data provided by GBS and includes the use of the construction equipment for LCA and the costs of site preparation, construction works and transportation costs for LCCA. For LCA, the machinery usage in hours has been provided by GBS (for all four buildings combined). Based on this data, as well as estimates of hourly fuel consumption for each of the machines, the environmental impacts were calculated based on the total emissions from the burning of diesel in an engine. Table 4.8 provides an overview of the estimated fuel consumption for each of the machines as well as the total per building.

Table 4.8: Overview of construction equipment fuel consumption for LC.

Equipment name	Equipment utilisation, hours	Fuel consumption, l/h	Total fuel consumption for all four buildings, l
Mixer	40	1.1	45.4
Excavator	40	11.4	454.2
Combined excavator	16	11.4	181.7
Dumper	16	5.7	90.8
Loader (Bobcat)	40	5.7	227.1
Rummer	24	5.7	136.3
Concrete pump	11	1.1	12.5
Autocrane	40	13.2	529.9
Total fuel consumption per building, l			419.5

For LCCA, GBS provided an overview of the construction costs incurred during the construction process. Those costs were documented by GBS for all four buildings combined. Since the buildings are essentially the same, the cost per building has been taken as $1/4^{\text{th}}$ of the overall costs. Those costs can be found in Table 4.9.

Table 4.9: Overview of construction costs for LCCA.

Costs category	Cost for 4 buildings, EUR
Site preparation and excavation works	4 575
Construction works	74 237
Transportation costs	35 789
Total costs	114 601

Use stage

The use stage of a building can include multiple parts related to building maintenance and the use of resources (water, electricity, gas, etc.). In this analysis, only electricity consumption within the use stage is considered. All electricity consumption in demonstrator buildings comes from HVAC units used for heating and cooling. All of the buildings have the same HVAC system installed, which includes two internal Daikin FTXM35R and two external Daikin RXM35R units [151] that can work for heating or cooling. The overall heating capacity of this configuration is 10.4 kW for heating and 8 kW for cooling for each of the buildings.

While there were sensors installed in the building that allowed to monitor the energy consumption by HVAC, the assessments presented in this dissertation rely on building energy simulations instead. There are several reasons for this. First of all, HVAC in the buildings has only been operating for several months over the whole period of monitoring and the rest of the time the units were off. This has been done to monitor the temperature and heat flows in the buildings to analyse the effect of insulation on the indoor climate. There is, thus, not enough energy measurement data. Furthermore, even if there will be energy monitoring data spanning over the whole year, the usability of this data for LCA/LCCA is still questionable. The reason for that is that LCA/LCCA is conducted over the whole life cycle of a building, which is normally assumed to be 50 or 60 years, but a single year of energy consumption data is not representative of the whole analysed timeframe. For this reason, LCA/LCCA normally rely on energy simulations that are based on so-called typical meteorological year (TMY) weather data [152]. TMY provides weather data for a given location that is averaged for a long period of time, normally around 15-20 years. This ensures that energy consumption estimations are not influenced by possible outliers present in single-year weather. In other words, TMY-based simulations are more representative of climatic conditions for a given location.

The energy simulations were performed in EnergyPlus software [95]. The building model for EnergyPlus simulations has been developed to represent the real demonstrator buildings as closely as possible. It is, however, not possible to make a carbon copy of the real-world building due to the uncertainty of some values or the unavailability of data. For example, thermal, solar and visible absorptance of plaster on the outer surface of the walls can have a significant effect on the overall energy consumption of a building. Yet, those properties are not obtainable via the producer's specifications and might depend on how the plaster is prepared and applied to an actual building. Furthermore, due to the manual nature of the construction process, the real-world buildings deviate from the architectural plans: there might be some air gaps, final thicknesses of materials might be different, etc. Those are just a couple of examples highlighting that a computer model of a building should only be treated as an approximation, and the modelled performance and the real-world performance would not necessarily be the same. Nonetheless, this possible deviation should not pose an issue for a comparative assessment of two materials in the context of a whole building as long as the same building model is used.

The final building models used in the assessments presented in this chapter were developed in cooperation with the project partner Centro de Investigación de Métodos Computacionales (CIMEC). The model includes all the necessary data for EnergyPlus to simulate the performance of the building over a single year and estimate the total energy consumption for heating and cooling. The key data necessary to be specified in the model file for EnergyPlus includes, but is not limited to:

- Building geometry
- Properties of all materials used in the building (thickness, thermal conductivity, density, specific heat, roughness, thermal absorptance, solar absorptance, visible absorptance)
- Construction of the building envelope (material layers for each of the walls, roof and ceiling)
- Parameters of the fenestration surfaces
- Parameters of the foundation
- HVAC parameters
- Ventilation and infiltration parameters
- Schedules for HVAC, occupancy, shading, etc.
- Parameters of thermal simulation algorithms

The geometry and the configuration of the building envelope that was used to build the model have already been presented in Figure 4.4. The parameters of the materials are shown in Table 4.10.

Table 4.10: Properties of materials used in demonstrator building envelope.

Construction	Material layer	Thickness, m	Thermal conductivity, W/mK	Density, kg/m ³	Specific heat, J/kgK	Roughness	Thermal absorptance	Solar absorptance	Visible absorptance
Walls	Plaster	0.01	0.47	1150	1000	Rough	0.9	0.4	0.4
	Insulation	EPS	0.1	0.04	15	1500	Rough	0.9	0.6
		NRG-Panels	0.1	0.06	174	1150	Rough	0.9	0.6
	Brick	0.25	0.31	500	900	Rough	0.9	0.6	0.6
	Gypsum-lime plaster	0.01	0.87	1750	1050	Rough	0.9	0.26	0.26
Roof	Bituminous sheet	Modelled as no-mass material with thermal resistance of 0.03 m ² K/W				Rough			
	Wooden board	0.015	0.17	550	2090	Rough	0.9	0.6	0.6
	Mineral wool	0.18	0.032	21	840	Rough	0.9	0.6	0.6
	Air buffer	Air gap with thermal resistance of 0.16 m ² K/W							
	Plasterboard	0.016	0.21	900	840	Rough	0.9	0.26	0.26
Floor	Gravel	0.6	0.6	1550	900	Rough	0.9	0.6	0.6
	Bituminous sheet	0.005	0.17	1100	1050	Rough	0.98	0.98	0.98
	XPS insulation	0.1	0.033	32	1500	Rough	0.9	0.6	0.6
	Waterproof tarp	0.002	0.17	600	1050	Rough	0.9	0.6	0.6
	Reinforced concrete slab	0.2	1.63	2400	960	Rough	0.88	0.6	0.6

Since NRG-Panels is a material that includes MPCM particles, in addition to the data presented in Table 4.10, it also requires the provision of supplementary information related to the properties of the embedded PCM to account for its dynamic properties and energy-storing capabilities. For the energy simulations in this chapter, two additional datasets were used and included in the model file for Building 2: temperature-enthalpy data pairs defining the enthalpy curve of PCM in the temperature range from -100°C to 100°C and temperature-thermal conductivity data pairs defining the variable nature of thermal conductivity of PCM. Those inputs were compiled based on the HFM testing of NRG-Panels conducted by the project partner Netzsch. Figure 4.6 shows those input data pairs in graphical form.

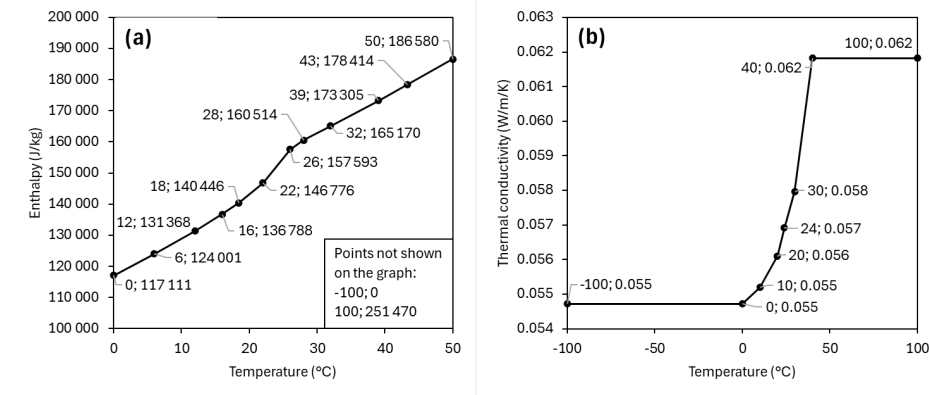


Figure 4.6: Enthalpy (a) and thermal conductivity (b) curves for NRG-Panels used in the demonstrator buildings.

The demonstrator buildings have two windows on the South-facing wall. The properties of the windows used as inputs in the model are taken from the datasheet provided by the supplier:

- U-factor – $0.7 \text{ W/m}^2\text{K}$
- Solar heat gain coefficient – 0.34
- Visible transmittance – 0.62

The foundation has been modelled as a Kiva foundation based on the architectural plans provided by GBS. Kiva is a tool built in EnergyPlus that is developed specifically to calculate heat losses and gains from a building foundation on a timestep basis using two-dimensional heat transfer calculations [153]. Using Kiva allows for more precise simulations of heat transfers between the building and the ground, but at the expense of increased building energy simulation times. The exact input parameters used to define the Kiva foundation can be found in Table B2 of Appendix B.

When it comes to the HVAC system, it has been modelled in EnergyPlus as an ideal loads air system that is a fitting option for mirroring the operation of thermostat-controlled air conditioners. The parameters of the system were specified based on the characteristics of the actual HVAC units installed in the demonstrator buildings: 10.4 kW of maximum sensible heating capacity and 8 kW of maximum sensible cooling capacity. The thermostat control setting for simulations has been set to dual setpoint mode with a 20°C heating setpoint and a 25°C cooling setpoint. The HVAC system was assumed to be always on. With those settings, the HVAC system will keep the temperature inside the demonstrator buildings between 20 °C and 25 °C at all times.

Apart from the above-mentioned, some other important model parameters to note include:

- The infiltration rate has been assumed to be 0.5 air changes per hour

- There is no occupancy
- There is an internal load of 200 W
- The conduction finite difference energy simulation algorithm has been used to simulate PCM performance correctly
- A very narrow simulation timestep of 30 timesteps per hour to precisely simulate the dynamic behaviour of PCM

In addition to the building model itself, another necessary input for running an energy simulation is weather data. As mentioned above, the simulations performed for this chapter relied on TMY weather data. More specifically, TMY for Sofia has been downloaded from the EU's Photovoltaic Geographical Information System (PVGIS) [154]. The TMY is based on the weather observations over the period from 2005 to 2020.

After running energy simulations with the inputs and settings described above, the total yearly energy demand for heating and cooling has been obtained. The lifetime of the buildings has been assumed to be 60 years, which is a typical value used in LCA/LCCA of buildings. The total energy consumption over the life cycle of a building is then calculated as yearly consumption times 60. The total life cycle energy consumption has then been used to calculate the overall economic and environmental impacts for both of the compared buildings. For LCCA, the price of electricity has been taken at 0.11 EUR/kWh based on the data from Eurostat [155]. The energy costs occurring in the future were adjusted to inflation using the average inflation rate in Bulgaria over the last 10 years of 2.7% obtained from Eurostat [156]. For LCA, environmental data from the ecoinvent database has been used. More specifically, it contains the dataset "*market for electricity, low voltage / electricity, low voltage*" that contains the emissions profile of 1kWh of electricity consumed by an end-user in Bulgaria. It is based on the average electricity generation mix for Bulgaria and also includes distribution and conversion losses in the network. The final impacts for this stage were calculated by multiplying the total life cycle energy consumption of a building by the corresponding economic/environmental impacts of 1 kWh of electricity consumed.

End of Life stage

The cost assessment of the end of life of demonstrator buildings was based on the expected deconstruction costs provided by GBS. Those costs were estimated at 21000 EUR for all four buildings. The costs then were equally distributed between the buildings, giving us an estimate of 5250 EUR per building. Since those costs are occurring 60 years in the future, they were adjusted for inflation using the same 2.7% inflation rate as in the case of energy use costs correction discussed in the previous section. The environmental assessment included two parts: the use of machinery for deconstruction, as well as the collection and treatment of waste construction materials. The use of deconstruction equipment in hours has been estimated by GBS. Those values were then converted into environmental impacts using

the same procedure as described in the *Construction process stage* section above. Table 4.11 provides an overview of the equipment used for deconstruction as well as corresponding fuel consumption.

Table 4.11: Overview of deconstruction equipment fuel consumption for LCA.

Equipment name	Equipment utilisation, hours	Fuel consumption, l/h	Total fuel consumption for all four buildings, l
Excavator with hydraulic hammer and clips	35	11.4	397.4
Dumper	24	5.7	136.3
Bucket-wheel excavator	30	11.4	340.7
Loader	20	5.7	113.6
Total fuel consumption per building, l			247.0

The environmental impacts of the EoL stage of the waste construction materials (their collection, transport and treatment), apart from insulation, were modelled based on the datasets available in the ecoinvent database. The database contains averaged values of environmental impacts of the collection and treatment of all the construction materials used in the demonstrator buildings. Where possible, the localised data for Bulgaria was used. Where localised data was not available, wide coverage datasets were used (Europe or the whole world). For the insulation materials - EPS and NRG-Panels - a more detailed assessment has been made, as already described in Scenario P6 of Section 4.2.5 above.

Benefits Beyond End of Life stage

The analysis of the benefits beyond EoL for EPS and NRG-Panels has already been described in Scenario P6 of Section 4.2.5 above. For the rest of the materials, the assessment of their benefits beyond EoL is not included in this work. Leaving this part away does not influence the outcomes of the comparison between the demonstrator buildings since their composition is the same apart from the insulation layer.

4.3 Results and discussion

4.3.1 Up-scaled LCA and LCCA of MPCM and comparison of different MPCM types

The up-scaled LCA and LCCA of MPCM were performed using the approach described in previous sections and by implementing all the up-scaling scenarios described in Section 4.2.3. As mentioned in the methodology section, the assessments were conducted for two types of MPCM slurry: IC

MPCM slurry and MF MPCM slurry. Those two slurry types have different fractions of solid MPCM: 15% for IC MPCM slurry and 25.1% for MF MPCM. In order to make the results of LCA/LCCA directly comparable, the results below are provided for 6.66 kg of IC MPCM slurry and for 3.98 kg of MF MPCM slurry: both contain exactly 1 kg of solid MPCM. The functional unit for LCA/LCCA is, thus, the production of 1 kg of solid MPCM in the form of slurry. Table 4.12 and Table 4.13 provide the inventories (amounts of inputs and outputs) for the production of those slurries in condensed form. The inventories extended with the names of ecoinvent datasets used can be found in Appendix B (Table B3 and Table B4).

Table 4.12: Inventory of MF MPCM slurry production.

Inputs		
Product	Amount	Unit
MF-Resin	0.21	kg
Isobutanol	0.15	kg
PCM (FAME)	0.75	kg
Water	2.83	kg
PVA	0.03	kg
Electricity	5.07	MJ
Transport	0.23	t*km
Ammonium chloride	0.00	kg
Outputs		
Product	Amount	Unit
MF MPCM slurry	3.98	kg
From which solid MPCM	1.00	kg

Table 4.13: Inventory of IC MPCM slurry production.

Inputs		
Product	Amount	Unit
Water	6.85	kg
PCM (FAME)	0.68	kg
Gelatine	0.11	kg
Electricity	7.12	MJ
Crosslinker	0.02	kg
Polymer 2	0.04	kg
Plasticiser	0.05	kg
Emulsifier	0.00	kg
Transport	0.21	t*km
Shell material	0.05	kg
Soda ash	0.05	kg
Outputs		
Product	Amount	Unit
IC MPCM slurry	6.66	kg
From which solid MPCM	1.00	kg

Based on those inventories and the rest of the inputs, the environmental impacts have been calculated for both types of MPCM. Figure 4.7 presents the overview of individual contributors (inputs) to the overall environmental impacts of MPCM production for MF MPCM, and Figure 4.8 - for IC MPCM. For each of the impact categories, the largest contributor is indicated and its relative contribution is shown in the corresponding bar of the chart. The absolute values of the impacts for both MPCM types can be found in Appendix B, Table B8 and Table B9.

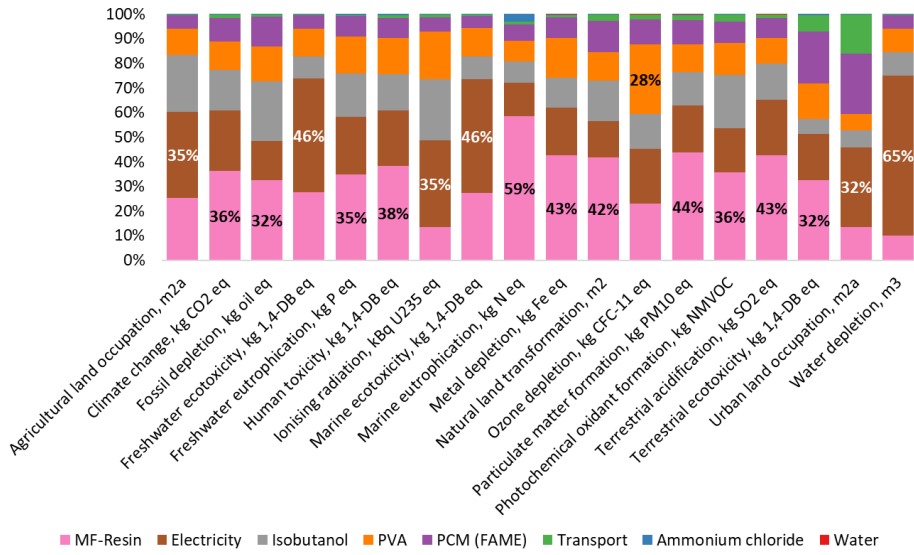


Figure 4.7: The structure of the environmental impacts of MF MPCM production.

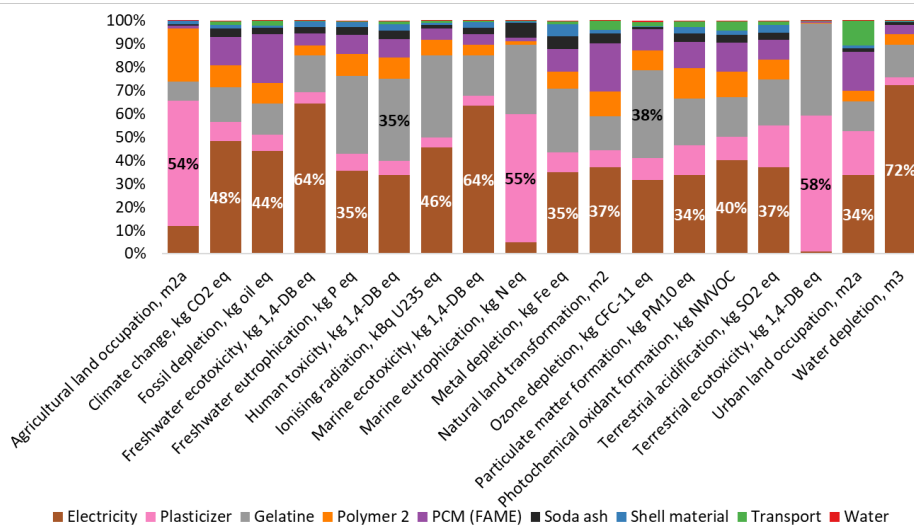


Figure 4.8: The structure of the environmental impacts of IC MPCM production.

For MF MPCM, MF-resin is the main contributor to most of the environmental impact categories. Electricity use is also a significant contributor and has a larger share of impact in six impact categories, and notably dominates the water depletion category, where it contributes to 65% of the total. Interestingly, within the Ozone depletion category, it is PVA that is the main contributor.

In the case of IC MPCM, the situation with the distribution of impacts is somewhat similar to MF MPCM, with three dominant processes. Electricity use is the main contributor in all but five environmental categories, while plasticiser is the highest contributor in three categories and gelatine – in the two remaining ones.

In addition to the environmental impacts in their native units, the environmental costs were also calculated using the Environmental Prices method introduced previously. Those environmental costs, as well as economic costs, are presented below in the form of impact matrices. In the rows of such a matrix are impact categories, and the columns contain all the contributors (chemicals, electricity, water, etc.). On the intersection of a column and a row, the corresponding environmental cost can be found. In the last row, the economic cost is presented. This matrix makes it easy to understand where costs are coming from and provides all the necessary information in a compact form. It also enables a direct comparison between contributors and across the impact categories within each MPCM type, as well as between two MPCM types.

Impact category	Environmental cost by contributor, EUR								Total
	MF-Resin	Electricity	Isobutanol	PVA	PCM (FAME)	Transport	Ammonium chloride	Water	
Agricultural land occupation	€ 0.003	€ 0.004	€ 0.003	€ 0.001	€ 0.001	€ 0.000	€ 0.000	€ 0.000	€ 0.011
Climate change	€ 0.045	€ 0.030	€ 0.020	€ 0.014	€ 0.012	€ 0.002	€ 0.000	€ 0.000	€ 0.123
Freshwater ecotoxicity	€ 0.001	€ 0.001	€ 0.000	€ 0.000	€ 0.000	€ 0.000	€ 0.000	€ 0.000	€ 0.003
Freshwater eutrophication	€ 0.000	€ 0.000	€ 0.000	€ 0.000	€ 0.000	€ 0.000	€ 0.000	€ 0.000	€ 0.001
Human toxicity	€ 0.022	€ 0.013	€ 0.008	€ 0.008	€ 0.005	€ 0.001	€ 0.000	€ 0.000	€ 0.057
Ionising radiation	€ 0.001	€ 0.003	€ 0.002	€ 0.002	€ 0.001	€ 0.000	€ 0.000	€ 0.000	€ 0.010
Marine ecotoxicity	€ 0.000	€ 0.000	€ 0.000	€ 0.000	€ 0.000	€ 0.000	€ 0.000	€ 0.000	€ 0.000
Marine eutrophication	€ 0.001	€ 0.000	€ 0.000	€ 0.000	€ 0.000	€ 0.000	€ 0.000	€ 0.000	€ 0.002
Ozone depletion	€ 0.000	€ 0.000	€ 0.000	€ 0.000	€ 0.000	€ 0.000	€ 0.000	€ 0.000	€ 0.000
Particulate matter formation	€ 0.057	€ 0.025	€ 0.017	€ 0.014	€ 0.013	€ 0.003	€ 0.000	€ 0.000	€ 0.129
Photochemical oxidant formation	€ 0.003	€ 0.001	€ 0.002	€ 0.001	€ 0.001	€ 0.000	€ 0.000	€ 0.000	€ 0.008
Terrestrial acidification	€ 0.028	€ 0.015	€ 0.010	€ 0.007	€ 0.005	€ 0.001	€ 0.000	€ 0.000	€ 0.066
Terrestrial ecotoxicity	€ 0.001	€ 0.000	€ 0.000	€ 0.000	€ 0.000	€ 0.000	€ 0.000	€ 0.000	€ 0.002
Urban land occupation	€ 0.000	€ 0.001	€ 0.000	€ 0.000	€ 0.000	€ 0.000	€ 0.000	€ 0.000	€ 0.002
Total environmental cost	€ 0.161	€ 0.094	€ 0.063	€ 0.049	€ 0.037	€ 0.007	€ 0.001	€ 0.000	€ 0.413
Economic cost, EUR	€ 3.955	€ 0.352	€ 2.864	€ 0.102	€ 1.509	€ 0.000	€ 0.002	€ 1.131	€ 9.91

Figure 4.9. Cost matrix for MF MPCM slurry (3.98 kg of slurry or 1 kg of dry MF MPCM equivalent).

Impact category	Contributor											Total
	Electricity	Plasticizer	Gelatine	Polymer 2	PCM (FAME)	Soda ash	Shell material	Transport	Water	Crosslinker	Emulsifier	
Agricultural land occupation	€ 0.005	€ 0.025	€ 0.004	€ 0.010	€ 0.001	€ 0.000	€ 0.001	€ 0.000	€ 0.000	-	-	€ 0.045
Climate change	€ 0.042	€ 0.007	€ 0.013	€ 0.008	€ 0.011	€ 0.003	€ 0.001	€ 0.002	€ 0.000	-	-	€ 0.087
Freshwater ecotoxicity	€ 0.002	€ 0.000	€ 0.000	€ 0.000	€ 0.000	€ 0.000	€ 0.000	€ 0.000	€ 0.000	-	-	€ 0.003
Freshwater eutrophication	€ 0.000	€ 0.000	€ 0.000	€ 0.000	€ 0.000	€ 0.000	€ 0.000	€ 0.000	€ 0.000	-	-	€ 0.001
Human toxicity	€ 0.018	€ 0.003	€ 0.018	€ 0.005	€ 0.004	€ 0.002	€ 0.001	€ 0.001	€ 0.000	-	-	€ 0.053
Ionising radiation	€ 0.005	€ 0.000	€ 0.004	€ 0.001	€ 0.001	€ 0.000	€ 0.000	€ 0.000	€ 0.000	-	-	€ 0.010
Marine ecotoxicity	€ 0.000	€ 0.000	€ 0.000	€ 0.000	€ 0.000	€ 0.000	€ 0.000	€ 0.000	€ 0.000	-	-	€ 0.000
Marine eutrophication	€ 0.000	€ 0.004	€ 0.002	€ 0.000	€ 0.000	€ 0.000	€ 0.000	€ 0.000	€ 0.000	-	-	€ 0.007
Ozone depletion	€ 0.000	€ 0.000	€ 0.000	€ 0.000	€ 0.000	€ 0.000	€ 0.000	€ 0.000	€ 0.000	-	-	€ 0.000
Particulate matter formation	€ 0.035	€ 0.013	€ 0.021	€ 0.013	€ 0.012	€ 0.004	€ 0.003	€ 0.002	€ 0.000	-	-	€ 0.103
Photochemical oxidant formation	€ 0.002	€ 0.000	€ 0.001	€ 0.001	€ 0.001	€ 0.000	€ 0.000	€ 0.000	€ 0.000	-	-	€ 0.005
Terrestrial acidification	€ 0.021	€ 0.010	€ 0.011	€ 0.005	€ 0.005	€ 0.002	€ 0.002	€ 0.001	€ 0.000	-	-	€ 0.057
Terrestrial ecotoxicity	€ 0.001	€ 0.037	€ 0.025	€ 0.000	€ 0.000	€ 0.000	€ 0.000	€ 0.000	€ 0.000	-	-	€ 0.063
Urban land occupation	€ 0.001	€ 0.000	€ 0.000	€ 0.000	€ 0.000	€ 0.000	€ 0.000	€ 0.000	€ 0.000	-	-	€ 0.002
Total environmental cost	€ 0.132	€ 0.100	€ 0.100	€ 0.044	€ 0.034	€ 0.012	€ 0.009	€ 0.006	€ 0.001	-	-	€ 0.44
Economic cost	€ 0.495	€ 0.069	€ 0.628	€ 0.124	€ 1.369	€ 0.046	€ 0.198	€ 0.000	€ 2.739	€ 0.187	€ 0.020	€ 5.87

Figure 4.10: Cost matrix for IC MPCM slurry (6.66 kg of slurry or 1 kg of dry IC MPCM equivalent).

As can be seen from the cost matrices, IC MPCM slurry has significantly lower (41% lower) economic costs and almost the same level of environmental costs. A major part of the costs of MF MPCM slurry comes from MF resin and isobutanol. In fact, those are two components of the MF resin solution – the most essential component of MF MPCM production. In contrast, the largest part of the economic costs of IC MPCM slurry comes from demineralised water. This highlights one of the main advantages of IC MPCM – the materials used in its production are abundant and inexpensive.

The obtained economic cost of MF MPCM (9.9 EUR/kg of MPCM) is very close to the actual quoted large-batch price of Nextek 24D that RIB received from Microtek (9.8 EUR/kg of MPCM). While Nextek 24D is a commercial product with an MF-based shell and its production process is a commercial secret, it can be expected that it is similar to the particles modelled here. It is important to note here that the result of LCCA cannot be directly compared to the market prices of commercial MPCM, but it still provides a good reference point. The fact that the obtained LCCA results are of the same order of magnitude is already a good indicator of the assessment consistency. Furthermore, the sufficiently lower costs of IC MPCM highlight its market potential as a lower-cost alternative to the existing MPCMs and their manufacturing processes.

From the environmental perspective, the overall environmental costs of IC MPCM are 6% greater than those of MF MPCM. This is mostly due to a significantly larger contribution of electricity consumption. The reason for that is the higher water content required for the production process. This elevated water content results in higher energy requirements for dispersion and homogenisation of the solution, as well as necessitating an additional evaporation step. This higher energy consumption, however, is almost fully compensated for by the lower impacts of the chemicals used in the production process of IC MPCM.

4.3.2 Up-scaled LCA and LCCA of NRG-Panels and comparison with conventional insulation materials

Up-scaled LCA and LCCA of NRG-Panels with different types of MPCM

Based on the mix design that was chosen for the production and testing at demonstrator buildings in Sofia, as well as the methodology and scenarios described in the previous sections, the final production system of NRG-Panels has been built, and the inventories for NRG-Panels production were compiled. Figure 4.11 presents a simplified scheme of the NRG-Panels production system.

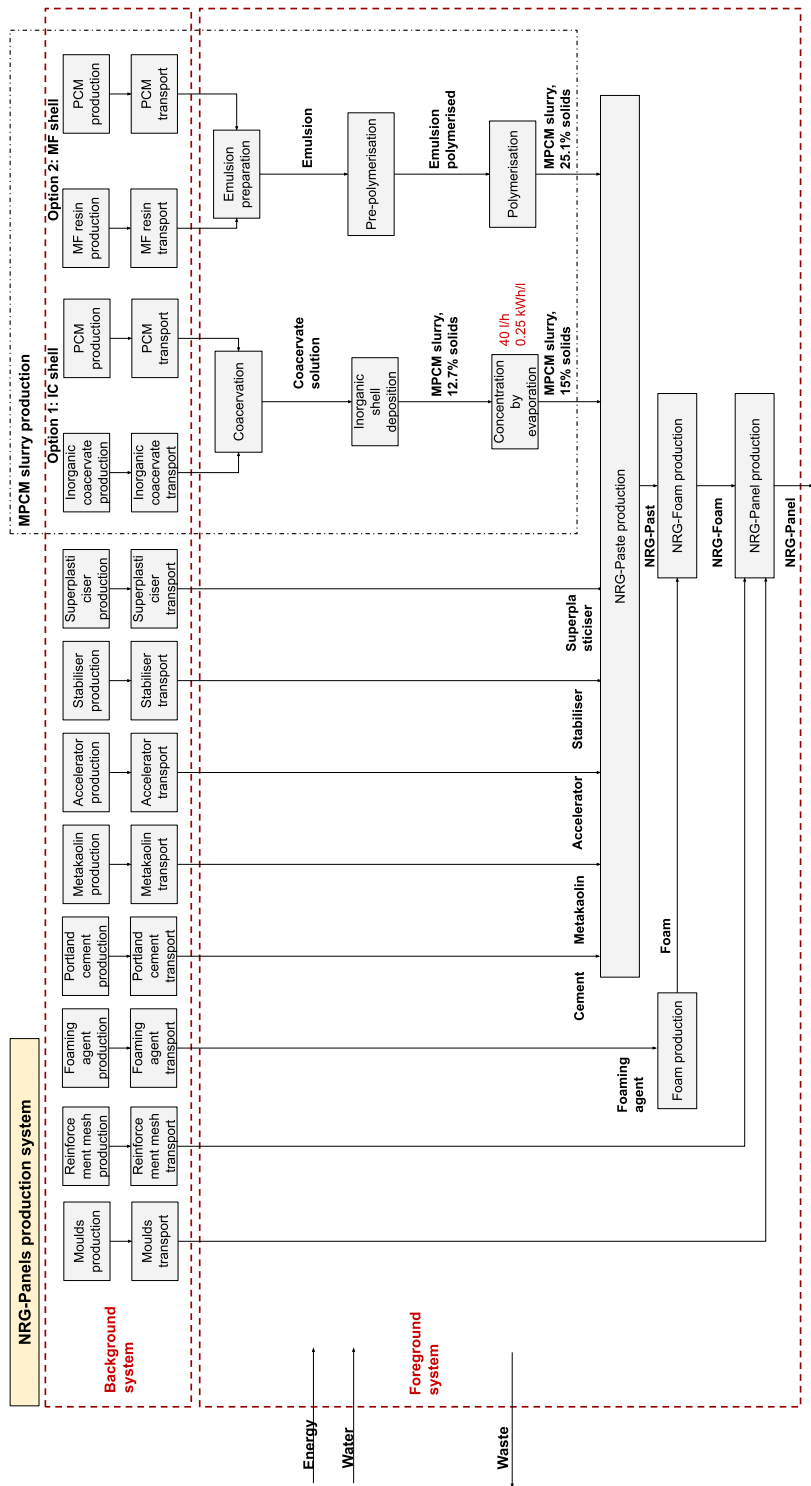


Figure 4.11: The overall scheme of the NRG-Panels production system.

Detailed information on inputs and outputs and their volumes can be found in Table 4.14. The inventory is provided for 10 m² of 10 cm thick NRG-Panels. Names of the corresponding ecoinvent datasets used can be found in the extended version of the inventory provided in Table B5 of Appendix B.

Table 4.14: Inventory of NRG-Panels production with MF and IC MPCM.

Inputs			
Product	Amount (MF MPCM)	Amount (IC MPCM)	Unit
MPCM Slurry (equiv. to 10.19 kg of dry MPCM)	42.71	71.51	kg
Cement CEM III/C	143.69	143.69	kg
Stabiliser	4.84	4.84	kg
Accelerator	3.35	3.35	kg
Foaming agent	1.27	1.27	kg
Metakaolin	23.65	23.65	kg
Superplasticiser	0.83	0.83	kg
Tap water	85.42	64.06	kg
Electricity	0.88	0.88	MJ
Rainwater	13.16	13.16	kg
Electricity PV	2.46	2.46	MJ
Reinforcement mesh	3.30	3.30	kg
Steel	2.40	2.40	kg
Outputs			
Product	Amount (MF MPCM)	Amount (IC MPCM)	Unit
MPCM Panels	1	1	m3
Waste cement slurry	1.10	1.10	kg
Waste water	0.08	0.08	m3
Waste steel	2.40	2.40	kg

As the next step, environmental and economic costs were calculated in accordance with the methodology described. Similarly to the MPCM assessment above, the results were compiled into cost matrices that are shown in Figure 4.12 and Figure 4.13. The matrices provide all the environmental impacts recalculated as environmental costs, but the impacts are also provided in their respective units in Appendix B (Table B9 and Table B10).

Impact category	Contributor																Total
	Cement CEM III/C	MF MPCM Slurry	Foaming agent	Reinforcement mesh	Metakaolin	Steel	Accelerator	Superplasticizer	Waste cement slurry	Electricity PV	Electricity	Waste water	Waste steel	Tap water	Rainwater	Stabilizer	
Agricultural land occupation	€ 0.193	€ 0.121	€ 0.325	€ 0.095	€ 0.036	€ 0.017	€ 0.025	€ 0.003	€ 0.015	€ 0.000	€ 0.001	€ 0.000	€ 0.000	€ 0.000	€ 0.000	-	€ 0.832
Climate change	€ 2.116	€ 1.555	€ 0.181	€ 0.717	€ 0.572	€ 0.261	€ 0.301	€ 0.052	€ 0.013	€ 0.004	€ 0.007	€ 0.002	€ 0.001	€ 0.002	€ 0.000	-	€ 5.784
Freshwater ecotoxicity	€ 0.025	€ 0.030	€ 0.005	€ 0.010	€ 0.005	€ 0.009	€ 0.010	€ 0.001	€ 0.000	€ 0.001	€ 0.000	€ 0.000	€ 0.001	€ 0.000	€ 0.000	-	€ 0.097
Freshwater eutrophication	€ 0.020	€ 0.012	€ 0.001	€ 0.006	€ 0.004	€ 0.004	€ 0.002	€ 0.000	€ 0.000	€ 0.000	€ 0.000	€ 0.000	€ 0.000	€ 0.000	€ 0.000	-	€ 0.051
Human toxicity	€ 0.992	€ 0.715	€ 0.084	€ 0.612	€ 0.195	€ 0.207	€ 0.177	€ 0.026	€ 0.007	€ 0.007	€ 0.011	€ 0.002	€ 0.003	€ 0.002	€ 0.000	-	€ 3.040
Ionising radiation	€ 0.222	€ 0.119	€ 0.004	€ 0.042	€ 0.038	€ 0.010	€ 0.011	€ 0.004	€ 0.000	€ 0.000	€ 0.001	€ 0.000	€ 0.000	€ 0.000	€ 0.000	-	€ 0.451
Marine ecotoxicity	€ 0.005	€ 0.005	€ 0.000	€ 0.002	€ 0.001	€ 0.002	€ 0.002	€ 0.000	€ 0.000	€ 0.000	€ 0.000	€ 0.000	€ 0.000	€ 0.000	€ 0.000	-	€ 0.018
Marine eutrophication	€ 0.019	€ 0.022	€ 0.052	€ 0.012	€ 0.004	€ 0.005	€ 0.005	€ 0.000	€ 0.000	€ 0.000	€ 0.000	€ 0.005	€ 0.000	€ 0.000	€ 0.000	-	€ 0.124
Ozone depletion	€ 0.000	€ 0.000	€ 0.000	€ 0.000	€ 0.000	€ 0.000	€ 0.000	€ 0.000	€ 0.000	€ 0.000	€ 0.000	€ 0.000	€ 0.000	€ 0.000	€ 0.000	-	€ 0.001
Particulate matter formation	€ 2.273	€ 1.767	€ 0.248	€ 0.985	€ 0.519	€ 0.653	€ 0.287	€ 0.048	€ 0.030	€ 0.008	€ 0.003	€ 0.005	€ 0.002	€ 0.002	€ 0.000	-	€ 6.833
Photochemical oxidant formation	€ 0.126	€ 0.114	€ 0.011	€ 0.089	€ 0.023	€ 0.024	€ 0.011	€ 0.003	€ 0.001	€ 0.000	€ 0.000	€ 0.000	€ 0.000	€ 0.000	€ 0.000	-	€ 0.404
Terrestrial acidification	€ 1.125	€ 0.848	€ 0.111	€ 0.418	€ 0.212	€ 0.122	€ 0.214	€ 0.021	€ 0.006	€ 0.003	€ 0.002	€ 0.002	€ 0.001	€ 0.001	€ 0.000	-	€ 3.086
Terrestrial ecotoxicity	€ 0.034	€ 0.039	€ 4.232	€ 0.074	€ 0.003	€ 0.003	€ 0.004	€ 0.000	€ 0.000	€ 0.001	€ 0.000	€ 0.000	€ 0.000	€ 0.000	€ 0.000	-	€ 4.391
Urban land occupation	€ 0.071	€ 0.054	€ 0.002	€ 0.010	€ 0.002	€ 0.003	€ 0.003	€ 0.000	€ 0.000	€ 0.000	€ 0.000	€ 0.000	€ 0.000	€ 0.000	€ 0.000	-	€ 0.147
Total environmental cost	€ 7.223	€ 5.401	€ 5.256	€ 3.070	€ 1.614	€ 1.320	€ 1.050	€ 0.160	€ 0.074	€ 0.026	€ 0.026	€ 0.018	€ 0.009	€ 0.008	€ 0.001	-	€ 25.26
Economic cost	€ 21.55	€ 106.34	€ 7.82	€ 5.00	€ 5.39	€ 1.51	€ 11.11	€ 1.32	€ 0.00	€ 0.00	€ 0.07	€ 0.00	€ 0.00	€ 0.43	€ 0.00	€ 14.19	€ 174.74

Figure 4.12: Cost matrix for NRG-Panels with MF MPCM.

Impact category	Contributor																Total
	Cement CEM III/C	IC MPCM Slurry	Foaming agent	Reinforcement mesh	Metakaolin	Steel	Accelerator	Superplasticizer	Waste cement slurry	Electricity PV	Electricity	Waste water	Waste steel	Tap water	Rainwater	Stabilizer	
Agricultural land occupation	€ 0.193	€ 0.501	€ 0.325	€ 0.095	€ 0.036	€ 0.017	€ 0.025	€ 0.003	€ 0.015	€ 0.000	€ 0.001	€ 0.000	€ 0.000	€ 0.000	€ 0.000	-	€ 1.212
Climate change	€ 2.116	€ 1.391	€ 0.181	€ 0.717	€ 0.572	€ 0.261	€ 0.301	€ 0.052	€ 0.013	€ 0.004	€ 0.007	€ 0.002	€ 0.001	€ 0.001	€ 0.000	-	€ 5.619
Freshwater ecotoxicity	€ 0.025	€ 0.033	€ 0.005	€ 0.010	€ 0.005	€ 0.009	€ 0.010	€ 0.001	€ 0.000	€ 0.001	€ 0.000	€ 0.000	€ 0.000	€ 0.000	€ 0.000	-	€ 0.101
Freshwater eutrophication	€ 0.020	€ 0.012	€ 0.001	€ 0.006	€ 0.004	€ 0.004	€ 0.002	€ 0.000	€ 0.000	€ 0.000	€ 0.000	€ 0.000	€ 0.000	€ 0.000	€ 0.000	-	€ 0.051
Human toxicity	€ 0.992	€ 0.772	€ 0.084	€ 0.612	€ 0.195	€ 0.207	€ 0.177	€ 0.026	€ 0.007	€ 0.007	€ 0.011	€ 0.002	€ 0.003	€ 0.001	€ 0.000	-	€ 3.096
Ionising radiation	€ 0.222	€ 0.144	€ 0.004	€ 0.042	€ 0.038	€ 0.010	€ 0.011	€ 0.004	€ 0.000	€ 0.000	€ 0.001	€ 0.000	€ 0.000	€ 0.000	€ 0.000	-	€ 0.477
Marine ecotoxicity	€ 0.005	€ 0.006	€ 0.000	€ 0.002	€ 0.001	€ 0.002	€ 0.002	€ 0.000	€ 0.000	€ 0.000	€ 0.000	€ 0.000	€ 0.000	€ 0.000	€ 0.000	-	€ 0.018
Marine eutrophication	€ 0.019	€ 0.081	€ 0.052	€ 0.012	€ 0.004	€ 0.005	€ 0.005	€ 0.000	€ 0.000	€ 0.000	€ 0.000	€ 0.005	€ 0.000	€ 0.000	€ 0.000	-	€ 0.183
Ozone depletion	€ 0.000	€ 0.001	€ 0.000	€ 0.000	€ 0.000	€ 0.000	€ 0.000	€ 0.000	€ 0.000	€ 0.000	€ 0.000	€ 0.000	€ 0.000	€ 0.000	€ 0.000	-	€ 0.001
Particulate matter formation	€ 2.273	€ 1.787	€ 0.248	€ 0.985	€ 0.519	€ 0.653	€ 0.287	€ 0.048	€ 0.030	€ 0.008	€ 0.003	€ 0.005	€ 0.002	€ 0.002	€ 0.000	-	€ 6.852
Photochemical oxidant formation	€ 0.126	€ 0.107	€ 0.011	€ 0.089	€ 0.023	€ 0.024	€ 0.011	€ 0.003	€ 0.001	€ 0.000	€ 0.000	€ 0.000	€ 0.000	€ 0.000	€ 0.000	-	€ 0.397
Terrestrial acidification	€ 1.125	€ 0.864	€ 0.111	€ 0.418	€ 0.212	€ 0.122	€ 0.214	€ 0.021	€ 0.006	€ 0.003	€ 0.002	€ 0.002	€ 0.001	€ 0.001	€ 0.000	-	€ 3.102
Terrestrial ecotoxicity	€ 0.034	€ 0.706	€ 4.232	€ 0.074	€ 0.003	€ 0.003	€ 0.004	€ 0.000	€ 0.000	€ 0.001	€ 0.000	€ 0.000	€ 0.000	€ 0.000	€ 0.000	-	€ 5.058
Urban land occupation	€ 0.071	€ 0.086	€ 0.002	€ 0.010	€ 0.002	€ 0.003	€ 0.003	€ 0.000	€ 0.000	€ 0.000	€ 0.000	€ 0.000	€ 0.000	€ 0.000	€ 0.000	-	€ 0.178
Total environmental cost	€ 7.223	€ 6.491	€ 5.256	€ 3.070	€ 1.614	€ 1.320	€ 1.050	€ 0.160	€ 0.074	€ 0.026	€ 0.026	€ 0.018	€ 0.009	€ 0.006	€ 0.001	-	€ 26.35
Economic cost	€ 21.55	€ 63.69	€ 7.82	€ 5.00	€ 5.39	€ 1.51	€ 11.11	€ 1.32	€ 0.00	€ 0.00	€ 0.07	€ 0.00	€ 0.00	€ 0.32	€ 0.00	-	€ 14.19
																	€ 131.98

Figure 4.13: Cost matrix for NRG-Panels with IC MPCM.

As expected based on the results assessment of MPCM, NRG-Panels produced with IC MPCM have sufficiently lower (by 24%) economic costs compared to MF MPCM panels. In both cases, MPCM dominates total economic costs. In the case of NRG-Panels with MF MPCM, the share of MPCM is 61% and in the case of IC MPCM – 48%. Cement, stabiliser and accelerator are three other major contributors to the economic costs.

On the side of environmental costs, cement has the highest share of those. Even though CEM III/C is assumed to be used in this up-scaled LCA, it still has relatively high environmental impacts. MPCM is the second largest contributor to the environmental costs, followed by foaming agent and reinforcement mesh. The foaming agent is an interesting case since it shows a very high peak impact in the Terrestrial ecotoxicity impact category but a low impact across the rest of the categories. This high impact can be traced to the chemical Cypermethrin, which is sometimes used as an insecticide in coconut farming and has been included in the dataset used in this assessment. While it is possible to obtain the same biomaterials necessary for the production of a foaming agent from sources that do not use Cypermethrin, in this study, the dataset is kept unmodified. It is, however, worth keeping in mind that the environmental impact of the foaming agent might be overestimated. Another possible point of improvement is the use of an alternative material for the reinforcement mesh, since it has relatively high environmental impacts per unit of weight.

While the analysis highlights that IC MPCM would be a better choice for use in NRG-Foam and NRG-Panels, due to certain technical complications that occurred during the project, the final NRG-Panels were produced with MF MPCM. Due to this, the following assessments on the building level will only include MF MPCM as a part of NRG-Panels. The results of this assessment, however, show great potential for bio-based IC MPCM as an affordable energy-storing filler for construction materials.

Comparison of NRG-Panels with conventional insulation materials

Using the results of up-scaled LCA and LCCA of NRG-Panels, it is possible to compare them against some conventional insulation materials. For that, the environmental costs of conventional insulation materials have been calculated based on the data available in the ecoinvent database. The datasets used provide averaged values of environmental impacts and are not specific to a particular product/producer. Table 4.15 provides the environmental costs of different insulation materials available in the ecoinvent database, as well as calculated values for NRG-Panels.

Table 4.15: Environmental costs of different insulation materials. The densities provided in the column "Assumed density kg/m³" were used to recalculate the impacts per kg to impacts per m³.

Insulation material	ecoinvent dataset	Assumed density, kg/m ³	Environmental cost, EUR/ m ³
PUR - World Average	market for polyurethane, rigid foam polyurethane, rigid foam Cutoff, S RoW	30	€ 47.0
Foam glass - World Average	market for foam glass foam glass Cutoff, S GLO	120	€ 46.2
PUR - Europe Average	market for polyurethane, rigid foam polyurethane, rigid foam Cutoff, S RER	30	€ 38.1
XPS - World Average	market for polystyrene, extruded polystyrene, extruded Cutoff, S GLO	35	€ 33.9
Stone wool - World Average	market for stone wool stone wool Cutoff, S GLO	100	€ 33.8
Glass wool - World Average	market for glass wool mat glass wool mat Cutoff, S GLO	40	€ 26.4
Foam glass, renewable energy sources - World Average	market for foam glass, electricity from renewable energy products foam glass, electricity from renewable energy products Cutoff, S GLO	120	€ 17.2
EPS - World Average	market for polystyrene foam slab for perimeter insulation polystyrene foam slab for perimeter insulation Cutoff, S GLO	20	€ 13.1
EPS with graphite, 6% recycled - World Average	market for polystyrene foam slab with graphite, 6% recycled polystyrene foam slab with graphite, 6% recycled Cutoff, S GLO	20	€ 9.5
EPS, 10% recycled - World Average	market for polystyrene foam slab, 10% recycled polystyrene foam slab, 10% recycled Cutoff, S GLO	20	€ 9.5
Autoclaved aerated concrete - World Average	market for autoclaved aerated concrete block autoclaved aerated concrete block Cutoff, S - RoW	115	€ 7.1
Glass wool, Saint-Gobain - Switzerland	market for glass wool mat, uncoated, Saint-Gobain ISOVER SA glass wool mat, uncoated, Saint-Gobain ISOVER SA Cutoff, S CH	25	€ 6.4
NRG-Panels with MF MPCM	-	-	€ 25.3
NRG-Panels with IC MPCM	-	-	€ 26.4

As can be seen from Table 4.15, the environmental costs of NRG-Panels are comparable with conventional insulation materials. Autoclaved aerated concrete provides an interesting reference point for NRG-Panels as another cement-based material. The table shows that it has significantly lower environmental impacts compared to NRG-Panels, which is caused by two main factors. First of all, it has a sufficiently lower density compared to the analysed configuration of NRG-Panels (115 kg/m³ versus 174 kg/m³). Secondly, NRG-Panels contain PCM and thus provide additional energy-storing qualities, unlike ordinary aerated concrete. In the basic configuration with no MPCM and high porosity, the environmental footprint of NRG-Panels is expected to be similar to or lower than such of autoclaved aerated concrete.

For the comparison of the economic prices, GBS acquired local prices for a set of insulation products available on the market. Those prices, together with the results of LCCA of NRG-Panels, are provided in Table 4.16.

Table 4.16: Prices of insulation materials and the results of LCCA of NRG-Panels.

Insulation material	Market name	Market price, EUR/m ³
PIR	PF - PIR boards 100mm coated with fiber glass fleece, 1200 x 600mm, straight edges	€ 229.6
XPS	XPS Ecostir 100x600x1250 mm	€ 147.1
Stone wool	Knauf Insulation - 100x600x1000 mm, FKD-N Thermal	€ 128.3
EPS	BAUMIT Open Plus 100x500x1000mm	€ 122.1
Autoclaved aerated concrete	YTONG Multipor 100x600x400	€ 121.7
Glass wool	Knauf Insulation 100x1200x9100 mm, NatuRoll Plus	€ 29.6
		LCCA result, EUR/m³
NRG-Panels with MF MPCM	-	€ 174.7
NRG-Panels with IC MPCM	-	€ 132.0

It is worth stressing again that the results of LCCA of NRG-Panels cannot be compared directly to the prices of insulation materials on the market due to the major differences in the calculation methodology and the composition of those. It is, however, possible to use the market prices as a rough consistency check of LCCA and its upscaling. If the results of LCCA were several times higher than market prices, that would indicate that there are either some issues in the assessment or the assessment needs to be upscaled further, and current upscaling scenarios are not enough. The table above shows that LCCA results of NRG-Panels production are comparable or lower

than the market prices of conventional insulation materials, indicating that the results are consistent and that there is a potential for the further development of the material into a competitively-priced market product.

End of Life and Benefits Beyond End of Life of NRG-Panels and comparison with EPS

The results presented so far focused only on the production process of NRG-Panels. It is, however, important to understand how the material can be treated when it is reaching the end of its service life and what kind of impacts and, possibly, benefits can be found there. This result section provides insight into EoL and the benefits beyond EoL of NRG-Panels. The methodological approach to this analysis is presented in Scenario P6 in Section 4.2.5.

The impacts of NRG-Panels' recycling have been calculated for three manufacturing scenarios developed in the paper by Klemczak et al. [147] and introduced in Section 4.2.5. Here, only environmental impacts are considered, since no data for the economic assessment is available. The recycling experiments in the study by Klemczak et al. [147] were conducted for NRG-Foam with MF MPCM, and the results presented below might thus not be representative of NRG-Panels with IC MPCM.

Figure 4.14 shows the environmental impacts (in the form of environmental prices) of EoL for EPS and three recycling scenarios of NRG-Panels, as well as associated benefits beyond EoL. The EoL impacts come from the need for energy for recycling, as well as emissions produced during the recycling process. Benefits beyond EoL represent possible benefits of substituting primary production with the production from waste insulation: energy substitution in the case of EPS and cement substitution in the case of NRG-Panels (more details can be found in Section 4.2.5).

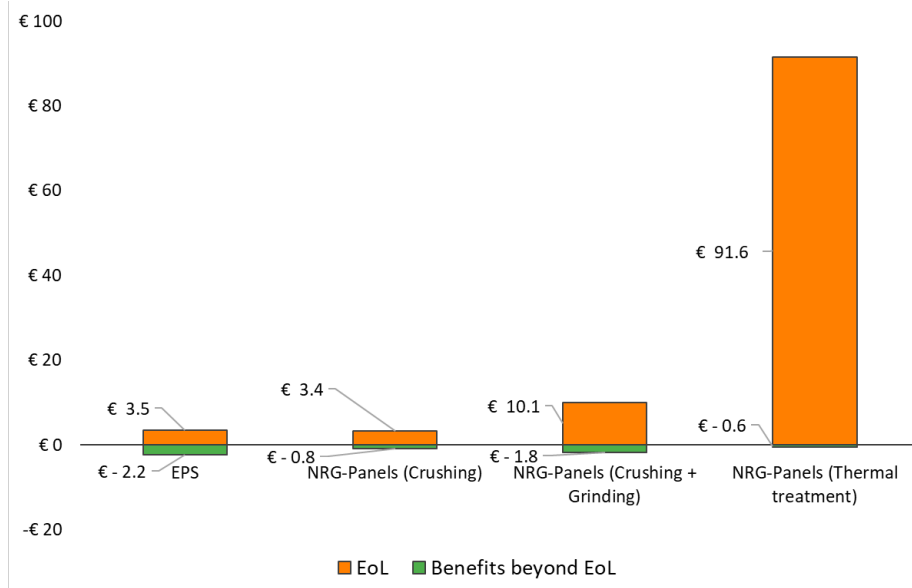


Figure 4.14: Environmental costs and benefits for EPS and three ways of NRG-Panels recycling. The results are provided for 1 m³ of insulation material.

As Figure 4.14 illustrates, the benefits beyond EoL are less than the impacts caused by the EoL stage for all of the analysed scenarios and materials. The overall ratio of environmental benefits to environmental costs is the best for EPS insulation, but the crushing scenario of NRG-Panels provides a close result. The environmental costs of the crushing scenario are the lowest across all the considered cases. The benefits are the highest for the Crushing + Grinding recycling scenario due to a very high final yield of 90%. However, the much higher energy requirement for grinding is overshadowing the gains in the benefits. The thermal treatment scenario is characterised by extremely high energy demand and low yield, leading to very high environmental costs compared to the rest of the cases. As Klemczak et al. [147] showed, while thermal treatment provides some benefits, there was no major difference in the performance of mortars produced using thermally-treated RFCP or via other methods. Due to this, in the current context, thermal treatment cannot be considered a feasible recycling strategy.

It is important to stress that relatively low values of benefits for NRG-Panels recycling are caused by a low substitution rate of 0.2 used in this assessment. However, as the NRG-Panels are developed further, it can be expected that this value could increase. For example, other types of MPCM (different shell, different core material) could have better compatibility with mortars, and it will be possible to produce them with a higher load of RFCP. Furthermore, the electricity demand for crushing, grinding and thermal treatment can potentially be decreased using more efficient machinery and/or the electricity demand can be covered by renewable energy sources. Nevertheless, even in the currently analysed case, NRG-Panels prove to be

easy to recycle and display the environmental costs and impacts comparable to conventional insulation materials.

4.3.3 LCA/LCCA of demonstrator buildings with EPS and NRG-Panels

With the results of the component-level LCA/LCCA obtained, it is possible to continue to the assessment on a building level. The methodology and input information required for the assessment of demonstrator buildings are provided in Section 4.2.7. All results below are provided per building unless stated otherwise. In the following text, the demonstrator Building 1 containing EPS insulation is referred to as EPS-building and the demonstrator Building 2 with NRG-Panels, as NRG-building. The overall inventories for both of the demonstrator buildings are not included here due to their large size, but are provided in Appendix B (Table B6 and Table B7).

Combining the results of assessments presented in the preceding sections and other necessary data obtained, a building-level assessment and comparison between EPS and NRG-Panels has been conducted. Figure 4.15 shows the comparison between the environmental and economic costs of EPS-building and NRG-building over their life cycle.

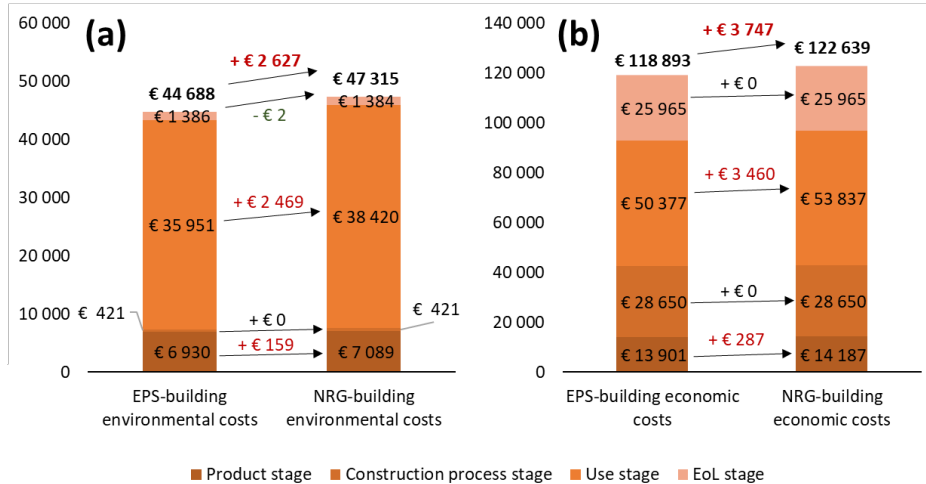


Figure 4.15: Comparison between environmental (a) and economic (b) costs of EPS-building and NRG-building.

The results show that the total environmental life cycle costs of the NRG-building are 6% (2 627 EUR) higher than those of the EPS-building, while economic costs are 3% (3 747 EUR) higher. The major part of environmental costs for both buildings comes from the Use stage, which is responsible for

more than 80% of the total in both cases. Economic costs are more equally distributed, but the use stage is still the largest contributor with a 42% share of total costs in the case of the EPS-building and 44% in the case of the NRG-building. It can also be observed that the differences in the overall impacts between the EPS-building and the NRG-building are largely driven by the Use stage as well. The cost difference occurring in the Production stage is due to the higher embedded costs of NRG-Panels, and this has already been discussed in Section 4.3.2.

The difference in environmental and economic costs in the Use stage is a direct consequence of the difference in the thermal performance of EPS insulation and NRG-Panels on the building level. This difference in building-level performance is then reflected in the heating and cooling demand. Figure 4.16 shows the comparison of the simulated energy demand for the EPS-building and the NRG-building.

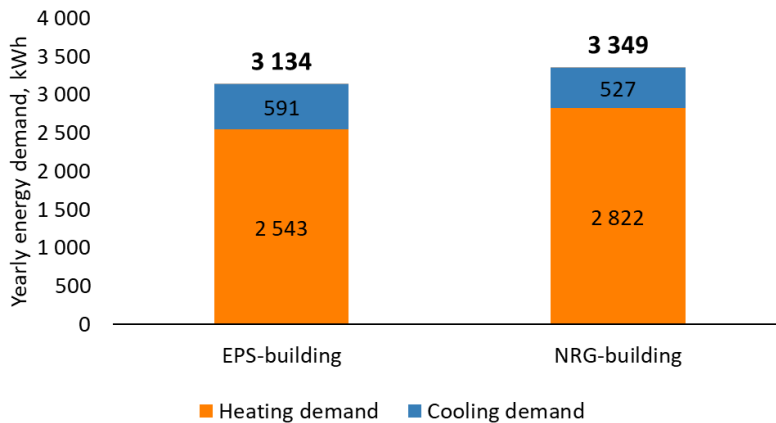


Figure 4.16: Comparison of yearly HVAC energy demand for EPS-building and NRG-building.

The figure above shows that under the given climatic conditions and with the final real-world configurations of the demonstrator buildings and NRG-Foam, NRG-building consumes 215 kWh more energy per year compared to EPS-building. NRG-building has a 64 kWh lower cooling demand, but this advantage is overshadowed by a significantly higher (279 kWh) heating demand. The cold-weather performance of NRG-Panels is thus the main cause of the difference in environmental and economic life cycle costs of the demonstrator buildings.

It is, however, important to stress that the configuration of NRG-Panels used in the demonstrator buildings has been impacted by tight project schedules and technological limitations. Consequently, the final selected configuration of NRG-Panels may not necessarily be the most suitable for the given building case and climatic conditions in Sofia, Bulgaria. To address this

issue, the following chapter will look into improving the building-level performance of NRG-Panels via case-specific design optimisation.

4.4 Concluding remarks

This chapter marks the shift in the development level of NRG-Foam from the lab scale to the prototype scale. It follows its transformation from NRG-Foam to NRG-Panels and their consecutive application in the demonstrator buildings in Sofia, Bulgaria. In this chapter, up-scaled environmental and cost assessments are conducted for MPCM production, NRG-Panels production and recycling and, finally, for the full lifecycle of demonstrator buildings including NRG-Panels. The obtained results allow for comparison between different types of MPCM as well as between NRG-Panels and conventional insulation materials. The key findings from the chapter are summarised below.

- Produced from abundant and inexpensive material, IC MPCM showed 41% lower economic costs compared to MF MPCM, with similar environmental costs.
- NRG-Panels with IC MPCM had 24% lower economic costs than those with MF MPCM but slightly higher environmental costs.
- The environmental and economic costs of NRG-Panels in both IC and MF configurations are comparable to conventional insulation materials.
- Even though under the up-scaling scenarios, CEM I cement has been substituted with low-emission CEM III/C cement, it has still been found to be the largest contributor to environmental costs in NRG-Panels' production.
- End-of-life analysis showed that NRG-Panels recycling had environmental impacts comparable to EPS recycling, but the benefits beyond EoL were lower, mostly due to a low substitution rate of primary production cement.
- The building-level assessment revealed that the use stage (electricity consumption for heating and cooling) was responsible for over 80% of total environmental costs and about 42-44% of economic costs for both buildings.
- Overall, NRG-building had 6% higher environmental costs and 3% higher economic costs over its lifecycle compared to EPS-building.

- The configuration of NRG-Panels that has been used in the prototype buildings might not have been well-suited for the climatic conditions in Sofia, Bulgaria.

5

CASE-SPECIFIC OPTIMISATION OF NRG-FOAM FOR IMPROVED BUILDING-LEVEL PERFORMANCE

This chapter investigates the hypothesis that has been formulated in Chapter 4: the configuration of NRG-Panels analysed was not optimal for the demonstrator building case at hand, leading to their underperformance. For that purpose, the static assessments developed in the previous chapter are first parametrised, making it possible to analyse the impacts of various material parameters on the final performance of the building. Then, using those parametric models, NRG-Panels' configuration is optimised for three objectives: lifecycle environmental costs, energy costs for heating and cooling, and construction and demolition costs. The results show that optimised NRG-Panels outperform the as-built configuration and comparable EPS insulation across all objectives. However, in all the cases, the optimal configuration favours high porosity with a non-significant MPCM inclusion or no MPCM at all. In such configurations, NRG-Panels have a very limited energy storage capacity, making them essentially a regular insulation material. The results of this chapter highlight the relative importance of the insulating properties of NRG-Panels over their energy-storing functionality in the specific climate conditions of Sofia with a heating-dominant energy consumption profile. Those findings emphasise the need for further investigation of NRG-Panels' performance in different climatic contexts, some of which might be more favourable for the utilisation of the NRG-Panels' heat-storing properties.

5.1 Introduction

Bringing a new construction material to life is impossible without extensive real-world testing where the prototype material is applied to a full-scale building, similarly to how it would be applied when it becomes a market product. However, due to the limited resources and time available, such full-scale testing is restricted to one or, at most, a small number of possible configurations of the prototype material. Ideally, the material configurations selected for real-world prototype testing should be optimised for the particular case at hand. Yet, predicting the real-world performance of a novel material is a complex task due to the limited availability and high uncertainty of the data at low TRL of the material. Furthermore, there might be technological, economic and time limitations that restrict the range of material configurations that can be produced. As a consequence, the prototype material that is produced for real-world testing might end up being suboptimal and not delivering the best possible performance.

While real-world testing of a prototype material provides essential data for its further development, even if the selected material configuration is suboptimal, some issues might arise when its performance is put against the existing commercial materials. More specifically, such comparisons might present the newly developed material in an unfavourable light. When it comes to NRG-Panels, their performance on the building level in the context of the demonstrator building in Sofia has been assessed in the previous chapter, and it has been revealed that NRG-Panels were underperforming compared to EPS panels. The final configuration of NRG-Panels used in the demonstrator buildings, however, has been greatly impacted by multiple manufacturing limitations that could not be resolved within the limited timeframe of the EU-backed project. This dissertation looks beyond the EU project, and from this standpoint, the configuration of NRG-Panels is still flexible and can be further optimised and improved to challenge the performance of the commercial materials.

This chapter focuses on the optimisation of NRG-Panels specifically for the demonstrator building case in Sofia. The optimisation process involves transitioning from static life cycle assessment (LCA), lifecycle costing assessment (LCCA) and energy models developed in previous chapters to dynamic ones where the configuration of NRG-Panels is not fixed but can be varied. Subsequently, an optimisation model is developed allowing us to find the optimal configuration of NRG-Panels providing the best possible building performance. Given that building performance can be defined in multiple ways, three different objectives are considered, each aligned with the interests of different stakeholders. As a result, three optimal configurations of NRG-Panels are found, and their performance in the context of the demonstrator building is compared against EPS insulation in a comparable thickness.

The results of this chapter allow for a more objective comparison between conventional insulation materials and NRG-Panels and provide an important

insight into their application potential from environmental, social and economic standpoints.

5.2 Methodology and modelling approach

5.2.1 Overview

This chapter builds on the results of the previous chapters. It uses the results of the building-level assessments presented in Chapter 4, but also implements parametrisation and optimisation techniques similar to those utilised in Chapter 2. Figure 5.1 presents the schematic overview of the approach used in this chapter.

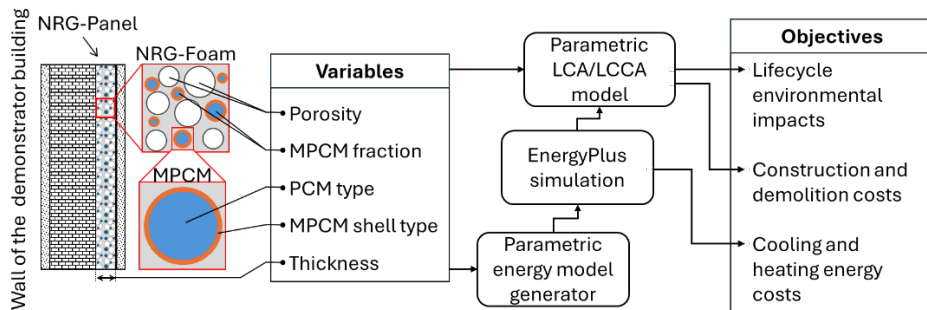


Figure 5.1: Overview of the methodological approach used in this chapter.

In the first step, LCA, LCCA and energy models used in Chapter 4 were parametrised. The parametrised energy model allows the calculation of the energy consumption for heating and cooling depending on the given set of NRG-Panels parameters. The parametric LCA/LCCA model calculates building-level environmental impacts and costs based on the NRG-Panels' parameters and the results of EnergyPlus simulations. The outputs of the parametric models are used to calculate three selected objectives quantifying the performance of the demonstrator building from the perspective of three different stakeholders. Each of the objectives is optimised separately to find three sets of optimal NRG-Panels configurations that are then compared to each other and against conventional insulation materials.

5.2.2 Optimisation model setup

Case building

This chapter relies on the same demonstrator building case as already described in detail in Chapter 4. The only difference is that in this chapter, the configuration of the insulation layer is not fixed. The following sections will describe in more detail how the parameters of the insulation layer are varied and how it is connected to the assessment of the building performance.

Variables definition

At this stage of the material development, we are not strictly constrained to a singular configuration, and many parameters could still be adjusted. It is thus possible to investigate the effects of tweaking those parameters on the overall performance of the material and the demonstrator building as a whole. In this chapter, the fixed-configuration models developed in Chapter 4 are parametrised with five key parameters of NRG-Panels selected for the assessment and optimisation:

- Material porosity, $0.05 \leq x_1 \leq 0.95$ (fixed at 0.87 for NRG-Panels in the demonstrator buildings)
- Fraction of MPCM, $0.001 \leq x_2 \leq 0.6$ (fixed at 0.1 for NRG-Panels in the demonstrator buildings)
- Type of PCM used as the core material in MPCM particles, x_3 . Overall, 11 different PCMs with melting temperatures from 4 °C to 37 °C were considered (a PCM with a melting temperature of 24 °C has been used in the demonstrator buildings)
- Material of MPCM shell, inorganic coacervate (IC) or melamine-formaldehyde (MF), x_4 (MF MPCM in the demonstrator buildings)
- Thickness of NRG-Panels layer in the walls, $0.02 \text{ m} \leq x_5 \leq 0.3 \text{ m}$ (0.1 m in the demonstrator buildings)

Those parameters define the material on micro (PCM and MPCM properties), meso (fractions of air and MPCM in the overall volume) and macro levels (thickness of the panels in the building wall) and are determine the overall building performance. By varying those parameters, it is possible to find a configuration of NRG-Panels that would result in the best possible building performance – an optimum configuration. While in the context of LCA and LCCA, the term “parameter” is commonly used for such variable values that impact the result of the assessment, in the context of mathematical optimisations, “variable” is a more correct term. Since this chapter revolves around the optimisation of NRG-Panels and the performance of the demonstrator building, further in the text, only the term “variable” will be used to avoid confusion. Within the equations and other mathematical formulations below, the variables will be denoted as x_1 , x_2 , etc., according to the list of variables above.

The micro-level variables were implemented as follows. For the type of PCM, the properties of commercially available bio-based PureTemp PCM were obtained from the manufacturer's website [157]. From all of the PCMs available, only 11 were taken for this study based on their reported melting temperatures: PT4, PT8, PT15, PT18, PT20, PT23, PT25, PT27, PT28, PT29, and PT37 (the number in the name of PCM represents the melting temperature in degrees Celsius). PCMs with higher or lower melting temperatures than those selected were not considered since they fall beyond the regular building operation temperatures. From the datasheets, the properties of each PCM necessary for further calculations were extracted: density, thermal

conductivity and the differential scanning calorimetry (DSC) curve. The DSC curves have then been digitised to extract the numerical data from them using WebPlotDigitizer v4 software [158]. The resulting tabular DSC has then been further processed to fit the specific requirements of EnergyPlus: it has been converted to specific enthalpy, fitted using 12-segmented linear regression (*piecewiselm* function from MATLAB Central File Exchange has been used [159]) and extrapolated to cover the range of temperatures from -100 °C to 100 °C. The type of PCM has been assumed to only have an impact on the thermal performance of the building, but the embodied emissions and costs were considered to be the same among all the PCMs. Compared to the PCM with a melting temperature of 24 °C that has been used in the actual demonstrator buildings, selecting another PCM could potentially lead to reduced energy consumption of the building.

The second micro-level variable, MPCM shell material, has been considered to have two possible options: inorganic coacervate (IC) and melamine-formaldehyde (MF). Those two kinds of encapsulation techniques differ greatly in their manufacturing processes and, consequently, the resulting environmental impacts and costs, as it has been presented in detail in Chapter 4. This variable will thus have an impact on the overall building-level environmental costs as well as the economic costs of building construction. Furthermore, from the building energy performance standpoint, the MPCM shell type will have a significant impact on the overall heating and cooling demand due to the difference in the PCM load factors (the volumetric fraction of PCM core in an MPCM particle): 0.685 for IC MPCM and 0.755 for MF MPCM.

The meso-level variables are both related to the volumetric fractions and proportions of the different components in NRG-Foam and NRG-Panels. NRG-Foam can be divided into three main components: cementitious matrix, MPCM particles and air bubbles. The cementitious matrix and MPCM particles together form a cementitious paste, which makes up the solid part of NRG-Foam, and the rest is considered to be air. When the volumetric fraction of MPCM particles in the cementitious paste increases, those particles replace cementitious matrix material. From LCA and LCCA perspectives, this results in an increase in embodied environmental emissions and costs. From the thermal whole-building performance, this increase in MPCM fraction affects the effective thermal conductivity of NRG-Panels, reduces their density, as well as leads to an increase in their heat storage capacity. The final effect of those changes on energy consumption is not straightforward and is assessed using energy simulations in EnergyPlus. Higher porosities, in turn, lead to lower environmental impacts and costs as well as to lower thermal conductivity, but at the cost of decreasing heat storage capacity. The overall effect of porosity on the building energy consumption for heating and cooling can also be explored via EnergyPlus simulations.

The macro-level variable, NRG-Panel thickness, represents the thickness of the insulation layer in the wall of the demonstrator building. While the impact of the thickness on the overall construction and demolition costs is

straightforward, the connection to the lifecycle environmental impacts and energy consumption for heating and cooling is more complex and depends on a multitude of other factors. The overall effect of NRG-Panels' thickness on the energy costs and environmental costs objectives can only be obtained from energy simulations.

Objectives definition

The essential part of any optimisation is defining what should be optimised, or, in mathematical terms, the objective function. When it comes to building performance, there are multiple ways to define it and, consequently, many possible objectives that either should be maximised or minimised. In Chapter 4, the building performance has been evaluated in environmental and economic terms using whole lifecycle environmental and economic costs. This chapter takes those metrics as a basis and defines three objectives to be optimised:

- Lifecycle environmental costs, EUR
- Lifecycle economic costs of energy use for heating and cooling, EUR
- Construction and demolition costs, EUR

A notable change compared to Chapter 4 is the separation of the lifecycle costs into two objectives. This change is to better reflect the real-world nature of construction projects where multiple stakeholders are interested in different aspects of building performance and, consequently, seek to optimise different objectives. In the context of the case study presented here, the Lifecycle environmental costs objective is representative of the interests of the environmental agency, Construction and demolition costs – building owner and Lifecycle economic costs of energy use for heating and cooling – of the building occupant. It can also be argued that those objectives roughly represent the triple-bottom line of sustainability. Lifecycle environmental costs are clearly attributable to the environmental sustainability domain, and construction and demolition costs – to the economic. The heating and cooling costs arise from the necessity to keep the temperature in the building within the comfortable range for the occupant and thus relate to the social aspect of sustainability.

Building energy simulation model parametrisation

The simulation of the energy performance of the demonstrator buildings in Sofia in Chapter 4 has been performed using EnergyPlus software [95]. In this chapter, the same software and general approach are used. EnergyPlus relies on two main input files: one contains information on the building configuration, constructions, materials, etc. and the other one – the weather data. Since the configuration of the insulation layer is not fixed in the case presented in this chapter, the building configuration input file will need to be generated dynamically depending on the set of input variables described

above. More specifically, the following parameters of NRG-Panels will need to be calculated, recorded in the file and passed to EnergyPlus for the simulation:

- Thickness of the panels
- Thermal conductivity
- Temperature-thermal conductivity table for materials with temperature-dependent thermal conductivity
- Density
- Temperature-enthalpy table
- Specific heat

The thickness of the panels is simply the same as the thickness variable defined above and does not need any processing. It is just passed directly to the EnergyPlus model.

The thermal conductivity of NRG-Panels depends on the PCM material, porosity and fraction of MPCM. The final thermal conductivity of NRG-Panels was calculated using the Lewis-Nielsen model [82], [83] already described in Section 2.2.4. However, in this study, the model has been applied twice. In the first step, the thermal conductivity of the solid fraction of NRG-Panels has been calculated based on the thermal conductivities of cementitious paste (matrix) and MPCM particles (filler). NRG-Panels are composed of the solid fraction and air bubbles, and so the final thermal conductivity of the panels can be calculated using the thermal conductivity of the solid fraction obtained in the previous step and the thermal conductivity of air. It is also important to mention that the thermal conductivity of PureTemp PCM material differs between liquid and solid states. Consequently, the final thermal conductivity of NRG-Panels will also be different depending on the temperature. EnergyPlus allows the provision of such variable thermal conductivity, and the final thermal conductivity of NRG-Panels has been specified as Temperature – Thermal conductivity table rather than a single value. This allows to better account for the real-world behaviour of PCM. Table 5.1 lists the parameters and other input variables for the Lewis-Nielsen models used for calculations in this chapter.

Table 5.1: Parameters used for the calculation of thermal conductivity of NRG-Panels.

Parameter	Step 1 (Cementitious foam + MPCM)	Step 2 (Solid fraction + air)
Shape coefficient, A	1.5	1.5
Maximum packing fraction, ϕ_m	0.601	0.7405
Thermal conductivity (matrix), $W \cdot m^{-1} \cdot K^{-1}$	0.588 (cement paste)	Calculated in Step 1
Thermal conductivity (filler), $W \cdot m^{-1} \cdot K^{-1}$	From the PureTemp datasheets, depends on the value of x_3	0.025 (air)
Volumetric fraction of filler	x_2	x_1

The density of NRG-Panels depends on the densities of all the components in the mix design and their volumetric fractions. The volumes of all components that NRG-Panels comprise are also necessary for the calculations within the parametric LCA/LCCA model. Within the optimisation model developed as a part of this chapter, the calculation of the final density of NRG-Panels has been performed together with LCA/LCCA calculations and then passed to the parametric building energy model.

As it has been described in the section above introducing the variables used in this study, the enthalpy curve of PCM has been built based on the DSC measurements provided in the manufacturer's datasheets. The final enthalpy of NRG-Panels is dependent on the individual enthalpies of its components and their volumetric fractions and can be calculated using the mixture law. The approach here is the same as in Chapter 2 (see Section 2.2.4 and Equations 2.5, 2.6 and 2.7) with two differences related to the requirements of EnergyPlus. First of all, in Chapter 2, the Enthalpy has been a singular value and has been calculated on a given interval of temperatures. For EnergyPlus simulations, enthalpy should be provided in tabular form with multiple Temperature - Enthalpy pairs covering the interval of temperatures from -100 °C to 100 °C. Secondly, while in Chapter 2 volumetric enthalpy has been used, EnergyPlus works with specific enthalpy. Specific enthalpy of NRG-Panels (h_{eff}) can be calculated by simply dividing their volumetric enthalpy (H_{eff}) by the density of the panels (ρ_{eff}):

$$h_{eff} = H_{eff} / \rho_{eff} \quad (4.1)$$

The resulting Temperature - Specific enthalpy data pairs are then passed to EnergyPlus. Finally, the specific heat of NRG-Panels has been calculated based on their specific enthalpy as follows:

$$c_{eff} = \min \frac{\Delta h_{eff}}{\Delta T} \quad (4.2)$$

where Δh_{eff} and ΔT are the distances between data points in the abovementioned Temperature – Specific enthalpy table. The minimum value is taken because specific heat capacity is temperature-dependent and is influenced by the phase transition of PCM, but the required value is the specific heat capacity only including sensible heat.

LCA and LCCA parametrisation

The parametrised LCA/LCCA model has been built on the basis of the model presented in the previous chapter. Unlike the solution introduced in Chapter 2, where LCA and LCCA models were parametrised in OpenLCA software and then connected to a MATLAB optimisation model, in this chapter, all calculations are performed in MATLAB. This change has been necessary due to the slow speed of OpenLCA calculations, leading to extremely long optimisation times.

The parametric model developed in this chapter works as follows. First, the overall LCA inventory over the whole building lifecycle has been divided into two parts: fixed and variable. The variable part of the inventory consists of all the individual processes that are impacted by the variables. In the case presented in this chapter, the variable inventory includes everything related to the production, use and EoL of NRG-Panels. For each individual process in the variable inventory, its impact per unit of measurement (e.g., environmental/economic impacts per kg of material for production of materials or per kWh for electricity consumption) is known and is already obtained in Chapter 4. The amounts of each of the components of the variable inventory can be calculated based on the values of the variables. Denoting the known environmental impacts as a vector $e = [e_1, e_2, \dots, e_n]$, economic impacts (costs) – as vector $c = [c_1, c_2, \dots, c_n]$ and calculated amounts for each process in the inventory – as vector $a = [a_1, a_2, \dots, a_n]$, the final total variable impacts can be calculated as the dot product of two vectors: $E_v = e \cdot a$ for environmental impacts and $C_v = c \cdot a$ for costs.

The fixed part of the inventory is not impacted by the variables and includes, e.g., manufacturing and EoL of demonstrator building materials other than NRG-Panels, as well as construction and demolition processes of demonstrator buildings. The impacts from the fixed part of the inventory can be grouped together and then added to the calculated impacts of the variable inventory. The final impacts of the demonstrator buildings can thus be calculated as $E = E_v + E_f$ for environmental impacts and $C = C_v + C_f$ for economic impacts where E_f and C_f are the fixed environmental and economic costs, respectively.

In total, the inventory used for calculations in this chapter includes 23 variable components and one fixed component. Table 5.2 provides an overview of those as well as the associated environmental and economic costs.

Table 5.2: Overview of inventory components and their economic and environmental costs.

Level	Inventory component	Unit	Environmental cost per unit	Economic cost per unit
Macro (building-level)	Fixed impacts	1 building	8.65E+03	6.76E+04
Impacts of inventory processes that are used for the calculation of variable costs				
Micro (MPCM-level)	MF MPCM slurry	kg	5.32E-02	7.39E-01
	IC MPCM slurry	kg	1.04E-01	2.49E+00
	Energy used for concentration of MPCM slurry	kWh	6.67E-02	2.50E-01
	Transport of MPCM	t*km	3.03E-02	0.00E+00
Meso (NRG-Panels-level)	Cement	kg	5.03E-02	1.50E-01
	Metakaolin	kg	6.82E-02	2.28E-01
	Accelerator	kg	3.14E-01	3.32E+00
	Superplasticiser	kg	1.92E-01	1.58E+00
	Stabiliser	kg	0.00E+00	2.93E+00
	Tap water for paste production	kg	9.00E-05	5.00E-03
	Foaming agent	kg	4.14E+00	6.16E+00
	Tap water for foam production	kg	9.00E-05	5.00E-03
	Electricity use for panels production, renewable	kWh	3.86E-02	0.00E+00
	Electricity use for panels production, non-renewable	kWh	1.06E-01	3.00E-01
	Rainwater for panels production	kg	6.96E-05	0.00E+00
	Hazardous waste from panels production	kg	6.76E-02	0.00E+00
	Wastewater	kg	2.36E-04	0.00E+00
	Reinforcement mesh	kg	9.30E-01	1.52E+00
	Steel moulds	kg	5.50E-01	6.30E-01
	Panel transport	t*km	3.03E-02	0.00E+00
	Waste steel moulds for recycling	kg	3.69E-03	0.00E+00
	Waste panels for recycling	m ²	4.04E-01	3.00E-01
Macro (building)	Electricity use for heating and cooling	kWh	1.91E-01	1.10E-01

In order to be able to calculate the required amounts for each inventory component, in addition to the values of the variables, some other parameters of NRG-Paste, NRG-Foam and NRG-Panels should be specified. For example, the amount of cement required not only depends on the values of the variables but also on the water-to-binder ratio, cement-to-metakaolin ratio, as well as proportions of other additives (accelerator, superplasticiser, stabiliser) relative to the total amount of binder used. Similarly, the amount of moulds needed depends on the thickness of the panels variable but also their width and height. Those constants necessary for calculations were obtained based on the experiments and tests conducted by various project partners and are provided in Table 5.3.

Table 5.3: Constant parameters related to the production process of NRG-Panels.

Constant parameter	Value
Weight ratio of metakaolin to cement	0.146
Water-to-binder ratio	0.4
Weight ratio of accelerator to binder	0.02
Weight ratio of superplasticiser to binder	0.005
Weight ratio of stabiliser to binder	0.029
Ratio of foaming agent in the foam	0.02
NRG-Panel width (m)	0.4
NRG-Panel height (m)	0.3

To calculate the amounts of each of the components of the inventory, a script has been written in MATLAB. As it was mentioned, parametric energy models and LCA/LCCA models are interconnected. The parametric energy model requires the provision of the final density of NRG-Panels, and it can be calculated when the amounts of all of the inventory parts are known. In the opposite direction, one required part of the variable inventory is the electricity consumption for heating and cooling. Thus, both LCA/LCCA calculations and energy simulations are performed alongside each other within the same function.

Foam stability constraint

In Chapter 2, the foam stability constraint has been introduced. This constraint defines the relation between the maximum possible fraction of MPCM and the porosity of NRG-Foam: with increasing MPCM fraction, the maximum achievable porosity of the foam decreases. This constraint is based on the experimental investigations of NRG-Foam. Similarly to Chapter 2, the impact of this stability constraint on the optimisation results is also analysed in this chapter. First, the optimisations are run without taking the constraint into account. This can be seen as the ideal case. After that, the constraint is introduced, and optimisations are run again. Compared to Chapter 2, where the stability constraint covered the range of porosities from 0.4 to 0.92, in this

chapter, it has been extrapolated to cover the whole range of porosities from 0 to 0.95. Figure 5.2 shows the graphical representation of the final extended stability constraint.

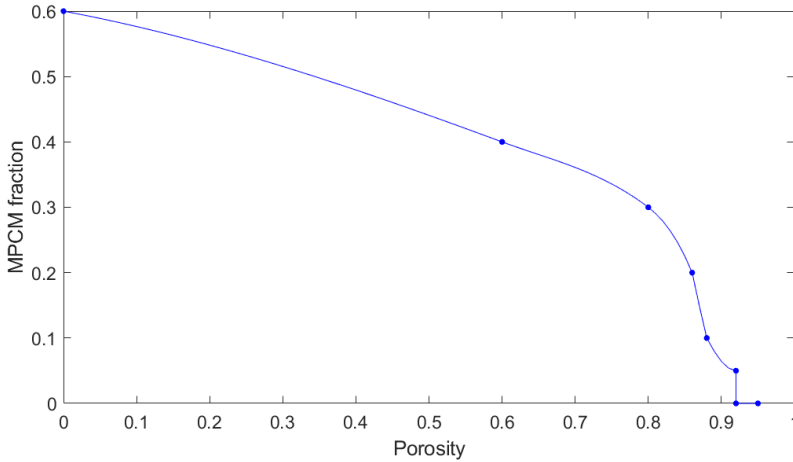


Figure 5.2: NRG-Foam stability constraint.

Optimisation problem setup in Matlab

Due to the complex nature of the optimisation problem (non-convex mixed-integer problem with high dimensionality), the genetic algorithm has been chosen as an optimisation algorithm. More specifically, the *ga* function in MATLAB has been used. The optimisation has been run in a parallelised mode using all 24 cores of the Intel Core i9-13700KF processor simultaneously. Parallelisation allows for performing simulations much faster compared to a regular single-threaded option. Further, the optimisation has been run in two steps with slightly different settings. First, it has been run for 12 hours with a relatively low crossover fraction setting of 0.6 and a large population of 480 members. This allows the genetic algorithm to better explore the solution space. The optimal solution from this first step has been saved as an intermediate best. After that, the crossover fraction has been changed to 0.85, and the population has been reduced to 72 members. The genetic algorithm has then been run with those new settings, with the starting point set at the intermediate best obtained in the previous step. This allowed it to converge closer to the actual optimal solution located on the edge of the solution space. The result of the second optimisation step has been taken as the final optimum solution. The optimisation has been performed this way for each of the three objectives described before. Table 5.4 provides an overview of parameters used in the genetic algorithm setup in MATLAB.

Table 5.4: Genetic algorithm parameters.

Parameter	Setting (Step 1)	Setting (Step 2)
Population size	480	72
Crossover fraction	0.6	0.85
Time limit, sec.	43 200	3600
Function tolerance	1E-6	1E-6

5.3 Results and discussion

5.3.1 Optimal configurations

The resulting optimal configurations of NRG-Panels for each of the three objectives are provided in Table 5.5 alongside the reference configuration that has been used in the demonstrator buildings in Sofia.

Table 5.5: Optimised configurations of NRG-Panels.

NRG-Panels configuration	Porosity	Fraction of MPCM in paste	PCM melting temperature, °C	Shell type	Thickness, m
Minimised lifecycle environmental costs	0.95 (maximum possible)	0.6 (maximum possible)	18	MF	0.3 (maximum possible)
Minimised economic costs of energy consumption	0.95 (maximum possible)	0.6 (maximum possible)	18	MF	0.3 (maximum possible)
Minimised construction and demolition costs	0.95 (maximum possible)	0	-	-	0.02 (minimum possible)
Reference					
Real-world demonstrator buildings configuration	0.87	0.1	24	MF	0.1

The optimal configurations for the minimisation of lifecycle environmental costs and economic costs of energy consumption turned out to be the same. Those have the highest possible porosity of 0.95, maximum possible fraction of MPCM of 0.6 and maximum possible thickness of 0.3 m. The optimal MPCM is PT18 with a melting temperature of 18 °C and a melamine-formaldehyde shell. The fact that those two configurations are the same signifies that in this particular case, environmental and social components of building performance are aligned, and there is no trade-off between them.

In the case of the minimisation of construction and demolition costs, the optimal configuration is also the one with maximum porosity, but in contrast to the first two objectives, without MPCM included and with the minimal possible thickness. This highlights the existence of a trade-off between the interests of the building owner and the other two stakeholders (building user and environmental agency).

The optimal configurations of NRG-Panels are significantly different from the real-world panels used in the demonstrator buildings in Sofia. First of all, all optimised results favour higher porosities. The actual values of MPCM fraction (0.1) and panel thickness (0.1 m) of NRG-Panels in the demonstrator building were between the optimal configurations but much closer to the configuration which minimises construction and demolition costs. However, since the main goal of real-world testing is showcasing the energy and environmental performance of NRG-Panels, increased thickness and fraction of MPCM would have been beneficial. It is also interesting to point out a large gap in PCM melting temperatures between the optimised configurations and the reference one. While in the test NRG-Panels PCM with a melting temperature of 24 °C have been used, the optimised material includes PCM with a 6 °C lower melting temperature.

5.3.2 Optimal configurations in the constrained case

When the stability constraint is introduced, the optimal results change drastically. Table 5.6 provides the optimal NRG-Panels configurations in the constrained case.

Table 5.6: Optimised configurations of NRG-Panels with the foam stability constraint taken into account.

NRG-Panels configuration	Porosity	Fraction of MPCM in paste	PCM melting temperature, °C	Shell type	Thickness, m
Minimised lifecycle environmental costs	0.95 (maximum possible)	0	-	-	0.3 (maximum possible)
Minimised economic costs of energy consumption	0.95 (maximum possible)	0	-	-	0.3 (maximum possible)
Minimised construction and demolition costs	0.95 (maximum possible)	0	-	-	0.02 (minimum possible)
Reference					
Real-world demonstrator buildings configuration	0.87	0.1	24	MF	0.1

As can be seen from the table, the optimal configuration is now the foam without MPCM and with maximum porosity for all of the objectives. This result highlights the fact that, in the given case, increasing porosity provides larger benefits than the addition of MPCM. For example, the configuration with 0.95 porosity and no MPCM performs better than a configuration with 0.92 porosity and 0.05 fraction of MPCM, which is also feasible.

5.3.3 Optimised building performance and comparison with EPS

Having obtained the optimal configurations of NRG-Panels, it is now possible to compare the building-level performance of the demonstrator buildings in the as-built case, optimised case (both unconstrained and constrained), as well as with the building containing EPS insulation of a comparable configuration. Figure 5.3 below shows such a comparison across three analysed objectives.

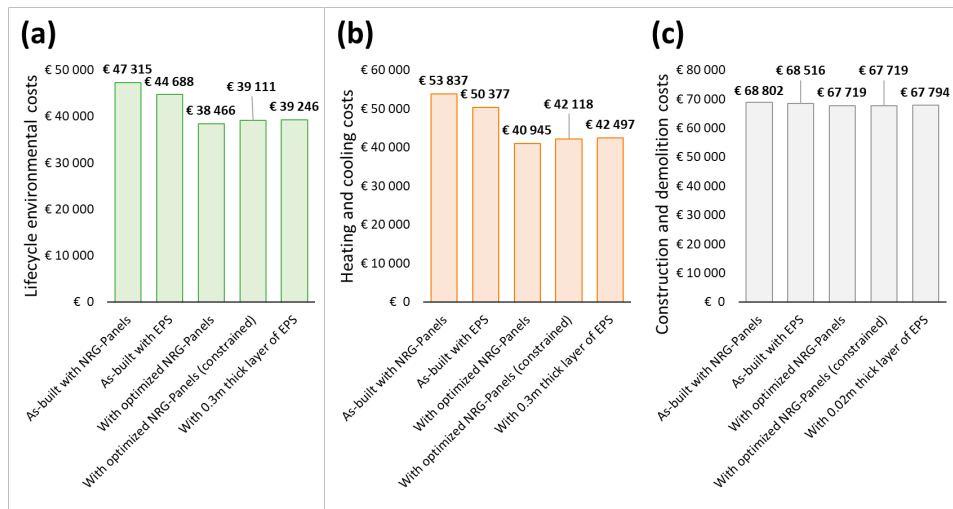


Figure 5.3: Building performance comparison between the reference as-built case, buildings with optimised NRG-Panels and a building with a comparable EPS layer. The comparison is provided for three objectives: Lifecycle environmental costs (a), Economic costs of energy consumption for heating and cooling (b) and Construction and demolition costs (c).

As Figure 5.3 shows, optimising the configuration of NRG-Panels provides great benefits for building performance, especially when it comes to environmental performance and the economic costs of energy for heating and cooling. In the optimised configuration, those are reduced by 19% and 24% respectively. With the stability constraint taken into account, the performance shows a minor dip, but even in this case, the building with optimised NRG-Panels would have 17% better environmental costs and 22% lower energy costs compared to the real-world reference case. In the case of

construction and demolition costs, the change is not as drastic as in the case of the other two objectives, and the resulting optimised building would demonstrate 2% lower costs.

In all of the cases across all three objectives, the building with optimised NRG-Panels shows better performance than a building with a comparable layer of EPS insulation (0.3 m thick for the first two objectives and 0.02 m for the third). In the case of environmental costs and energy costs, the improvement in the building performance is driven by the reduction of energy consumption. More specifically, the reduction of heating demand. While the optimised results demonstrate that the addition of MPCM is beneficial (the optimal unconstrained case had 0.6 fraction of MPCM), those benefits do not come from the energy-storing properties of PCM. In reality, the improvement is caused by the reduction in thermal conductivity of NRG-Panels: the cementitious matrix that NRG-Panels are based on is sufficiently more thermally conductive than MPCM particles, and their addition has a great impact on the final effective thermal conductivity of NRG-Panels. Consequently, it can be argued that the resulting optimal configurations – while demonstrating performance comparable with EPS – are essentially analogous to already existing cementitious foams that only provide insulating functionality with negligible energy-storing performance.

While the results obtained in this chapter might seem negative when it comes to the perspective of NRG-Panels and especially the benefits of their energy-storing functionality, it must be stressed that all the results presented so far were focused on a very narrow case: the demonstrator buildings that were built in Sofia, Bulgaria and their current-day performance. From a climate standpoint, Sofia is characterised by relatively long and cold winters, which, in turn, results in high energy demand for heating. In such conditions, the insulating performance of NRG-Panels is more important than their energy-storing performance, and the best material is the one with the lowest thermal conductivity. However, the area of material application is not limited to Bulgaria, and it could be expected that NRG-Panels would perform differently in other climates. Furthermore, as it was mentioned before, the assessments and optimisations presented so far were based on energy simulations that utilised typical meteorological year (TMY) weather data. This data provides a good representation of historical climatic conditions in the given location, but does not take into account the effects of climate change. Yet, buildings are characterised by long lifetimes during which the climatic conditions will most likely drift away from the historical ones. Thus, in order to accurately assess the potential of NRG-Panels, it is essential to extend the scope of the analysis to other geographical locations as well as investigate the effects of climate change on their performance. The following chapter provides such a scope extension and identifies the areas of the best potential for NRG-Panels application across Europe.

5.4 Concluding remarks

Following the hypothesis proposed in Chapter 4, which suggests that the configuration of NRG-Panels in the demonstrator buildings in Sofia has not been well-suited for the local climatic conditions, this chapter presents a case-specific optimisation of NRG-Panels design. First, LCA and LCCA models were parametrised, allowing to calculate the final environmental and economic costs based on the variable parameters of NRG-Panels. Then, on the basis of those models, three objectives were defined describing the building performance from the perspective of three different stakeholders. Consequently, each of the objectives has been optimised to find the best possible configuration of NRG-Panels from the viewpoint of each respective stakeholder. The main findings of this chapter are listed below.

- In the unconstrained case, optimal configurations for environmental costs and energy costs objectives were identical, favouring high porosity (0.95), maximum MPCM fraction (0.6), and maximum thickness (0.3 m).
- The constrained optimisation resulted in configurations without MPCM and maximum porosity for all objectives, highlighting the importance of porosity (insulating function) over MPCM content (heat-storing functions) in the climatic conditions of Sofia.
- Optimised NRG-Panels configurations showed improved performance compared to the as-built case and EPS insulation across all objectives.
- The improvement in building performance was primarily driven by reduced thermal conductivity rather than the energy-storing properties of PCM.
- While NRG-Panels can outperform EPS insulation, their optimal configurations in this specific case resemble existing cementitious foams with minimal energy-storing functionality.
- The findings suggest that the climatic conditions in Sofia might not be optimal for NRG-Panels, indicating that further analysis of NRG-Panels' performance under various climatic scenarios is necessary.

6

CLIMATE-DEPENDENT DESIGN OF NRG-PANELS AND IDENTIFICATION OF FAVORABLE LOCATIONS FOR NRG-PANELS APPLICATION

Following the suggestion originating from Chapter 5, that climatic conditions of Sofia were suboptimal for NRG-Panels, this chapter focuses on climate-specific analysis of NRG-Panels' performance and their optimisation in different climatic contexts. Using multi-objective optimisation techniques, NRG-Panels were optimised for 53 locations across Europe. Furthermore, for a selected subset of locations, optimisations were also performed using future climate projections to investigate the effects of climate change. For all analysed cases, the building-level performance of NRG-Panels was compared to EPS. The results showed that NRG-Panels' performance is highly dependent on local climatic conditions, with the Mediterranean region characterised by the Csa climate under the Köppen-Geiger climate classification showing the highest potential for NRG-Panels application. Moreover, climate change was observed to significantly impact the optimal configuration and performance of NRG-Panels, highlighting the importance of taking it into account in decision-making related to thermal materials' design and thermal performance of buildings in general.

6.1 Introduction

The final building-level performance of thermal performance materials (insulating and energy-storing) is strongly dependent on the climatic conditions of the location where the material is applied or is expected to be applied (see, e.g., [38], [160], [161]). Yet, when a novel thermal material is developed, it generally cannot be tested in the whole possible range of climates. In reality, when such a material is being tested at the prototype level, the testing is usually limited to just one or small number of locations due to unavoidable budget and time limitations. The envisioned geographical area of application of a novel thermal material, however, is potentially wider and is not limited to selected test locations. To investigate the potential of a novel thermal material on a larger scale, it thus becomes essential to utilise computational models and simulate the behaviour and performance of the material in a variety of climatic settings where physical testing is not possible.

In the context of this dissertation, as it has been illustrated in the preceding chapters, NRG-Panels were shown to have limited applicability in the demonstrator buildings' physical location (Sofia, Bulgaria). While the addition of MPCM in the material has provided some benefits, those benefits originated from the associated reduction in thermal conductivity and not from the improved thermal storage capacity. Furthermore, taking into account the constraint associated with the stability of the NRG-Foam, the best feasible configuration of NRG-Panels in the context of the climate in Sofia is the one with maximum porosity and no MPCM added, which is essentially equivalent to already existing materials such as autoclaved aerated concrete.

To a large extent, those results are prompted by the cold climatic conditions, resulting in high space heating demand. In such conditions, the low thermal conductivity of the envelope is more beneficial than the increased heat storage capacity of it. However, even within Europe, a variety of different climatic conditions can be observed that differ in temperatures, solar radiation levels, precipitation, and wind speeds, and it can be expected that NRG-Panels would perform differently under those conditions. Moreover, in the context of NRG-Panels' design optimisation, the optimal configuration of NRG-Panels might also vary significantly depending on the location of the building to which they are applied.

Furthermore, beyond the spatial variability of the climate, it is important to investigate its temporal variability and the associated effects on the performance of NRG-Panels. Indeed, the climate in a given geographical location is not fixed; it is constantly evolving, and research shows that this change is accelerating [162], [163]. Given the rates at which the climate changes and the long lifetime spans of buildings, the performance of new construction and especially insulation materials should be analysed in the context of the future climate. Further, in the context of material design optimisation, the material that is optimised for the current or historical climate might become suboptimal if the climate change effects are taken into

account. Moreover, the application potential of NRG-Panels might also be different depending on whether the current or future climate is considered: a geographical location that does not look promising currently might become so in the future.

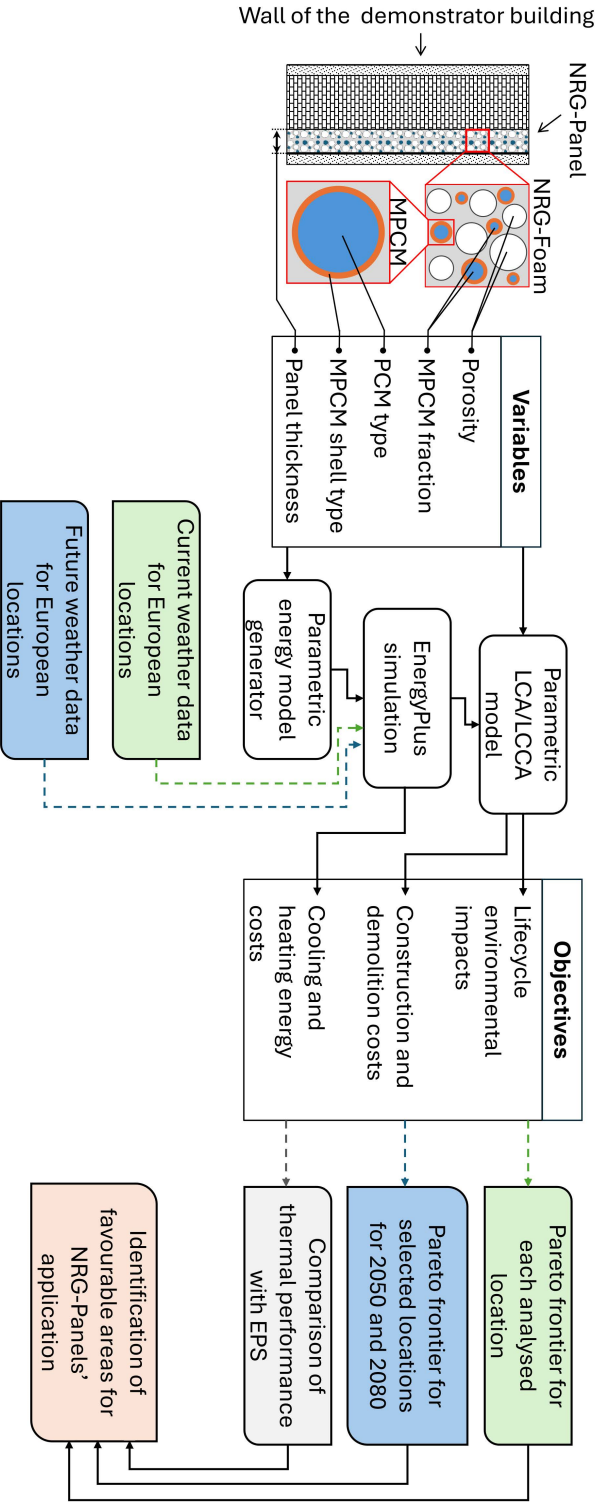
This chapter is focused on the climate-dependent design of NRG-Panels, where they are optimised with the extended geographical and temporal scopes. For the extended geographical scope, multiple locations across Europe are selected, and NRG-Panels are optimised using weather data representative of the climatic conditions in those locations. For the temporal scope extension, a subsample of locations is created, and the weather data for those locations is then modified to embed the climate change projections from the Intergovernmental Panel on Climate Change (IPCC) for the years 2050 and 2080. Based on the results of the optimisations, the favourable areas for NRG-Panels application are identified.

6.2 Methodology and modelling approach

6.2.1 Overview

Figure 6.1 shows the graphical representation of the overall approach used in this chapter.

As can be observed, the methodology is very closely resembling the one introduced in Chapter 5, with extra layers added to it. Namely, instead of using the weather data for a single geographical location and the present climate in this location, the scope of the analysis has been extended to include multiple locations as well as future climate projections. Furthermore, while the objectives stayed the same, this chapter implements multi-objective optimisation resulting in Pareto frontiers for each of the analysed climatic conditions. The chapter concludes with the identification of the promising areas for NRG-Panels application based on the obtained Pareto frontiers and a comparison of thermal performance against EPS. The following sections describe this methodology in detail.



6.2.2 Geographical scope extension

For extending the geographical scope of NRG-Panels' performance assessment and optimisation, 53 locations spanning across Continental Europe, Ireland, the United Kingdom and Turkey have been selected. Those locations include all cities with populations larger than 1 000 000 inhabitants, as well as all of the capitals, excluding those with populations smaller than 20 000 inhabitants. The population data has been taken from the GeoNames database [164] and only accounts for the city population, excluding the suburbs. Figure 6.2 shows all of the selected locations on the map.



Figure 6.2: Map of geographical locations selected for the analysis.

To ensure consistency with the previous chapters, the typical meteorological year (TMY) weather data files for each of the locations have been obtained from the same source (PVGIS [154]). Those weather files were then used to run EnergyPlus simulations within the optimisation problem.

6.2.3 Temporal scope extension and generating weather data for future climates

To explore the effects of climate change on the performance of NRG-Panels, the CCWorldWeatherGen tool [165], [166] has been used. This tool allows the generation of future climate weather files based on the current (baseline) weather files by using climate change projections developed by the

Intergovernmental Panel on Climate Change (IPCC). It has scenarios built in to make projections for 2050 as well as for 2080. The tool works by adjusting the weather data in the input file (temperature, irradiation, cloud cover, precipitation rate, humidity, atmospheric pressure, wind speed) to align with IPCC projections and then generates an output morphed file that can be used to run energy simulations and to conduct assessments of future scenarios.

Due to the high computational load and time requirement for running optimisations, only a part of all 53 locations have been selected for extended temporal scope analysis. More specifically, only the following subset of cities has been analysed: Athens, Barcelona, Berlin, Istanbul, Lisbon, Madrid, Paris, Podgorica, Sofia, and Tirana. From those, Sofia has been selected since it is the actual location of the demonstrator buildings. Paris and Berlin represent cities with a milder climate and less contrasting yearly temperatures compared to Sofia. Other locations have been selected based on the analysis of the results of geographical scope extension, and represent the locations with an elevated applicability potential of NRG-Panels.

6.2.4 Optimisation model setup

Unconstrained optimisation model setup

As mentioned earlier, the optimisation model used in this chapter is largely the same as the one described in Chapter 5, except for two major differences. First of all, while the objectives are the same as in Chapter 5 (Lifecycle environmental costs, Lifecycle economic costs of energy use for heating and cooling, Construction and demolition costs), in this chapter, multi-objective optimisation (MOO) is performed instead of multiple single-objective optimisations. MOO has already been used in Chapter 2 and, as discussed there, it is a convenient way of identifying and showing the trade-offs between the objectives. The presence of trade-offs has already been suggested in Chapter 5 since the optimal configuration of NRG-Panels was different depending on the analysed objective. Furthermore, looking at the optimisation problem from the standpoint of stakeholders, using single-objective optimisation results in three potentially different solutions, each of which is optimal for one stakeholder but does not take into account the interests of others. In reality, in case trade-offs are present, none of those extreme solutions would likely be selected as the final configuration. Instead, a solution somewhere in between has a higher chance of being accepted by all stakeholders. The exact choice is dependent on multiple factors such as the method of selection, the number of stakeholders and objectives, and the power (or weight) of each stakeholder. However, at the prototyping stage, there is no such information available. Stakeholders and objectives are not set in stone yet, and their weights are not certain either. And while some assumptions about the stakeholders and objectives representing their interests could be made already at the prototyping stage, their weights are specific to a particular construction project. The benefit of MOO in this context is that it allows one to find a set of optimal solutions (Pareto frontier),

each of which is representative of a particular distribution of weights between the stakeholders and their objectives. The analysis of the Pareto frontier provides a broad overview of the potential of NRG-Panels application as it highlights all possible configurations that are both feasible and attractive to stakeholders (or, in other words, optimal depending on their weights).

From the technical perspective, MOO has been implemented in MATLAB using the built-in *gamultiobj* function, which is based on the NSGA-II elitist multi-objective genetic algorithm [167]. For each input weather data file (current and future), the optimisation has been run on a computer with a 24-core Intel Core i9-13700KF processor in parallelised mode on all 24 cores simultaneously for 12 hours. At each generation, the whole population and the associated scores (values of objective functions) have been saved into a file. After the optimisation has been terminated, the final Pareto frontier has been obtained using a similar approach already described in Section 2.2.4.

In addition to MOO, in order to find extreme points of the Pareto frontier that the *gamultiobj* function might be struggling to reach in the given time, three single-objective optimisations have been run for each of the climatic conditions. It has been done in the following manner. First, the results of MOO have been analysed, and three configurations of NRG-Panels (each configuration is represented by a set of variable values) have been found that minimise each of the three objectives. Then, for each of the objectives, a single-objective optimisation using a genetic algorithm has been run using the corresponding configurations found from MOO as the starting point. This single-objective optimisation has been run for one hour. To illustrate the purpose of such a two-step approach to optimisation, let us imagine that after running MOO, it has been found that an extreme point of Pareto frontier that minimises energy consumption is provided by NRG-Panels with porosity of 0.94, MPCM fraction of 0.55, PCM type 4, MPCM shell type 2 and thickness of 0.27 m (this vector of values will be denoted as $x_{MOO} = [0.94 \ 0.55 \ 4 \ 2 \ 0.27]$). It can be seen that this solution is very close to the edge of the solution space, but is not exactly on the edge. This might be an actual optimal solution, but it also might be that the algorithm did not have enough time to converge and reach the optimum. Now it is possible to start a single-objective optimisation using x_{MOO} as the starting point. If x_{MOO} is an actual optimum point, the result of this second-round single-objective optimisation will be very close to or equal to it. On the other hand, if MOO did not manage to converge to an actual optimum, the result of the second-round single-objective optimisation will be closer to this actual optimum. For example, in the theoretical case used above, the resulting configuration might end up being $x_{SOO} = [0.949 \ 0.6 \ 4 \ 2 \ 0.299]$, which is located on the very edge of the solution space. This final configuration is a more precise representation of the extreme corner point of the Pareto frontier. Table 6.1 provides an overview of the parameters that were used to set up the optimisation in MATLAB.

Table 6.1: Key optimisation parameters used in this chapter.

Parameter	Multi-objective optimisation	Single-objective refinement optimisation
Population size	720	48
Crossover fraction	0.7	0.85
Time limit, sec.	43 200	3 600
Function tolerance	1E-6	1E-6
Starting point	Random	Obtained from MOO

The second difference between the optimisation setup in this chapter compared to Chapter 5 is the utilisation of multiple weather data files. There are 53 cities selected for the analysis with the extended geographical scope, and NRG-Panels' design has been optimised for each of those locations separately. This resulted in 53 Pareto frontiers. Further, a subset of 10 cities has been selected for the analysis with the extended temporal scope. For each of those cities, two weather files were generated: one representing the projected climatic situation in 2050 and another in 2080. NRG-Panels were then optimised using 2050 climate projections and 2080 climate projections, resulting in a total of 20 Pareto frontiers. Further, the constrained Pareto frontiers have been built for both current and future climates, for all the analysed locations. Thus, overall, 146 Pareto frontiers were obtained that were then analysed, compared with each other and used for the identification of the areas suitable for the application of NRG-Panels.

It is important to note that the purpose of this chapter is solely to investigate the impacts of different climatic conditions on the NRG-Panels' performance and application potential. Thus, the difference between LCA, LCCA and energy models presented in Chapter 5 and this chapter is limited to the input weather files, while the rest (environmental impacts of different processes, costs of materials and resources, transportation distances, etc.) is kept the same. The analysis presented in this chapter should thus not be perceived as a regionalised study but more like a sensitivity analysis. The results of such a study provide an initial indication of the potential of NRG-Panels in different climatic settings, but each of the locations requires a more in-depth follow-up analysis akin to the one presented in Chapters 4 and 5. Such an in-depth analysis, however, is highly time-consuming and, given the large number of locations under consideration, is beyond the scope of this work.

Integration of the foam stability constraint

Similar to the previous chapters, this chapter also examines the impact of the foam stability constraint on the optimisation results. The constraint itself has already been introduced in detail in Chapters 2 and 5, and this section will only focus on describing the approach to the integration of this constraint in

the study. As it has been mentioned above, the Pareto frontier in this chapter is obtained in a similar way to that described in Chapter 2. More specifically, as the genetic algorithm runs, every population member in every generation is recorded in a separate file (a member represents a possible configuration of NRG-Panels). After optimisation has finished, such a file would contain not only the resulting Pareto frontier but also every single intermediate NRG-Panel configuration that the optimisation algorithm has checked. It is then possible to take all of those recorded points and extract non-dominated solutions that would form the final Pareto frontier. This is done using the *getNonDominated* function in MATLAB [168]. This approach allows us to find a more detailed and full Pareto frontier. When the stability constraint is integrated, an additional step is introduced. All of the points recorded in the aforementioned file are first filtered based on the values of porosity and MPCM fraction: those configurations of NRG-Panels that do not satisfy the constraint are removed. The remaining configurations are then processed using the *getNonDominated* function to obtain the final constrained Pareto frontier.

It should be noted that the approach described above is simplified and cannot produce a detailed Pareto frontier. A more thorough way would be to introduce the constraint into the optimisation problem from the very beginning. However, this approach would imply that every optimisation problem for every geographical location must be run twice: without constraint and with constraint. Due to an extremely high computational time requirement for running the optimisations, such an approach has not been feasible within this work.

6.2.5 Assessment of NRG-panels' applicability in different climatic contexts

The assessment of the NRG-Panels' applicability is performed by combining two approaches: the analysis of the Pareto frontiers and the comparison of the performance with EPS insulation. While it is not possible to give a definitive answer to the question of whether NRG-Panels are suitable for a given geographical location or not, the provided analysis could help filter out the least promising locations and narrow down the scope for further in-depth assessments.

Analysis of material configurations in the Pareto frontier

As it has been outlined in previous sections, the main output of each optimisation performed in this study is a Pareto frontier, and the potential of NRG-Panels' application can be evaluated based on this Pareto frontier. Each point in the Pareto frontier is a possible configuration of NRG-Panels defined by 5 variables: porosity (x_1), MPCM fraction (x_2), type of PCM (x_3), MPCM shell material (x_4), panel thickness (x_5). From those variables, the ones defining the

applicability potential are porosity (x_1), MPCM fraction (x_2) and panel thickness (x_5). The following criteria can be identified:

- Porosity (x_1)

If the optimal NRG-Panel configuration has extremely high porosity (just like in the case presented in Chapter 5), such a material has a very limited energy storage capacity and is functionally very similar to already existing insulation materials such as aerated concrete. At very low porosities (close to 0.05), the material configuration is a cement/MPCM mix that has very limited insulating properties. Since NRG-Panels are developed as a dual-function material that possesses both insulating and energy-storing properties, the indicator of NRG-Panels' applicability can be argued to be higher for the cases where the obtained Pareto solutions have porosity somewhere in the middle between the lower bound of 0.05 and the upper bound of 0.95.

- MPCM fraction (x_2)

If obtained Pareto solutions have a low MPCM fraction, this would also indicate that NRG-Panels do not have great potential in this particular case: NRG-Panels without MPCM or with a very low fraction of MPCM are essentially just a regular foamed concrete.

- Panel thickness (x_5)

Very low panel thickness values of the obtained Pareto solutions indicate low potential for NRG-Panels as well. This implies that in this particular case, insulation might not be necessary altogether or necessary but in very limited amounts. This kind of situation might arise in mild warm climates where the implementation of insulation brings only minor benefits.

When looking at the visual representation of the Pareto frontier, it is easy to apply the criteria described above and distinguish between the cases with lower and higher potential for NRG-Panels application. However, if the number of analysed cases is large, it might be more convenient to define an indicator that would quantify this potential. There might be many ways to define such an indicator, but the one used in this chapter is expressed as follows:

$$P = \frac{1}{n} \sum_{i=1}^n \frac{(1 - x_1^i) * x_2^i * x_5^i}{0.95 * 0.6 * 0.3} \quad (6.1)$$

where n is the number of solutions in the Pareto frontier, x_1^i is the porosity value of the i -th Pareto solution, x_2^i is the MPCM fraction value of the i -th Pareto solution, x_5^i is the panel thickness value of the i -th Pareto solution.

This indicator calculates the average volume of MPCM across all Pareto solutions relative to the maximum possible volume of MPCM (0.95 is the maximum possible volume of paste, 0.6 is the maximum possible fraction of

MPCM and $0.3 \text{ m} \times 68 \text{ m}^2$ is the total volume of insulation in the demonstrator building). It is important to mention that this indicator should only be considered as the screening indicator and not as the definitive criterion of NRG-Panels' potential. Estimation of the actual potential (technical or market) requires an in-depth region-specific analysis.

6.2.6 Comparison of performance with EPS insulation in different climatic contexts

The comparison between the performance of NRG-Panels and EPS is performed based on the total building energy demand for heating and cooling. While a more comprehensive way would be to compare based on the full set of the objectives outlined above, this would require an in-depth regionalised study. This falls beyond the scope of this chapter, which is focused solely on the effects of different climatic conditions on the performance of NRG-Panels in the context of a demonstrator building.

The comparison between NRG-Panels and EPS has been performed as follows. For each of the climatic conditions analysed, a corner point of the Pareto frontier that results in the minimum building energy consumption has been extracted. Each of those points is an NRG-Panels configuration with specific porosity, MPCM fraction, PCM type, MPCM shell type and thickness. Next, the EPS-based comparison point should be selected. While the comparison between buildings containing NRG-Panels and EPS insulation of the same thickness is logical and straightforward, it can be argued that it is not accurate since NRG-Panels' configuration has been optimised for each given location, and EPS configuration (thickness) has not. In reality, there might be a different value of EPS layer thickness that would provide a lower energy consumption, and it would not necessarily match the optimal NRG-Panels thickness. To account for that, the comparison has been made between the optimised configuration of NRG-Panels and the optimised configuration of EPS. To obtain an optimal configuration of EPS, another optimisation problem was set up where the objective was the total energy consumption of the building for heating and cooling, and the single variable was EPS layer thickness. This optimisation problem has been solved for every analysed geographical location. Then, for each of the locations, the comparison has been made between the energy consumption of a demonstrator building containing optimised NRG-Panels and containing optimised EPS insulation.

For the comparison between NRG-Panels and EPS in future climates, the same approach has been utilised: EPS panels' thickness has been optimised for each analysed climate projection and the energy performance of demonstrator buildings containing optimised (for future climates) NRG-Panels and optimised EPS has been compared.

For both current and future climates, the comparison has been done with and without taking into account the effects of the NRG-Foam stability constraint on the optimal design of NRG-Panels. The resulting difference in

total energy consumption between a building with NRG-Panels and EPS can then be used as an indicator of the NRG-Panels' applicability potential under given climatic conditions: the larger the difference, the higher the potential. It is worth stressing again, however, that the discussed potential is tied to the given demonstrator building and is not indicative of the applicability potential in general.

6.3 Results and discussion

6.3.1 Results of optimisations with an extended geographical scope under current climatic conditions

Optimisation results and assessment of NRG-Panels' applicability in the unconstrained case

After running optimisations for all 53 geographical locations around Europe, the obtained Pareto frontiers were first visualised and compared to each other. This initial assessment of the results showed that for most analysed locations, the Pareto frontiers were nearly identical. It has also been observed that the indicator P defined by Equation 6.1 can act as a good determinant of (dis)similarity of Pareto frontiers for different locations: most of the locations with similar P -value showcased visually similar Pareto frontiers. Figure 6.3 provides an overview of the values of indicator P for each analysed location.

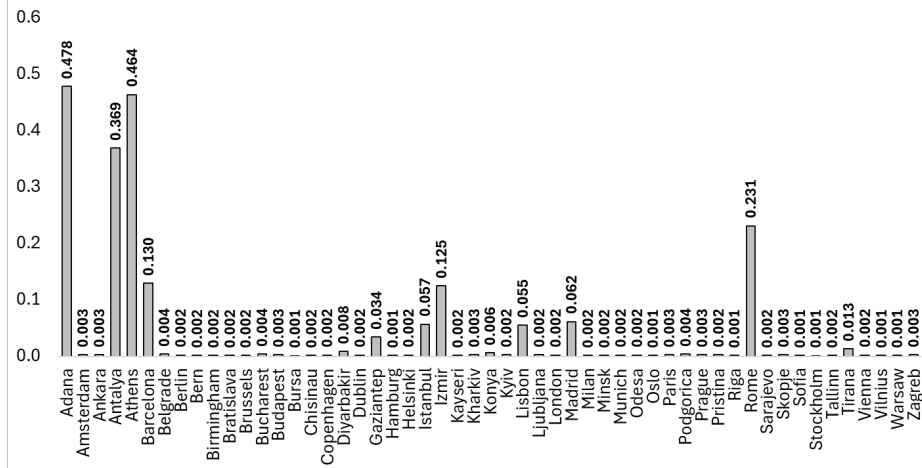


Figure 6.3: The values of indicator P for the analysed geographical locations.

For Sofia and multiple other locations, the calculated value of indicator P is similar and very small. It has been observed that up until the value of P approximately equal to 0.01, the Pareto frontiers were visually almost

identical and differed only in the values of objective functions (e.g., some locations had higher energy consumption). It is thus possible to use only one of those low-P locations as a representative case for all of them. Since Sofia has been the originally analysed location, it has further been used as a reference case.

Now let us take a closer look at the obtained Pareto frontiers for a selection of locations featuring different values of the indicator P. Figures 6.4, 6.5 and 6.6 show the Pareto frontiers for Sofia, Diyarbakir, Madrid, Rome, Adana and Lisbon. The first five of those cities are presented in the ascending order of the indicator P, and Lisbon is selected as a stand-out case that differs from other locations. The figures provide the Pareto front in the function space as well as in the variable space. The plots in the function space can be used to identify the trade-offs between different objectives. On the other hand, the variable space plots provide information on what possible material configurations are best suited to the given climatic conditions.

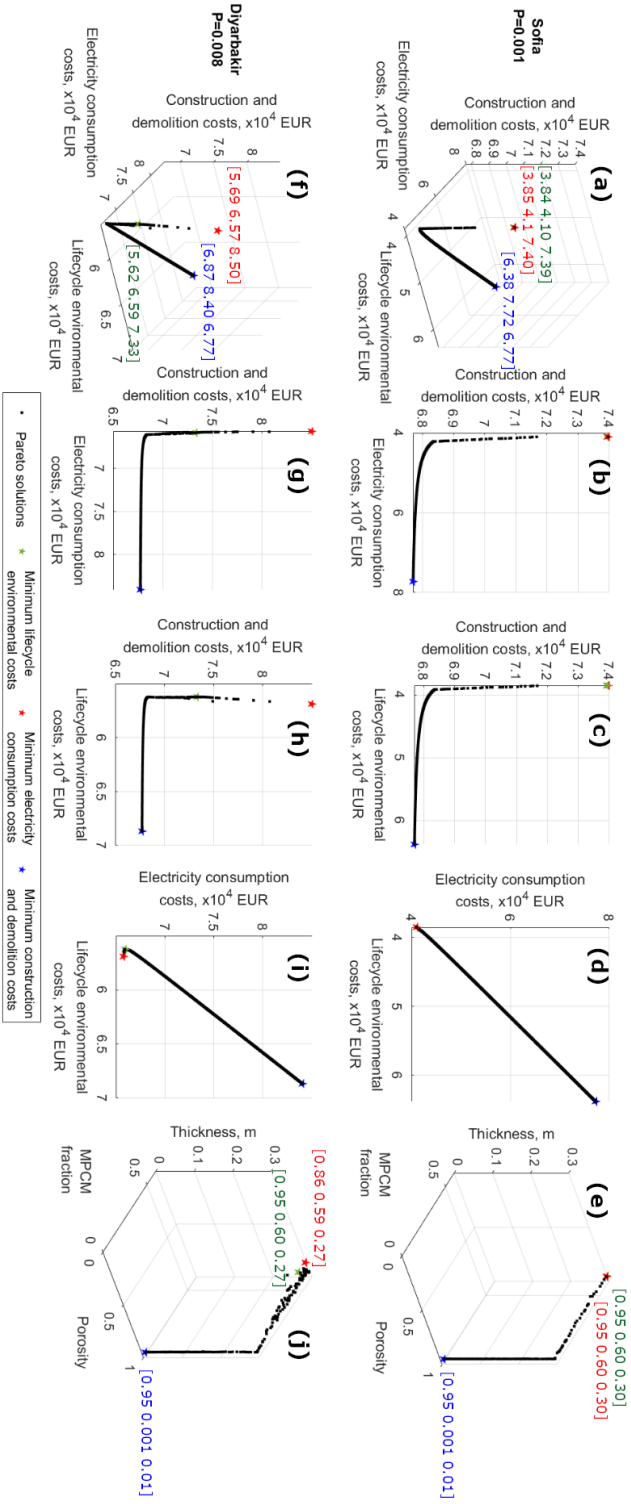


Figure 6.4: Pareto frontiers for Sofia (panels a–e) and Diyarbakir (panels f–j). Panels a–d and f–i show Pareto frontiers in the function space, and panels e and j – in the variable space. Panels a and f depict the Pareto frontier in three-dimensional space, while panels b–d and g–i show two-dimensional projections of the corresponding Pareto frontiers. Star-shaped markers indicate the location of the corner points of the Pareto frontier: green is the point corresponding to the minimum achievable lifecycle environmental costs, red – to the minimum achievable electricity consumption costs and blue – to the minimum achievable construction and demolition costs. In the variable space (panels e and j), the star-shaped points show the material configurations at which the corresponding Pareto corner points are achieved. The numerical vectors next to the star-shaped points provide the corresponding values of objective variables. The order of values in the vector is [lifecycle environmental costs; energy costs; construction and demolition costs] for the objective space and [porosity; MPCM fraction; panel thickness] in the variable space. Note that the scales are different between the axes and different cities.

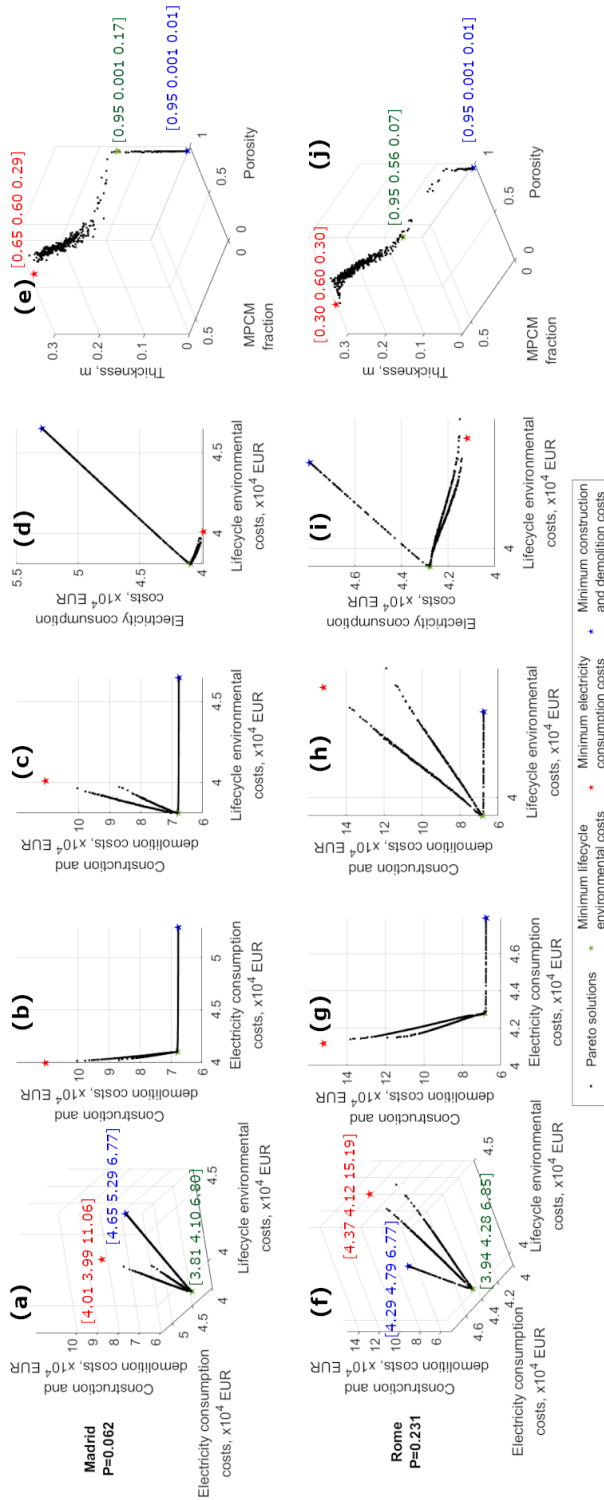


Figure 6.5: Pareto frontiers for Madrid (panels a-e) and Rome (panels f-j). Panels a-d and f-i show Pareto frontiers in the function space, and panels e and j - in the variable space. Panels a and f depict the Pareto frontier in three-dimensional space, while panels b-d and g-i show two-dimensional projections of the corresponding Pareto frontiers. Star-shaped markers indicate the location of the corner points of the Pareto frontier: green is the point corresponding to the minimum achievable lifecycle environmental costs, red - to the minimum achievable electricity consumption costs and blue - to the minimum achievable construction and demolition costs. In the variable space (panels e and j), the star-shaped points show the material configurations at which the corresponding Pareto corner points are achieved. The numerical vectors next to the star-shaped points provide the corresponding values of objectives or variables. The order of values in the vector is [lifecycle environmental costs; energy costs; construction and demolition costs] for the objective space and [porosity; MPCM fraction; panel thickness] in the variable space. Note that the scales are different between the axes and different cities.

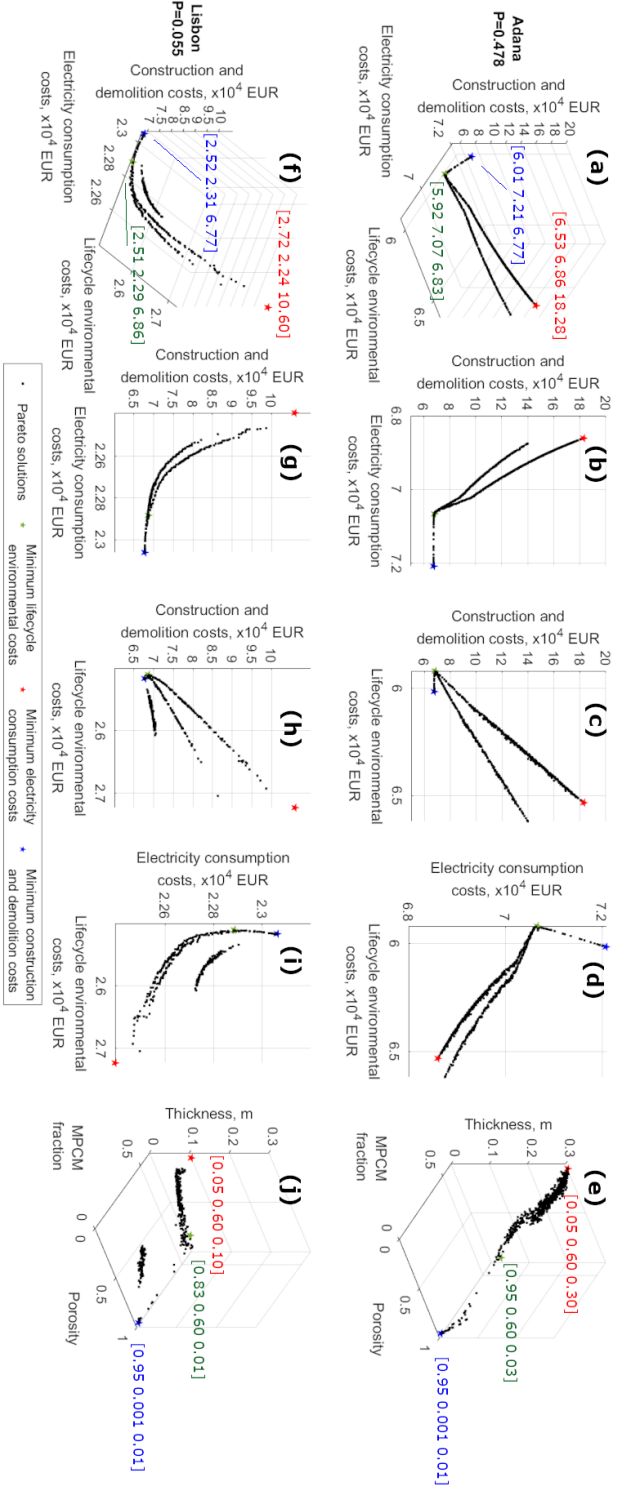


Figure 6.6: Pareto frontiers for Adana (panels a–e) and Lisbon (panels f–j). Panels a–d and f–i show Pareto frontiers in the function space, and panels e and j – in the variable space. Panels a and f depict the Pareto frontier in three-dimensional space, while panels b–d and g–i show two-dimensional projections of the corresponding Pareto frontiers. Star-shaped markers indicate the location of the corner points of the Pareto frontier: green is the point corresponding to the minimum achievable lifecycle environmental costs, red – to the minimum achievable electricity consumption costs and blue – to the minimum achievable construction and demolition costs. In the variable space (panels e and j), the star-shaped points show the material configurations at which the corresponding Pareto corner points are achieved. The numerical vectors next to the star-shaped points provide the corresponding values of objective variables. The order of values in the vector is [lifecycle environmental costs; energy costs; construction and demolition costs] for the objective space and [porosity; MPCM fraction; panel thickness] in the variable space. Note that the scales are different between the axes and different cities.

From comparing the presented Pareto frontiers for Sofia, Diyarbakir, Madrid, Rome and Adana and looking at them as a whole, some general trends can be observed (the case of Lisbon is, as mentioned, an outlier and will be discussed separately below). First of all, for all of the selected locations, there is a trade-off between electricity consumption and construction and demolition costs objectives (see panels b and g across the figures): the improvement in one of those objectives would always lead to a worsening of the other. Since those two objectives were taken as a representation of the interests of two different stakeholders – the building owner and building user – from the decision-making perspective, it would imply that between those two stakeholders, a compromise will always be necessary.

For the other two pairs of objectives, the situation is not as straightforward and differs depending on the location and the value of the indicator P. Lifecycle environmental costs and construction and demolition costs show a trade-off in the case of Sofia (Figure 6.4c), but the shape of the Pareto frontier is changing as the P value increases. The Pareto frontier becomes less smooth and starts featuring a turning point for the environmental costs. For example, in the case of Rome (Figure 6.5h), if we imagine moving along the Pareto frontier starting from the top right corner of it, construction and demolition costs and environmental costs would be first reduced simultaneously. On this part of the Pareto frontier, there is no trade-off between those two objectives. This will continue until we reach the corner point of environmental costs (green star in the figure), after which, further reduction in construction costs would lead to an increase in environmental costs – a trade-off occurs.

For the objective pair of lifecycle environmental costs and electricity consumption costs, there is no trade-off in the reference case of Sofia (see Figure 6.4d). Across the whole length of the Pareto frontier, the reduction in one of the objectives leads to the reduction in the other. Consequently, those two objectives share the same corner point: the NRG-Panels configuration that minimises electricity also minimises the lifecycle environmental costs. However, already in the case of Diyarbakir, two corner points get separated, and the Pareto frontier starts featuring an “appendix” – the area where the two objectives are in a trade-off state. With the increased value of indicator P, the trade-off part of the Pareto frontier is elongating, and the corner points for the lifecycle environmental costs and electricity consumption costs are drifting further apart. This highlights that the increase in the applicability potential of NRG-Panels might be leading to growing polarisation and conflict of interests between the building user and other stakeholders.

The Pareto frontiers in variable space (panels e and j) provide important insight as well. In the case of Sofia (Figure 6.4e), it is possible to see that all material configurations in the Pareto frontier are located at the very edge of the solution space, and all have the maximum possible porosity of 0.95. While the MPCM fraction of the obtained solutions varies from 0 to 0.6, at this level of porosity, MPCM does not provide any significant heat storage capacity, and such material can be considered an insulator (as it has been discussed in Chapter 5). In other climatic conditions, however, the situation is different.

Looking at the Pareto frontiers in the order the figures are presented, it is possible to see that Pareto solutions are gradually shifting towards the configurations with lower porosities. Consequently, the total volumetric fraction of MPCM in the material is increasing, leading to the associated increase in heat storage capacity. This also means that the applicability of NRG-Panels is increasing, as reflected by the increase in the value of indicator P .

Another important observation is that this shift of the overall Pareto frontier towards low porosities is driven by the shift of the corner point of the electricity consumption costs objective. In the reference case of Sofia, this corner point is characterised by a porosity of 0.95, MPCM fraction of 0.6 and panel thickness of 0.3 m (see red star marker in Figure 6.4e). In the case of Diyarbakir, it is shifting towards a lower porosity of 0.86 (Figure 6.4j). In the next figure for Madrid, it is already at 0.65 (Figure 6.5e), then at 0.3 in the case of Rome (Figure 6.5j), and, finally, reaching the lowest possible value of 0.05 in the case of Adana (Figure 6.6e). That indicates that for warmer climatic conditions, achieving the lowest possible energy costs for heating and cooling is only possible by increasing the heat-storing capacity of the material. In colder climates like Sofia and other cities with low P values (see Figure 6.3), the insulating properties play the dominant role in the energy consumption for heating and cooling, while in warmer climates, the energy-storing properties become more important.

In the case of the lifecycle environmental costs corner point, another kind of trend can be observed. The optimal configuration that minimises the environmental costs in the case of the Sofia reference case is the same as for the electricity objective ([0.95 0.6 0.3]). However, with increasing P value, this point is starting to move towards lower thickness values. The optimal NRG-Panel thickness that results in the minimum possible environmental costs is 0.27 m for Diyarbakir, 0.17 m for Madrid, 0.07 m for Rome and just 0.03 m for Adana. This can be explained by looking at the balance between the embodied environmental costs (environmental costs of producing the materials constituting the building) and the environmental costs arising from the energy consumption for heating and cooling. It is a well-known fact that the benefits of increasing the insulation layer thickness in buildings are not linear [38], [160], [161]. For example, in a cold climate, moving from no insulation to 0.05 m thick insulation layer would result in much larger energy savings than increasing the insulation layer thickness from 0.15 m to 0.2 m. Yet, the amount of added embodied emissions will be the same. With the benefits of added insulation diminishing, at some point, the environmental benefits from energy savings would become outweighed by the embodied emissions of the added insulation layer. Adding more insulation would lead to a net-positive change in the lifecycle environmental impacts (or environmental costs). The position of this turning point depends on multiple factors and is greatly influenced by climatic conditions. That is what is being observed in Figures 6.4-6.6. For example, in the Rome case, the corner point of lifecycle environmental costs is at 0.07 m thickness of NRG-Panels. Going from no insulation to 0.07 m results in an overall reduction in environmental

costs. Increasing the thickness of NRG-Panels beyond 0.07 m still results in reduced energy consumption and lower energy costs, but those benefits are outweighed by the embodied environmental costs of producing and transporting additional volume of NRG-Panels.

Another important aspect regarding the lifecycle environmental costs that should be noted is that for every analysed location, the NRG-Panels configuration resulting in the lowest possible environmental costs is the one with the maximum possible porosity of 0.95. As discussed before, such a material acts as an insulator but does not have sufficient heat-storing capacity. For locations with warmer climatic conditions, reduced porosity is beneficial from the standpoint of energy savings. However, the reduced porosity also means an increased solid fraction in the foam and a higher amount of embedded MPCM. As the LCA results presented in previous chapters showed, MPCM has a high environmental footprint. Furthermore, material configurations with lower porosity have higher density and, consequently, larger environmental impacts from the transport between production and construction sites. Due to those reasons, at least for the given optimisation problem and demonstrator building case, the energy savings from the increased volume of MPCM in NRG-Panels are not large enough to outweigh the negative environmental impacts arising from producing additional amounts of MPCM and transportation of heavier panels.

The case of Lisbon is different from all the rest of the analysed cities. As can be seen from Figure 6.6j, all Pareto solutions are characterised by a low thickness of panels. Even for the energy costs corner point (red star in the figure), the optimal thickness is just 0.1 m, while for all the other analysed locations, it was at 0.3 m. Moreover, two other corner points are located at the minimum possible thickness of 0.01 m. A possible explanation for that is that Lisbon has a relatively warm but mild climate, and under such conditions, the demand for heating and cooling is low. As a result, possible benefits from added thermal insulation or increased heat capacity are limited as well. Furthermore, under the climatic conditions of Lisbon, for the demonstrator building used in this research, an increase in NRG-Panels thickness beyond 0.10 m leads to energy consumption increasing as well. This can be attributed to the possible heat trap effect, where, depending on the building configuration, adding more insulation or increasing the thermal weight of a building (also by including heat storage materials like PCM) might increase the risk of overheating [169], [170]. This study has been built around a building with an ideal loads HVAC system, where the temperature is kept within the given range at all times, making overheating impossible. Instead, the heat trap effects in this case translate into increased energy demand for cooling. This is especially plausible in the analysed case since the demonstrator building used in this study has low ventilation and infiltration rates, making it susceptible to overheating effects.

Identification of the most favourable configurations of MPCM particles

While the discussion so far has concentrated on macro (panel thickness) and meso levels (porosity and MPCM fraction), it is also important to analyse the micro-level parameters – PCM type and MPCM shell material. Figure 6.7 provides a statistical overview of those two parameters in the form of two-dimensional histograms. There are in total 22 possible combinations of PCM type (11 PCMs with different melting temperatures) and shell material (inorganic coacervate and melamine-formaldehyde). Two-dimensional histograms in Figure 6.7 are based on the obtained Pareto frontiers and show how frequent each combination of PCM type and shell material is. To only analyse the cases where MPCM particles have a pronounced influence on the final properties of NRG-Panels, only those Pareto solutions were taken where the MPCM fraction has been higher than 0.01. Figure 6.7 shows the distributions for each analysed location as well as for all locations combined. Furthermore, it also shows the distribution only for the corner points of the Pareto frontier: one for the lifecycle environmental costs and another for the energy costs. For those distributions, for each location, the NRG-Panels configuration that results in the lowest possible lifecycle environmental costs/energy costs has been taken, and the corresponding PCM type and MPCM shell material were extracted. Then, all the extracted PCM types and MPCM shell material were grouped together and plotted in the histogram.

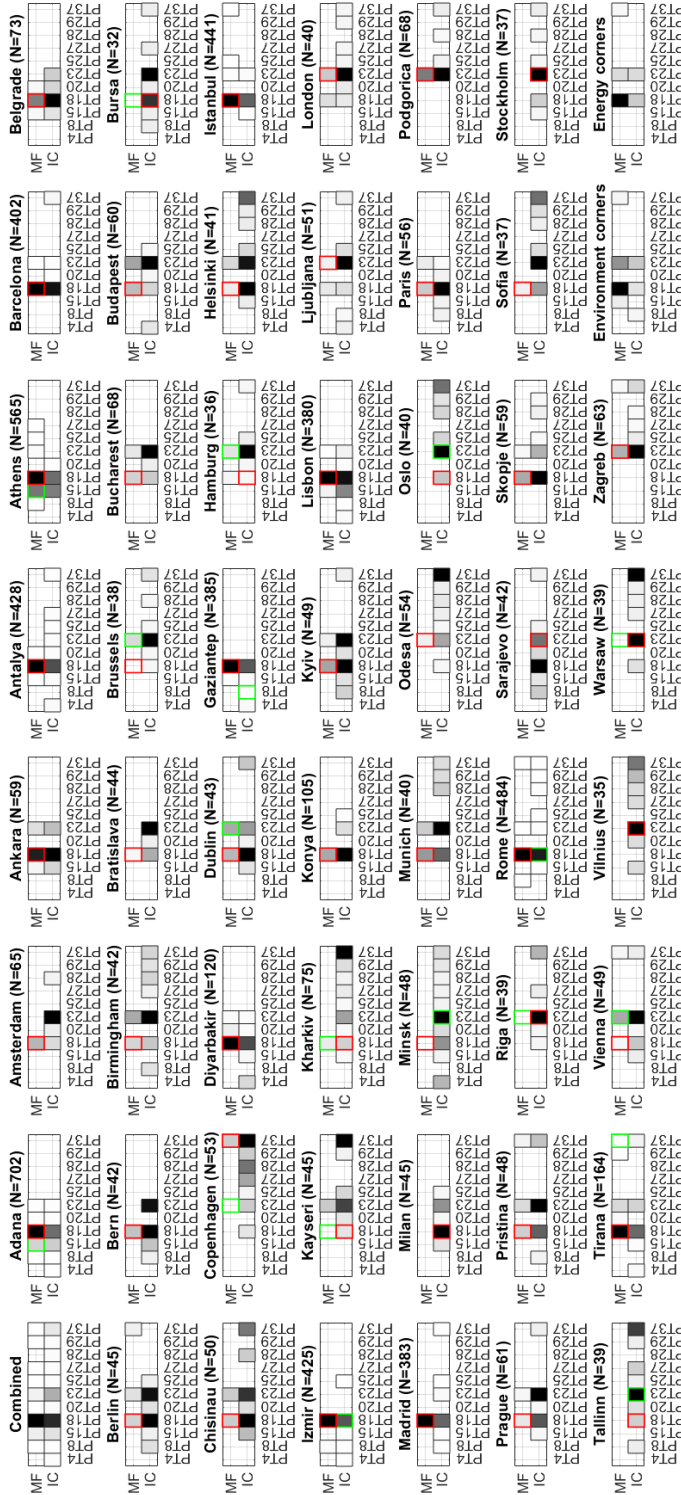


Figure 6.7: Two-dimensional distributions for MPCM parameters across Pareto solutions. The higher the frequency of occurrence is the darker the colour of the corresponding bin. The number next to the city name is the number of points (Pareto solutions) that have been used to build the corresponding distribution. The green edge around the bin marks the MPCM configuration that results in the minimum environmental costs corner point, red – minimum energy consumption costs. If only the red bin edge is present, the corner point MPCM configurations are the same for the environmental costs and energy consumption.

From the combined histogram, the most frequently found MPCM configuration is PT18 (PCM with melting temperature of 18 °C) with MF shell, closely followed by PT18 with IC shell. While the distributions vary quite greatly between the cities, for those locations that have a high P index value (refer to Figure 6.3), they are quite similar. For all of those locations, PT18 with MF shell is the most common MPCM configuration, and it is also the corner point for energy consumption costs. That means that PCM with a melting temperature of 18 °C is the optimal choice for those locations to ensure the lowest possible energy consumption and, consequently, costs of energy for heating and cooling. Interestingly, from the distributions of the corner points (see the two histograms in the bottom right corner of Figure 6.7), it can be concluded that PT18 with MF shell is also the most frequent. Thus, for most of the locations, no matter the difference in climatic conditions, PT18 with MF shell is the most promising MPCM configuration. The fact that PT18 is such a universally suitable option for a variety of locations with very different climatic conditions suggests that the indoor thermal climate in the building (the cooling and heating setpoints for HVAC) might be a more critical factor for PCM material selection than the local climatic conditions.

Optimisation results and assessment of NRG-Panels' applicability under the foam stability constraint

The results presented so far have been provided for the unconstrained case where any material configuration within the defined variable bounds is possible (0-0.95 porosity, 0-0.6 MPCM fraction, 0.01-0.30 m panel thickness). However, as it has been discussed, not all combinations of porosity and MPCM fraction are achievable in practice due to the issues with foam stability. If the foam stability constraint is introduced, some Pareto solutions might become infeasible, causing changes to the Pareto frontiers. Consequently, this also results in changes in indicator P, more specifically in its reduction, thus pointing out to the corresponding decline in the NRG-Panels' applicability potential. Figure 6.8 shows the values of indicator P after the stability constraint has been introduced.

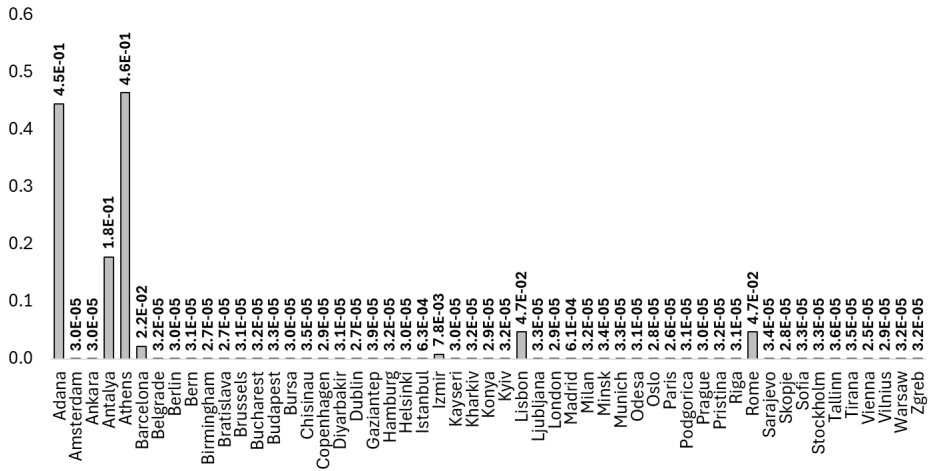


Figure 6.8: The values of indicator P for the analysed geographical locations in the constrained case.

Figure 6.8 demonstrates that for all locations except Athens and Adana, the introduction of the stability constraint led to a major reduction in the value of the indicator P . A closer look at the results of the constrained case shows that there are only 9 out of 53 analysed locations for which it is feasible to add any amount of MPCM to the foam in NRG-Panels: Madrid, Istanbul, Izmir, Barcelona, Lisbon, Rome, Antalya, Adana and Athens. For those cities, the value of the indicator P is larger than $1E-4$. For the remaining locations, all feasible Pareto configurations in the constrained case have an MPCM fraction equal to zero. Those zero-MPCM locations can be considered to be unfavourable for NRG-Panels application for the demonstrator building case when assessed using current climatic conditions.

Let us now zoom in on some of the locations and explore in more detail the influence of the stability constraint. Figure 6.9 and Figure 6.10 provide the Pareto frontiers for four selected locations for the constrained case alongside the unconstrained counterparts, thus providing a visual representation of the impact of the stability constraint.

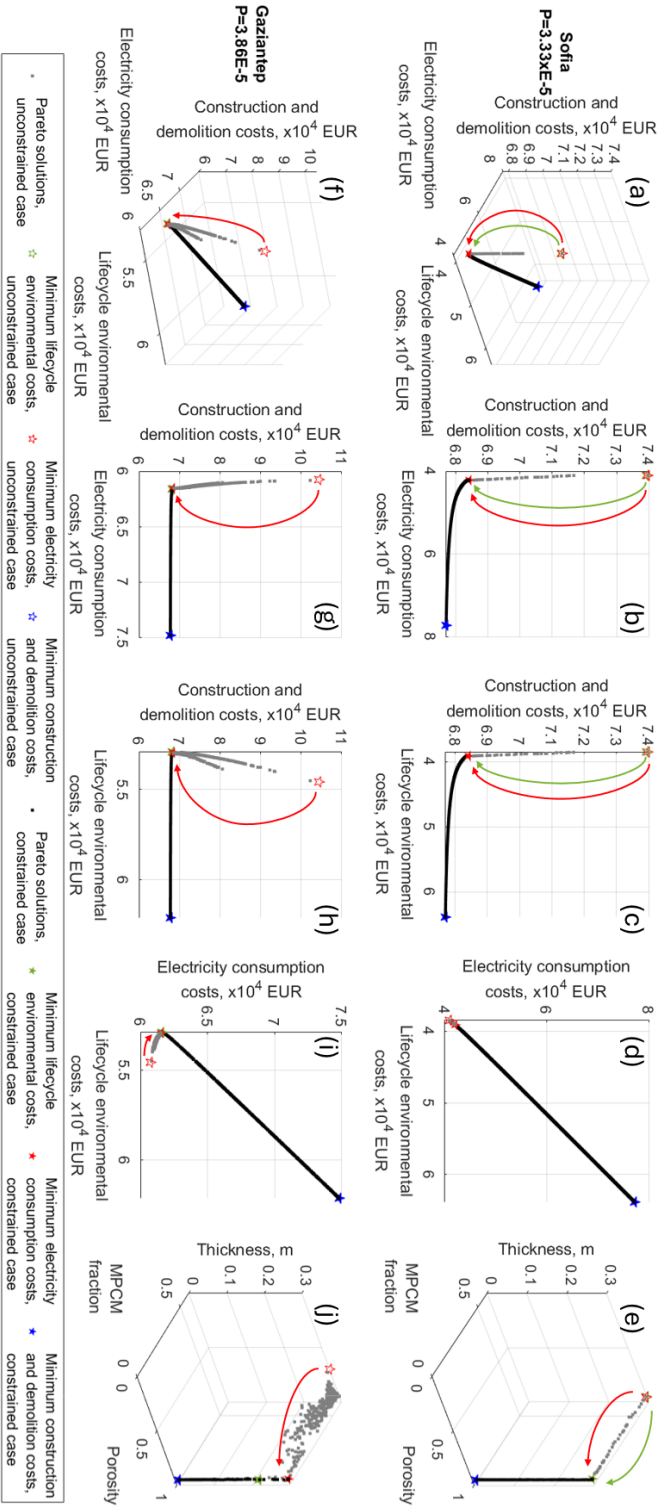


Figure 6.9: Unconstrained and constrained Pareto frontiers for Sofia (panels a–e) and Gaziantep (panels f–j). Grey points depict the unconstrained Pareto frontier, black – the constrained ones. Star-shaped markers with solid fill indicate the location of the corner points of the constrained Pareto frontier, while unfilled ones correspond to the corner points of the unconstrained Pareto frontier. The arrows indicate the change in the corner points when shifting from the unconstrained to the constrained case.

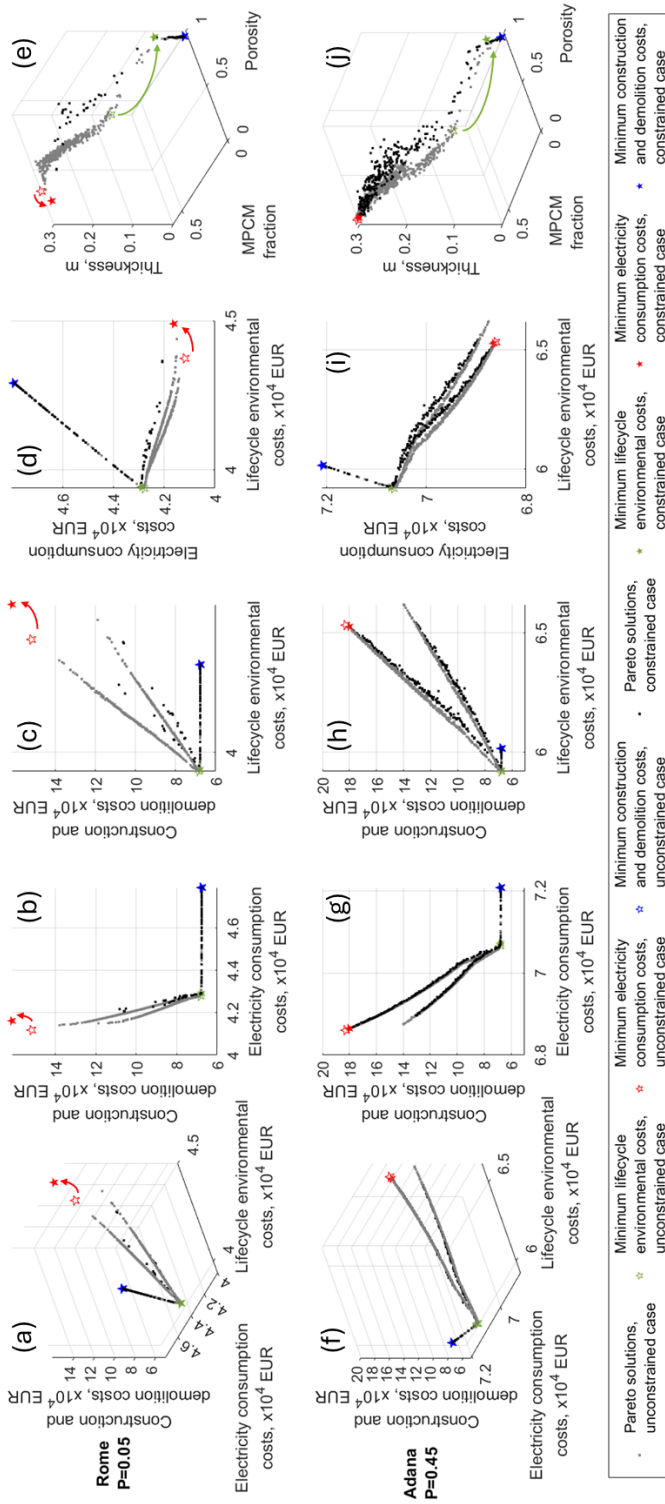


Figure 6.10: Unconstrained and constrained Pareto frontiers for Rome (panels a-e) and Adana (panels f-j). Grey points depict the unconstrained Pareto solutions, black – the constrained ones. Star-shaped markers with solid fill indicate the location of the corner points of the constrained Pareto frontier, while unfilled ones correspond to the corner points of the unconstrained Pareto frontier. The arrows indicate the change in the corner points when shifting from the unconstrained to the constrained case.

As Figure 6.9 shows, in the case of Sofia and Gaziantep, with the introduction of the foam stability constraint, many configurations of NRG-Panels become unachievable, rendering large parts of the Pareto frontiers unfeasible. It also leads to corner points moving in both functional and variable spaces. For Sofia, the corner point configurations for both lifecycle environmental costs and energy costs had porosity of 0.95, MPCM fraction of 0.6 and panel thickness of 0.3 m. However, with the foam stability constraint introduction, this configuration becomes unfeasible, and the corner points move to the configuration with 0.95 porosity, no MPCM and 0.3 m panel thickness. The case of Gaziantep is very similar to Sofia. The introduction of the constraint renders all Pareto solutions with non-zero MPCM fraction unfeasible, including the configuration that resulted in the lowest possible energy consumption with porosity of 0.7, MPCM fraction of 0.6 and 0.3 m thickness. Consequently, the value of indicator P has reduced from 0.03 to 4×10^{-5} , pointing to the same conclusion as in the Sofia case that there is no potential of NRG-Panels application for the analysed building configuration and current climatic conditions in Gaziantep.

On the other hand, those locations that exhibited a high value of the indicator P in the original unconstrained scenario, while also affected by the stability constraint, experienced this impact to a lesser extent. Figure 6.10 shows two examples of such locations: Rome and Adana. In the case of Rome, while due to the constraint, many Pareto solutions become unfeasible, this leads to a shift of the Pareto frontier away from the utopia point, whilst the overall shape gets preserved. In contrast, in the case of Sofia and Gaziantep, large parts of Pareto frontiers were essentially cut off by the constraint, causing a drastic change in shape. More specifically, the region with low porosities gets preserved in the case of Rome (as well as Adana), meaning that the NRG-Panel configurations with higher heat storage capacities are still feasible. From this viewpoint, the current climatic conditions in Rome can be considered as favourable for NRG-Panels application as the dual-function thermal material that provides both insulating as well as energy-storing functions. It is worth mentioning, however, that the corner points are still experiencing significant shifts when the constraint is introduced. The NRG-Panels configuration that resulted in the lowest possible energy costs (0.30 porosity, 0.60 MPCM fraction and 0.30 m panel thickness) becomes unfeasible and shifts to the configuration with 0.16 porosity, 0.56 MPCM fraction and 0.30 m panel thickness. This shift causes an increase in the minimum possible energy costs from 41 184 EUR to 41 622 EUR.

In the case of Adana, major changes can be observed in the variable space (see Figure 6.10j) and many Pareto configurations become unfeasible. However, this does not have a pronounced effect on the Pareto frontiers in the objective space (see Figure 6.10f-i). The middle points of the Pareto frontier are shifting slightly further away from the utopia point, but the corner points stay almost in the same position. Furthermore, the value of indicator P stays almost unchanged as well, reducing from 0.48 to 0.45. Those observations indicate that in the case of the current climatic conditions in

Adana, the applicability potential of NRG-Panels is high and is not sufficiently hindered by the stability constraint.

Another important observation from the analysis of the constrained Pareto frontiers is that for all of the locations, the corner point configurations for the lifecycle environmental costs and construction and demolition costs include no MPCM (see the green solid-filled star-shaped markers in Figure 6.9e, Figure 6.9j, Figure 6.10e and Figure 6.10j). Thus, from the perspective of two of the stakeholders, the optimum NRG-Panels configuration will be a regular, highly porous foamed concrete having no energy-storing function. On the other hand, in the warmer climates analysed (e.g., Athens, Adana, Rome, etc.) configuration minimising energy consumption is located on the opposite side of the solution space and is characterised by low porosity and high MPCM fraction. This results in a highly polarised situation where NRG-Panels (as a dual-function material) might be an attractive option from the point of view of one of the stakeholders, but will not make sense for the others. The selection of the final configuration would thus require major compromises. To avoid possible conflicts in situations like this, an equity-based decision-making approach can be used. This topic will be addressed in the following chapters of this dissertation.

Comparison between the energy performance of NRG-Panels and EPS

Figure 6.11 shows the difference in energy consumption of the demonstrator building with optimised NRG-Panels and optimised EPS configuration in different climatic contexts. The figure only shows the relative values, but the absolute values of energy consumption can be found in Appendix C, Table C1. Furthermore, Table C3 of Appendix C also lists the optimal EPS configurations (layer thickness) for each geographical location.



Figure 6.11: Comparison of electricity consumption for heating and cooling between the demonstrator building with NRG-Panels and EPS for unconstrained (a) and constrained (b) cases. Negative values mean that a building with NRG-Panels has lower energy consumption. Numbers in blue are the difference in heating demand, orange – heating demand and black – total demand.

As Figure 6.11 shows, NRG-Panels perform at least as good or better than EPS under all analysed climatic conditions, but the difference in energy performance varies greatly depending on location. In the unconstrained case, the difference is between 26 kWh/year (Diyarbakir) and 179 kWh/year (Helsinki). This difference becomes lower when the stability constraint is introduced and ranges between 0 kWh/year (Tirana and Gaziantep) to 130 kWh/year (Adana). Overall, the average difference in energy demand across all analysed locations decreases from 78 kWh/year to 26 kWh/year when the stability constraint is taken into account. For some locations, however, the stability constraint is not influencing the outcomes or is influencing, but only slightly. Those locations include Adana, Antalya, Athens and Lisbon.

It is interesting to note that the benefits of using NRG-Panels are coming from either cooling savings or heating savings, depending on the location. In most cases, if a building with NRG-Panels has lower heating demand, it also has higher cooling demand. And the other way around, in cases where a building with NRG-Panels outperforms its EPS counterpart in cooling demand, it has higher energy consumption for heating. In the constrained case, there is only one location – Adana – where the building with NRG-Panels has both lower heating and cooling demands.

6.3.2 Results of optimisations with extended temporal scope under future climatic conditions

Optimisation results and assessment of NRG-Panels' applicability in the unconstrained case

In total, 10 locations have been selected for the optimisation of NRG-Panels under future climatic conditions and the assessment of NRG-Panels' applicability under those projected conditions. Figure 6.12 shows the calculated values of indicator P for those locations under climate projections for 2050 and 2080. For the comparison, the values for the current climatic conditions are provided as well, allowing to track the changes caused by climate change.

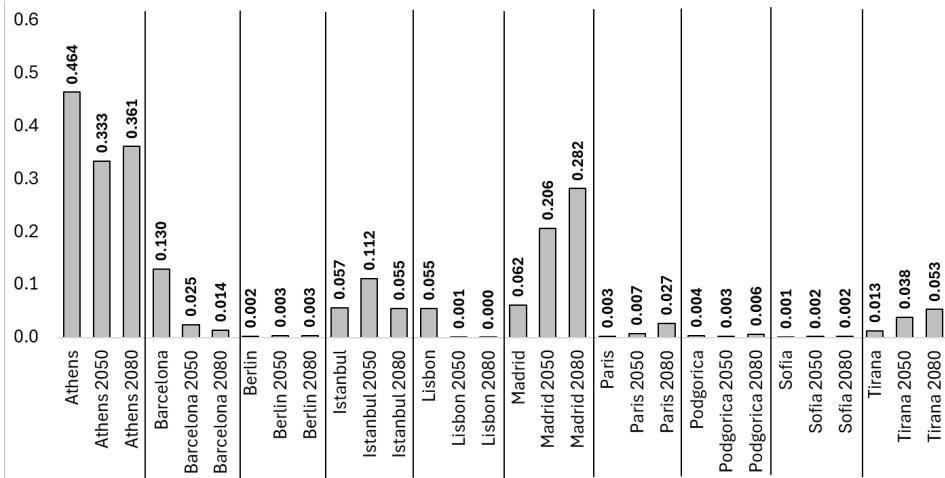


Figure 6.12: Values of index P for selected locations under current climatic conditions as well as under projected climatic conditions for 2050 and 2080.

In the case of Berlin, Podgorica and Sofia, climate change is not having a major impact, and the value of indicator P remains low. On the other hand, Paris, Tirana and especially Madrid demonstrated an increase in P value, pointing towards the growing potential of NRG-Panels' applicability in those locations. There were, however, locations where climate change resulted in a downward trend of indicator P values. In the case of Barcelona, the value of indicator P has been found relatively high in the current climatic conditions (0.130) but decreased to 0.025 in 2050 and then to 0.014 in 2080. Similarly, in Lisbon's case, the value shrank to almost zero in 2080. For the remaining two locations – Athens and Istanbul – there was no clear trend in the direction of changes.

To analyse the changes between the present and future climates in more detail, let us take a closer look at some of the locations mentioned above. Figures 6.13, 6.14 and 6.15 provide the Pareto frontiers obtained from multi-objective optimisations of NRG-Panels for Sofia, Paris, Madrid, Barcelona, Athens and Lisbon.

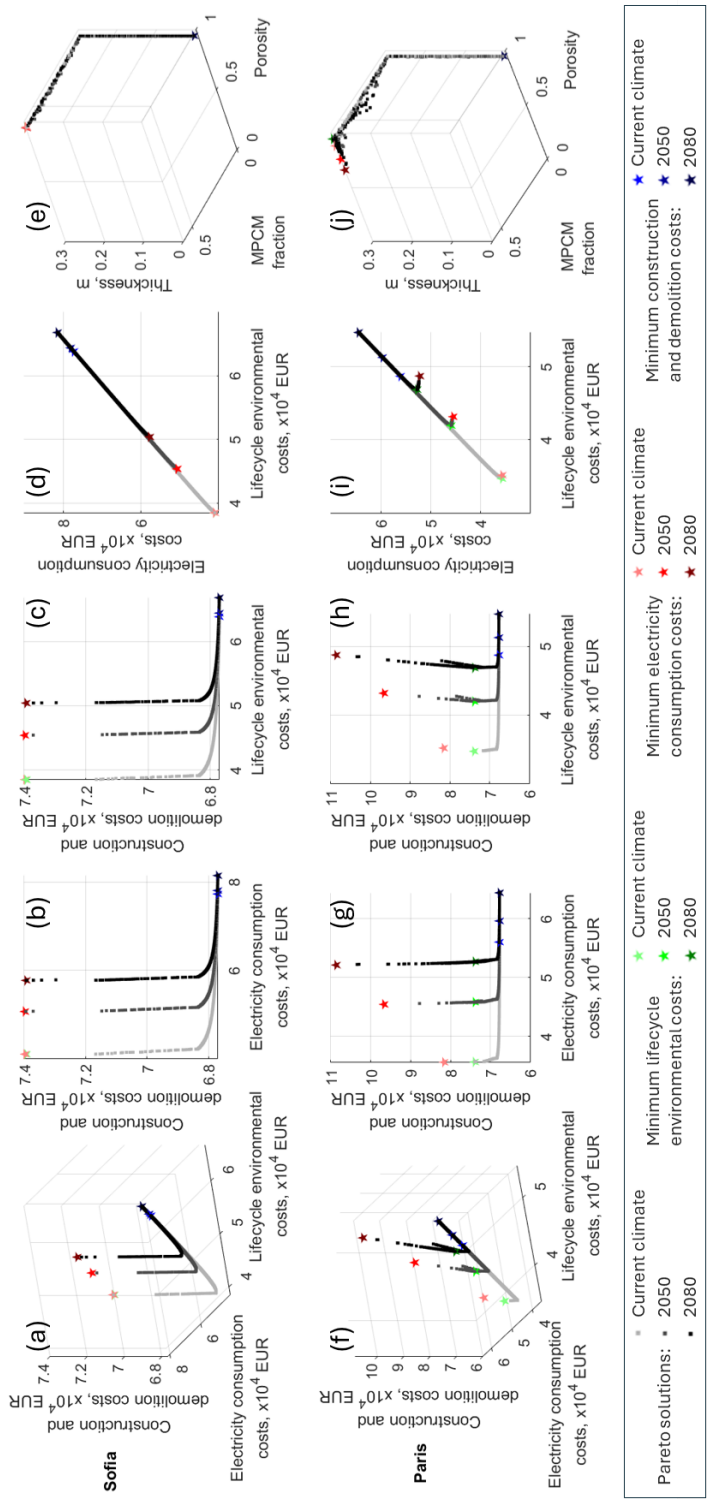


Figure 6.13: Pareto frontiers for Sofia (panels a–e) and Paris (panels f–j) under current and future climatic conditions.

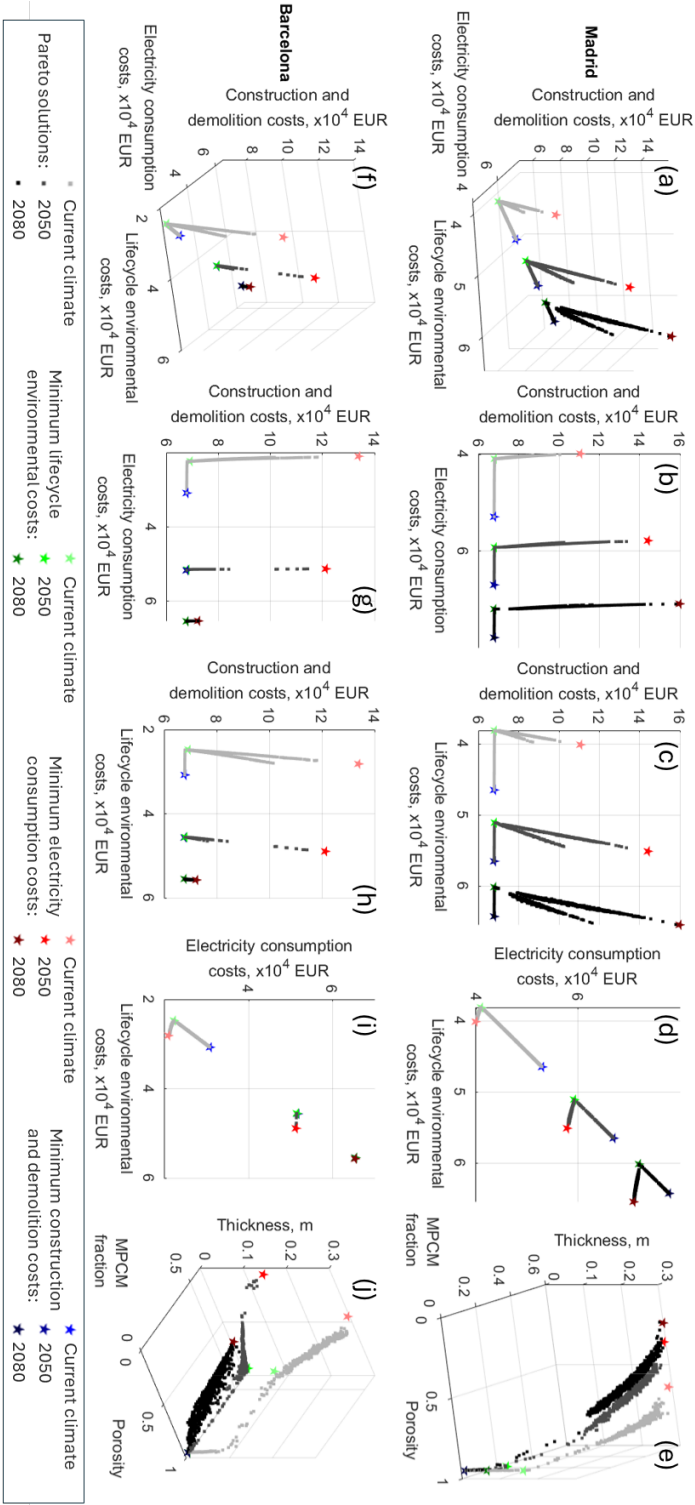


Figure 6.14: Pareto frontiers for Madrid (panels a–e) and Barcelona (panels f–j) under current and future climatic conditions.

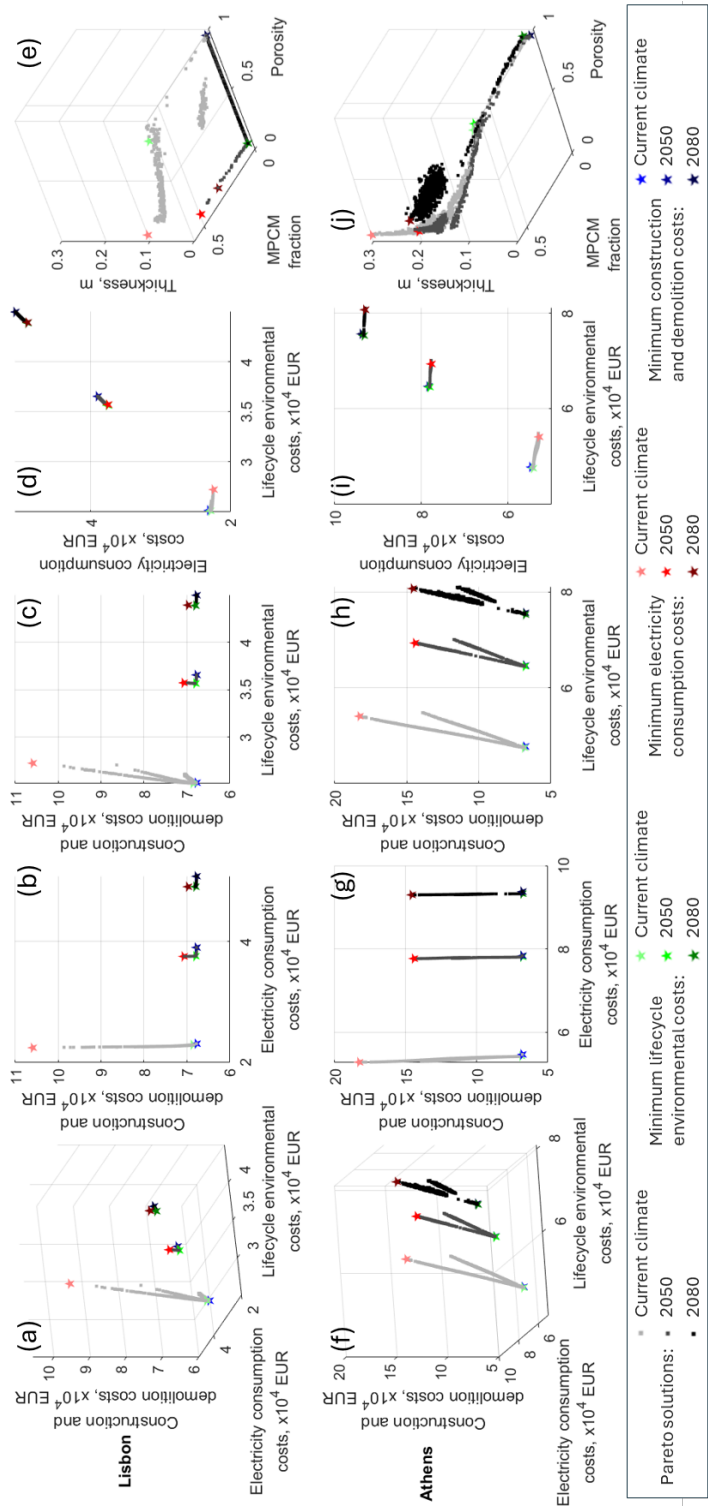


Figure 6.15: Pareto frontiers for Lisbon (panels a–e) and Athens (panels f–j) under current and future climatic conditions.

As Figures 6.13-6.15 show, for all locations, climate change leads to a significant increase in electricity consumption for heating and cooling. This, in turn, results in higher electricity consumption costs and lifecycle environmental costs and Pareto frontiers are shifting further away from the utopia point. In the case of Sofia, this is the only change that can be observed, but the Pareto frontier in variable space remains the same (see Figure 6.13e). Therefore, the optimal configurations of NRG-Panels for Sofia stay unchanged, and the applicability potential of NRG-Panels remains low. In the Paris case (Figure 6.13f-j), the changes in Pareto frontiers are more prominent, and a shift in optimal NRG-Panels configuration can be observed. More specifically, the configuration that results in the minimum electricity consumption costs is shifting towards lower porosity values (0.86 in the current climate, 0.76 in 2050 and 0.66 in 2080). Madrid (Figure 6.14a-e) shows a similar trend, but the change is more drastic. For this location, the NRG-Panels configuration that yields the lowest possible electricity consumption under current climatic conditions has a porosity of 0.64. Under the 2050 climate projection, it decreases to 0.36 and then to 0.24 under the 2080 climate projection. At the same time, the MPCM fraction and panel thickness stay the same (0.6 and 0.3 m respectively). This means that in the case of Madrid, climate change necessitates an increase in the heat storage capacity of NRG-Panels.

As mentioned before, Barcelona showcases the reverse trend in the value of indicator P compared to Paris and Madrid. Figure 6.14j depicts how this change occurs. The electricity consumption corner point is located at 0.45 porosity, 0.6 MPCM fraction and 0.3 m panel thickness in the current climatic conditions. Under the climate projection for 2050, the porosity is decreasing to 0.06 and the panel thickness to 0.14 m. Finally, in 2080, the porosity changes to 0.60 and the thickness further decreases to 0.03 m. Lisbon (Figure 6.15a-e) is characterised by a similar trend in the thickness of panels. However, compared to Barcelona, it reduces even further, and all Pareto-optimal configurations of NRG-Panels have the minimum possible thickness of 0.01 m in both 2050 and 2080. This is an important observation highlighting that in some locations, climate change might result in decreasing the applicability potential of NRG-Panels. And as the case of Lisbon shows, in some situations, it might be beneficial to not have any insulation layer at all. In those particular cases, the increased insulating performance or thermal weight of a building could result in heat-trapping effects and overheating. Those findings highlight the importance of taking the climate change effects into account when decisions regarding the optimal thermal performance of a building are made.

The last case presented above is Athens (Figure 6.15f-j). Some noticeable shifts can be observed in the NRG-Panel configurations in Figure 6.15j, but it is hard to extract some kind of trend or pattern from it. In general, the frontier seems to be shifting towards lower MPCM fractions and lower panel thicknesses, but the change is not as drastic as in other cases described above.

Identification of the most favourable MPCM configurations

In addition to the analysis of changes in optimal macro (panel thickness) and meso (porosity, MPCM fraction) parameters of NRG-Panels due to climate change, it is also important to investigate if it impacts the micro-level parameters as well (PCM type and MPCM shell material). This investigation is done in a similar manner to the case of assessment under current climatic conditions. Figure 6.16 shows the two-dimensional statistical distributions of all possible MPCM configurations for the current climate, the 2050 projection and the 2080 projection. Those distributions are shown for each location separately as well as for all locations combined. It also shows the distribution of Pareto corner points. Before the distributions were built, the Pareto solutions were filtered to only include those NRG-Panels configurations that have an MPCM fraction higher than 0.01.

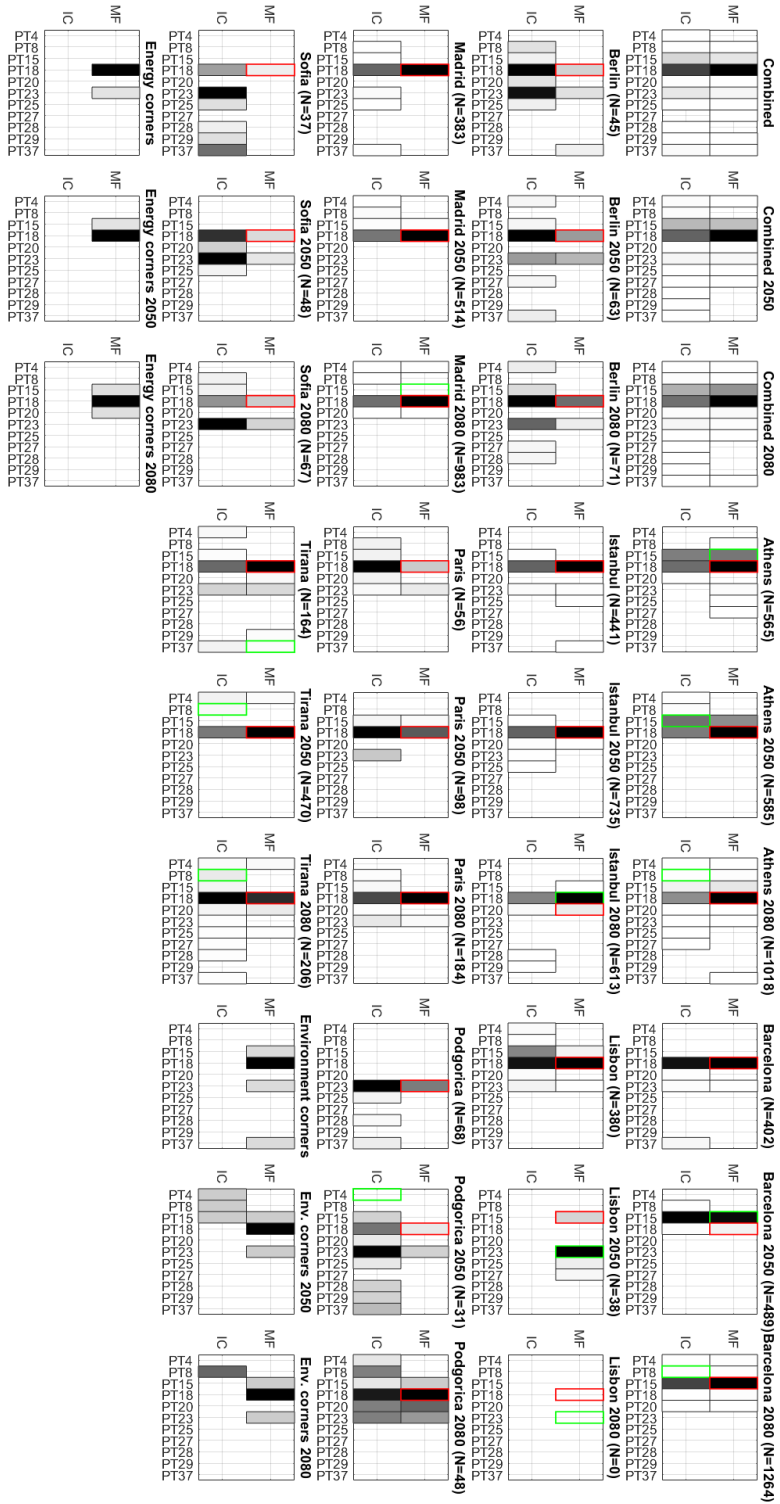


Figure 6.16: Two-dimensional distributions for MPCM parameters for current and future climates. The higher the frequency of occurrence is the darker the colour of the corresponding bin.

As Figure 6.16 indicates, there are no major changes in optimal MPCM configurations between current and future climates for the analysed locations. PT18 is still the dominant PCM type universally suitable for most of the locations under future climate projections as well. A notable exception is Barcelona, where the optimal PCM type is shifting from PT18 to PT15. On the other hand, in the case of Istanbul, the electricity consumption corner point is shifting towards higher melting temperatures, from PT18 to PT20. Overall, the optimal micro-level parameters of NRG-Panels seem to be less sensitive to the changes in climate compared to meso- and macro-level parameters. However, as the cases of Barcelona and Istanbul have shown, sometimes future climatic conditions might necessitate the use of a different PCM material compared to the current climate.

Optimisation results and assessment of NRG-Panels' applicability under the foam stability constraint

Just as in the assessment under the current climatic conditions presented above, the foam stability constraint makes some NRG-Panels configurations infeasible. The scale of this effect can be judged by the changes in the values of indicator P. Figure 6.17 shows the values of indicator P for the analysed locations with the constraint accounted for.

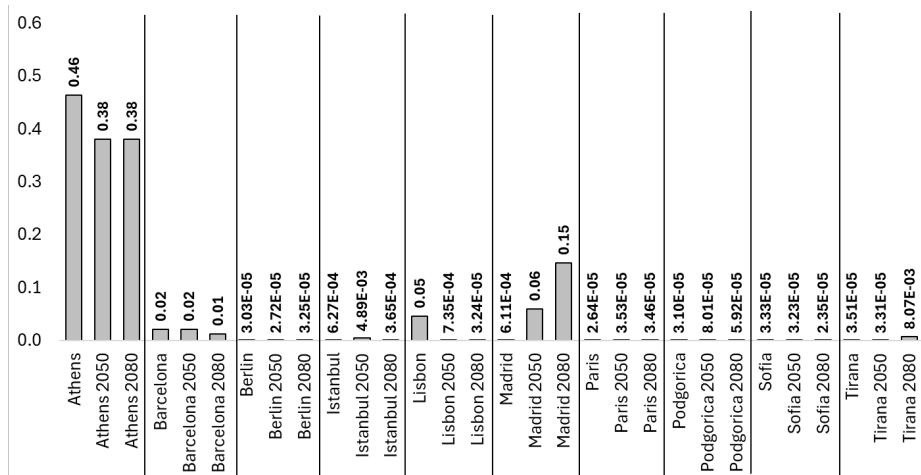


Figure 6.17: Values of index P for selected locations under current climatic conditions as well as under projected climatic conditions for 2050 and 2080 with the foam stability constraint taken into account.

The constraint has a major impact in all of the cases except for Athens. Amongst the analysed locations, only Athens, Barcelona, Madrid, Istanbul, and Tirana (in 2080) show some potential for NRG-Panels application in future climatic conditions. And from those, only for Madrid, the potential is increasing. For the rest, all Pareto solutions in the constrained case include no MPCM and perform solely the insulating function.

Comparison between the energy performance of NRG-Panels and EPS

The thermal performance of NRG-Panels has been compared against EPS under future climate projections as well. The comparison has been done for both unconstrained and constrained cases. Figure 6.18 provides an overview of the comparison results. The optimal thickness of EPS panels that has been used in the comparison, as well as the heating and cooling demand for each of the locations, can be found in Appendix C (Tables C2 and C4).

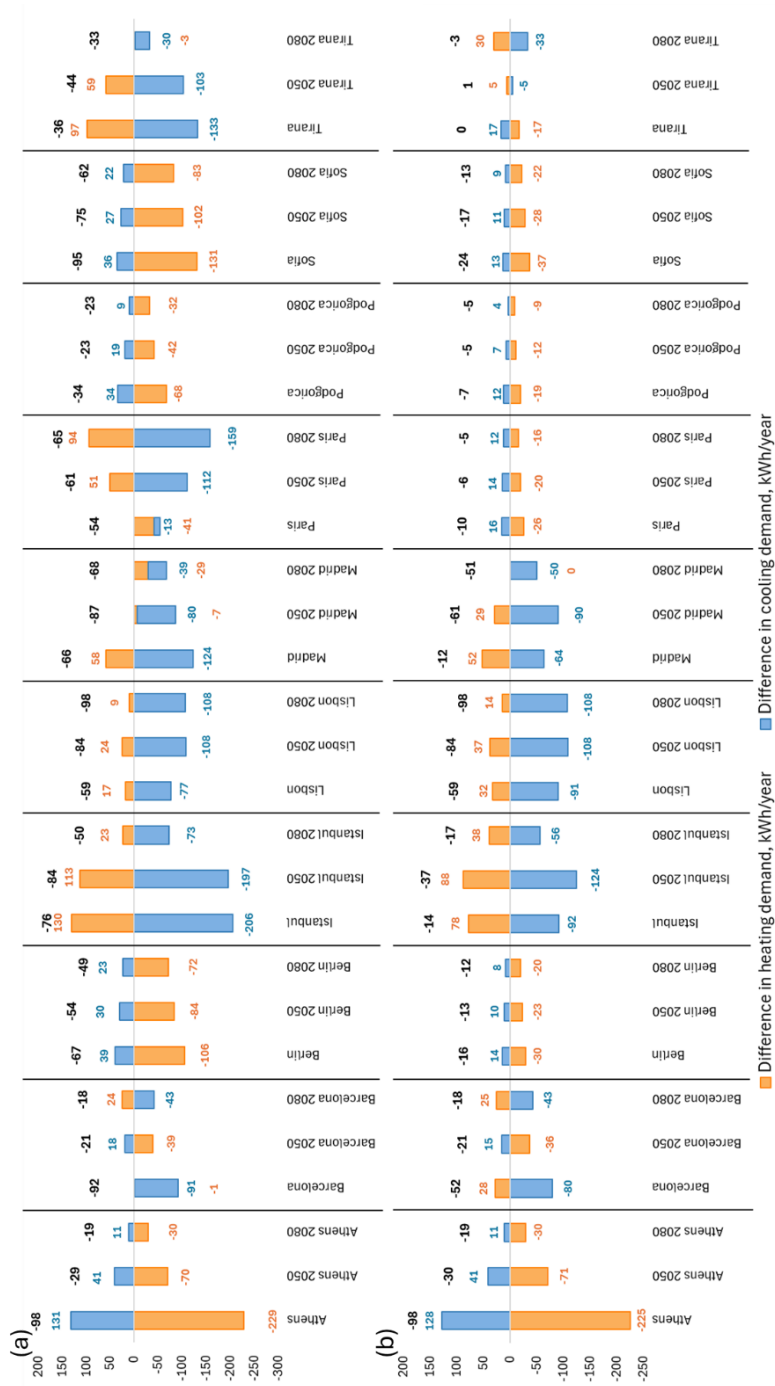


Figure 6.18: Comparison of electricity consumption for heating and cooling between the demonstrator building with NRG-Panels and EPS under current and future climatic conditions for unconstrained (a) and constrained (b) cases. Negative values mean that a building with NRG-Panels has lower energy consumption. Numbers in blue are the difference in cooling demand, orange – heating demand and black – total demand.

Figure 6.18 shows that climate change has a major impact on the energy performance difference between NRG-Panels and conventional insulation like EPS. Though no clear trend can be observed, in most cases, the gap in performance between NRG-Panels and EPS is shrinking under future climate projections. This is especially noticeable in the case of Athens, which under current climatic conditions showed high benefits from NRG-Panels use. Under the 2050 climate projection, however, the difference between NRG-Panels and EPS has shrunk more than three times, from 98 kWh/year to 30 kWh/year. Going from the 2050 climate projection to the 2080 projection caused a further reduction of benefits to just 19 kWh/year. This highlights the importance of taking climate change into account when analysing the applicability potential of NRG-Panels: the attractiveness of a particular location might change drastically within a relatively short period of time, not exceeding the lifetime of a typical building.

While Lisbon demonstrates a positive trend when it comes to the difference in thermal performance of NRG-Panels and EPS, it is not a sign of this location having good potential for NRG-Panels deployment. As it has been discussed before, Lisbon is an outlier case, and to ensure the minimum possible electricity consumption under future climatic conditions there, little to no insulation is needed. In this particular case, the comparison is done between NRG-Panels and EPS of the minimum possible thickness of 0.01 m and the benefits shown in Figure 6.18 are caused solely by the difference in thermal conductivity between the materials. In reality, the best possible solution for the demonstrator building under those thermal conditions would have been having no NRG-Panels or EPS layer altogether.

Another positive trend can be seen in the case of Paris, but only when analysing the results of unconstrained optimisations. If the foam stability constraint is taken into account, NRG-Panel configurations that minimise the demonstrator building energy consumption become unfeasible. As a result, the benefits of NRG-Panels compared to EPS are diminishing and become almost negligible in the constrained case.

Only in two cases, Istanbul and Madrid, the gap in thermal performance between NRG-Panels and EPS is seen to increase under future climatic conditions. In both cases, however, the initial surge in the NRG-Panels benefits when transitioning from the current climate to the 2050 climate has been followed by the consequent decrease in 2080 climatic conditions. Despite the drop, in the case of Madrid, the difference in thermal performance between NRG-Panels and EPS under future climatic conditions is still times higher than in the current climate (51 kWh/a in 2080 compared to 12 kWh/a in the current climate). In this regard, Madrid is a counter-case to Athens, showing that climate change could also make NRG-Panels more applicable in the future in certain locations.

6.3.3 Mapping the applicability potential of NRG-Panels

With all the obtained data at hand, it is now possible to map the applicability potential of NRG-Panels for the analysed locations to deduce the broader geographical extent of NRG-Panels' viability as a novel dual-function thermal material. Figure 6.19 shows two maps depicting the value of indicator P and the difference in electricity consumption between the demonstrator building equipped with NRG-Panels and the one with EPS. The map on top is based on the values calculated for the current climatic conditions, and the bottom one is for future climate projections. While two distinct climatic projections were analysed – 2050 and 2080 – a single set of values was necessary for mapping purposes. Thus, the value of indicator P and the electricity consumption difference presented in the map are the average between 2050 values and 2080 values. For both maps, the depicted values are calculated with the stability constraint taken into account.

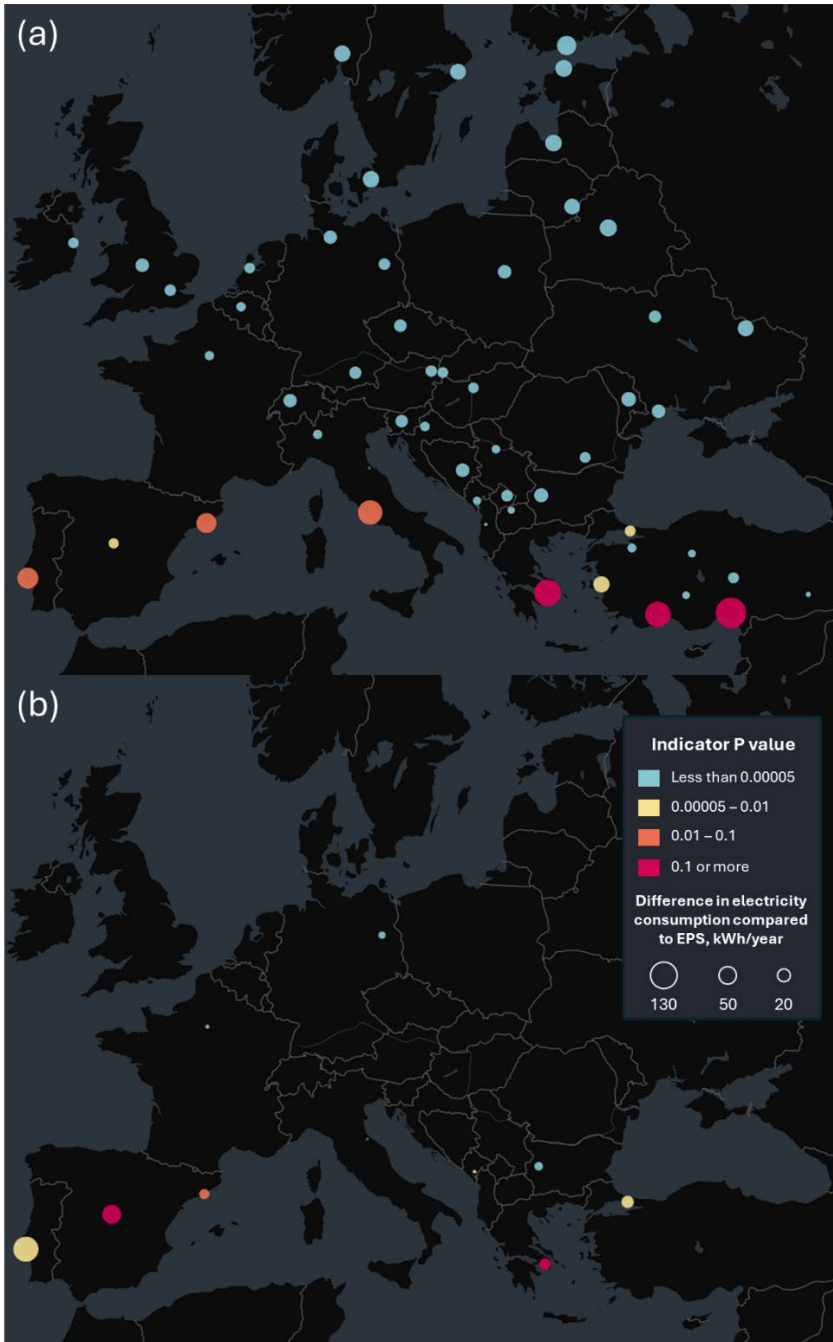


Figure 6.19: NRG-Panels applicability potential maps for the current climatic conditions (a) and for the future climates (b). The value of indicator P is colour-coded, and the size of the circles corresponds to the difference in thermal performance between NRG-Panels and EPS. The maps have been built using `kepler.gl` tool [171] with the basemap from MapLibre [172].

The maps presented in Figure 6.19 show that all of the locations that could be considered to be suitable for NRG-Panels deployment (in the context of the demonstrator building) are located in the South of Europe, in the Mediterranean area; this area does not seem to extend far inside the continent. This localisation becomes clearer when the maps in Figure 6.19 are compared against the Köppen-Geiger climate classification map presented in Figure 6.20.

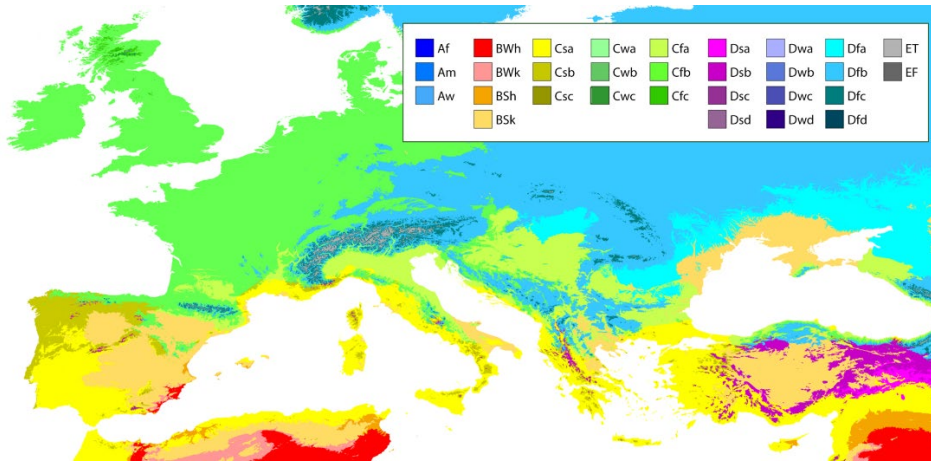


Figure 6.20: Köppen-Geiger climate classification map for Europe for the period from 1991-2020. The map is adapted from the publication by Beck et al. [173].

Evidently, the majority of potentially suitable locations for NRG-Panels application are situated in areas with a climate classified as Csa under the Köppen-Geiger climate classification system (temperate climate with dry and hot summer). Although Figure 5.20 categorises Barcelona and Madrid as having a cold semi-arid climate (BSk), both cities are located on the boundary between different climate types and, depending on the source, are occasionally classified as Csa as well (e.g., [174]). Therefore, it can be concluded that in the context of the chosen demonstrator building, NRG-Panels are most suitable for deployment in locations with Csa climate, encompassing large portions of Portugal, Spain, Italy, Greece, and Turkey, as well as Southern France and Mediterranean islands.

6.4 Concluding remarks

This chapter focused on exploring the influence of climatic conditions on the optimal configuration of NRG-Panels as well as on the estimation of the applicability potential of NRG-Panels in different climates, current and future. To do so, multi-objective optimisations have been performed for 53 locations across Europe under the current climatic conditions and for 10 of

those also under future climate projections. The main takeaways from this chapter are provided below.

- NRG-Panels' performance and optimal configurations are similar for colder and moderate climates, but vary significantly in warm and hot climates.
- From the three objectives analysed (environmental costs, energy costs, and construction and demolition costs), there are always trade-offs between at least one pair of objectives and often between all of them.
- PCM with a melting temperature of 18°C (PT18) is the most universally suitable option across various locations and climate projections, but in some cases, climate change might result in a shift of the optimal melting temperature towards lower or higher values.
- The foam stability constraint greatly affects the feasibility of certain NRG-Panel configurations, often reducing their applicability potential.
- In the constrained case, the configuration of NRG-Panels that minimises lifecycle environmental costs and construction and demolition costs is a regular foamed concrete with no MPCM embedded.
- From the standpoint of lifecycle environmental costs, energy savings from added MPCM are not large enough to compensate for the high embedded carbon emissions of MPCM production.
- The optimal configuration of NRG-Panels for a future climate often differs from the optimal configuration for the current climate.
- Climate change significantly impacts NRG-Panels' performance and applicability, with some locations becoming more suitable and others less suitable in future climate projections.
- Southern Europe and Mediterranean areas with Csa climate under Köppen-Geiger climate classification demonstrate the highest potential for NRG-Panels' application as a dual-function thermal material providing insulating and energy-storing functions.

7

BEST FIT FOR COMMON PURPOSE: A MULTI-STAKEHOLDER DESIGN OPTIMISATION METHODOLOGY FOR CONSTRUCTION MANAGEMENT

Previous chapters of the dissertation presented an in-depth analysis and optimisation of NRG-Foam and NRG-Panels on material as well as building levels. However, to further analyse the material on a construction project level, it becomes necessary to introduce the social factor into the equation. Indeed, at this level, the evaluation of a material's performance and applicability is guided not only by its technical performance but also depends heavily on whether this performance fits the subjective and often contradicting requirements of involved decision-makers. From this perspective, in order to evaluate the competitiveness of NRG-Panels as a thermal performance solution in real-world construction projects, it becomes especially important to apply decision-making methods that accurately account for the subjective preferences of decision-makers. This chapter presents a new preference-based decision-making methodology that is more representative of the real-life design and construction process. The application of the methodology is also demonstrated on a real-life decision-making case.

This chapter has been published in Buildings [175].

7.1 Introduction

The global challenges caused by global warming, rapid urbanisation, economic instability, and the ever-reducing affordability of housing call for rethinking and improvement of the ways we design and construct new buildings and renovate the existing ones. Aiming to answer this call, the research agenda of “better buildings” has been expanding rapidly over the last several decades, resulting in the development of multiple research domains and themes such as green buildings [176], [177], [178], [179], low- and zero-carbon buildings [180], [181], [182], [183], passive buildings [184], [185], sustainable buildings [186], [187], circular buildings [188], [189], resilient buildings [190], [191], smart buildings [192], [193], and healthy buildings [194], [195]. Some of the themes have made their way to statutes, building codes, standards, and certification schemes and certain ideas have been adopted by practitioners but there is still a very long way to go if we want to meet present and future challenges.

Moving towards practical implementation of “better construction” will have a major effect on the way construction projects are being developed. The project development and design processes in the construction industry are still often disconnected and based on individualistic principles where each involved party seeks to maximise their own local gains and optimise their own part of the project development chain, which can result in suboptimal performance on the project level [196], [197]. With the increasing complexity of the projects and a greater number of internal and external stakeholders and perspectives involved, it will become harder to come to a consensus and that, as a consequence, could result in conflicts, project delays, and expanding project costs [179], [198], [199], [200], [201]. Moving forward, the process will need to become more integrated, streamlined, and actively involve multiple stakeholders at all the stages of project development, starting from the earliest ones [21,25,27,28].

Further, effective implementation of “better construction” will not be possible without a shift away from the currently prevailing assessment-based project development approach. Assessments play an important role in the construction sector but, in their current form, they cannot ensure the optimality of the final design. For example, LCA is a well-developed and standardised assessment method that sees ever-increasing adaptation by the construction sector. In the Netherlands and France, it is now mandatory to conduct an LCA for all new construction projects [202]. However, it relies on comprehensive and detailed data that are often not available in the early stages of project development. Thus, LCAs (and other assessments) are often conducted in the late stages of project development when it is hard or not even possible to change the final design [203]. In addition, assessments often imply that the choice is made among a set of predefined alternatives, but this approach cannot guarantee that there is no superior design option that was for some reason not included in the assessment.

The shift from assessment-based methods to optimisation-based ones promises a number of major benefits. It can enable stakeholders’

collaboration from the early stages of the project's development, help in finding a consensus, ensure that the stakeholder's preferences (here and in the following text we use the term "preference" to define the expected value (economic, environmental, social, aesthetic, or any other) of the object designed for a stakeholder in an a priori optimisation-based design process) are reflected in the final design, speed up the project's development and delivery, and, ultimately, provide a higher value for stakeholders involved. Not surprisingly, this area has received a lot of attention in recent years; e.g., [204], [205] provided a review of algorithms and tools used in building design optimisation, [206] developed a review of simulation-based optimisation methods with a focus on the challenges that the field is facing, and [207] reviewed the energy-efficiency optimisation of buildings from the perspective of architects.

As pointed out above, the number of studies on optimisation in building design is quite large. Nevertheless, there are still some issues that have not been addressed and there is space for improvement. Most of the studies on building design optimisation that can be found in the literature focus on the technical aspect of the process, ignoring the stakeholders' involvement component and the group dynamics of the real-world design process. Those studies are predominantly based on a posteriori approaches and the construction of Pareto frontiers for multiple conflicting objectives (e.g., [205], [208], [209], [210], [211]). In such approaches, stakeholders are mostly seen as taking part at the end of the optimisation process and selecting an alternative from the Pareto frontier or are not even considered at all. However, in real-world design processes, stakeholders are an essential part of the process and if we want to fairly model a group decision-making process, the result of the optimisation should respect their preferences. Further, while a posteriori approaches have their advantages, they imply that stakeholders and their preferences come at the end of the optimisation process. In contrast, the real-world design process starts from stakeholders and their preferences and it is, thus, inherently an a priori preferences-first process. In addition, a posteriori optimisations can become very complex and hard for stakeholders to understand as the number of objectives increases. Those approaches are also generally very computationally demanding and slow as they rely on the calculation of multiple optimal solutions (and there can be hundreds or thousands) and each solution requires a separate optimisation run [212].

Some studies have coupled a posteriori optimisation and a Pareto frontier search with a consequent selection of the final solution utilising multi-criteria decision-making methods (MCDMs) (see, e.g., [213], [214], [215], [216]). While those approaches are a logical extension of pure a posteriori optimisation and make the decision-making process easier for stakeholders, they are still not without issues. The whole process becomes even more resource-demanding and complex as, in addition to the generation of multiple solutions, an MCDM process needs to take place. Making on-the-fly changes to the problem configuration (e.g., adding another objective) in such systems is hard and time-consuming as it would require a full recalculation of Pareto frontiers and re-evaluation of the consecutive MCDM process.

When it comes to a priori approaches where stakeholders provide their preferences up front and separate objectives are aggregated into one with a consequent single-objective optimisation run, only a few studies can be found that apply it to building design optimisation and decision-making [217], [218], [219]. Yet, those studies only consider objectives' weights as a form of representing stakeholders' preferences. In real-world scenarios, however, stakeholders also have some wishes and preferences regarding the numerical values of objectives they are willing to achieve but those considerations are not taken into account. For example, if a stakeholder wants to maximise the profit, they also normally have some expectations for the profit level they are targeting, the level that is below the target but still deemed to be acceptable, and the level that is not acceptable.

A priori approaches are sometimes criticised for their inability to illustrate the trade-offs between objectives in a way that a Pareto frontier can. However, making the a priori process iterative or adding a sensitivity analysis can help to resolve this. In particular, through an iterative approach stakeholders can learn how their inputs and changes are impacting the optimum and provide a similar illustration of the underlying trade-offs and interplays between the objectives. In addition, a priori approaches are more stakeholder-oriented, faster, and easier to understand. They are also sufficiently more flexible when it comes to making changes to the optimisation problem configuration. Due to these qualities, their application can make the design process more dynamic and flexible and foster collaboration.

Another general shortcoming of most of the studies on building design optimisation and decision-making is in their approach to measuring and modelling stakeholders' preferences for multiple objectives. As mentioned before, in building design optimisation studies, stakeholders' preferences at best are provided in the form of objectives' weights. A notable exception to this is a series of studies by Geyer [220], [221], [222] that utilised preference functions (or utility functions, as they are called by the author) to describe the variation in the desirability of different numerical values of objectives for stakeholders. However, those studies are still reliant on the building of Pareto frontiers with the associated downsides already mentioned above. When it comes to studies utilising MCDMs, most are based on methods (with the most common being analytic hierarchy process (AHP) [223], [224]) that, as was shown by Barzilai in [225], do not measure and aggregate preferences in a mathematically correct way and utilise the operations of addition and multiplication on scales where those operations are not defined. Barzilai has also proposed an alternative theory for preference modelling that overcomes the shortcomings of the existing methods, the preference function theory (PFM) [225]. Binnekamp [226] has made the first step in applying this theory within the built environment domain. However, this work only presented an initial proof of concept and not an operational optimisation-based design methodology that can be applied to real-world projects.

To address the abovementioned issues, this work aims to answer the following questions:

- How can early stage design optimisation be implemented?
- How can we ensure that the design optimisation properly reflects the real-world design and construction processes?
- How can we better involve stakeholders in the design optimisation process?
- How should stakeholders' preferences be measured and used within the optimisation?
- How can optimisation and stakeholder-driven design be integrated within a decision-making tool for construction management?

To answer these questions and fill the existing gaps, this paper focuses on the main objective of developing a novel methodology for integrated stakeholder-oriented building design optimisation that is based on an iterative a priori approach for finding the best-fitting design solution. The methodology is operationalised by means of a multi-criteria design optimisation and decision-making tool that:

- Reflects the real-world project design and construction process where stakeholders play an essential role;
- Automates the decision-making process within building design and construction;
- Uses a mathematically correct way of preference modelling by utilising the PFM theory;
- Is not computationally demanding, intuitive in use, and adaptive to changing stakeholders' demands;
- Can be applied to the early stages of design and construction development.

Tied to the main objective, this work also addresses the two ancillary objectives of applying the proposed methodology and the tool developed to a demonstrator case of early stage multi-storey building design optimisation and outlining the directions for the further development of stakeholder-oriented optimisation-based design.

7.2 Materials and methods

This section describes the developed methodology step-by-step and Figure 7.1 shows the overall flowchart of the methodology. The numbers in the figure refer to the steps below.

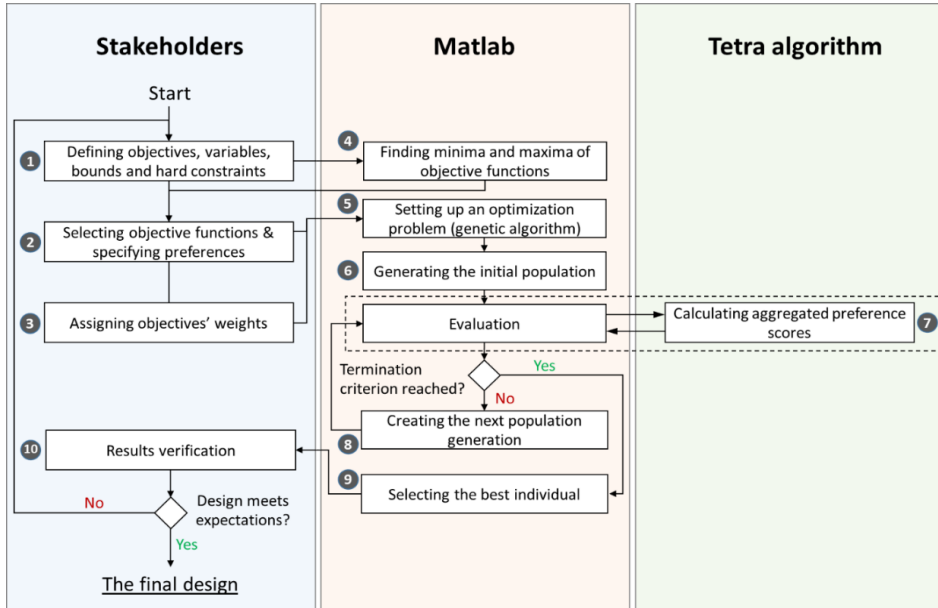


Figure 7.1: Methodology flowchart.

Step 1. Defining the design problem

Our method starts with stakeholders, who provide the necessary information to set up the design problem. They start by defining design variables (defined by a vector $\mathbf{x} = (x_1, x_2, \dots, x_N)$) that represent the design parameters that can be varied; the bounds of the design variables ($lb_i \leq x_i \leq ub_i, i = 1..N$) that provide the interval in which the design variables can change; objectives ($f_1(\mathbf{x}), f_2(\mathbf{x}), \dots, f_M(\mathbf{x})$) that quantify the performance of the design across different domains (economic, environmental, social, functional, aesthetic, and so on); inequality constraints ($g_j(\mathbf{x}) \leq 0, j = 1, 2, \dots, J$); and equality constraints ($h_k(\mathbf{x}) = 0, k = 1, 2, \dots, K$).

Step 2. Finding the minima and maxima of the objective functions

At the next step, we run multiple optimisations (the total number of which is equal to $2 * M$) in Matlab to find the minima and maxima of the objective functions given the data on design variables, bounds, and constraints. The optimisation problems are defined as follows:

$$\min_{\mathbf{x}} f_m(\mathbf{x}), \quad m = 1, 2, \dots, M \quad (7.1)$$

$$\min_{\mathbf{x}} -f_m(\mathbf{x}), \quad m = 1, 2, \dots, M \quad (7.2)$$

subject to

$$g_j(\mathbf{x}) \leq 0, \quad j = 1, 2, \dots, J \quad (7.3)$$

$$h_k(\mathbf{x}) = 0, \quad k = 1, 2, \dots, K \quad (7.4)$$

$$lb_i \leq x_i \leq ub_i, \quad i = 1, 2, \dots, N \quad (7.5)$$

For compactness, linear and nonlinear constraints are grouped together: $g_j(\mathbf{x})$ includes both linear and nonlinear inequality constraints and $h_k(\mathbf{x})$ includes

both linear and nonlinear equality constraints. The algorithm used in the optimisations is selected based on the objective functions on hand.

Step 3. Defining preferences

As was mentioned in the Introduction section, the studies that are currently available in the literature either do not utilise preferences at all (e.g., in most a posteriori studies based on building a Pareto frontier), utilise them only partially (e.g., only use objectives' weights as stakeholders' inputs), or rely on preference modelling approaches that were shown to have issues when it comes to the mathematical foundations. For example, in the case of one of the most commonly used decision-making methods—analytic hierarchy process (AHP)—the preference is measured by defining the ratio p_1/p_2 , where p_1 and p_2 are preferences for two alternatives. However, as Barzilai argues in [225], such a ratio is not well defined as a ratio is not defined for two time values or potential energies.

The design optimisation methodology proposed in this study is based on the PFM theory proposed by Barzilai [225]. Instead of commonly used utility and ratio scales, the method relies on measuring preferences on affine scales, thus making the mathematical operations possible. The affine scale is defined as:

$$k = \frac{p_1 - p_2}{p_3 - p_4} \quad (7.6)$$

where p_1, p_2, p_3, p_4 are four preference points on an affine scale defined by the scalar value k . The number of points needed to define the scale can be reduced to three (in this case, $k = \frac{p_1 - p_2}{p_2 - p_3}$) but not less than that. By measuring preferences in this way, we avoid issues related to the selection of the unit and the absolute zero of measurement that are inherent in other methods commonly used in the literature. This enables us to use preferences as a part of the design optimisation and group decision-making process. In this paper there is no room for an extensive description to the fundamentals of PFM theory and only the necessary high-level findings are incorporated. For further details the reader is referred to Barzilai [52].

In our method, the elicitation of preferences is implemented in a visual manner. In accordance with the PFM methodology, preferences are measured on a preference scale that ranges from 0 to 100. For each of the objectives, a stakeholder needs to provide three points that represent the worst possible case (measured at 0 on the preference scale), the best possible case (measured at 100 on the preference scale), and a point in-between. In order to simplify the task for the stakeholders, we calculate the minima and maxima of each of the objective functions (see the previous step) and select those as the worst and the best cases. Then, stakeholders need to provide only a single in-between point. However, there might be cases where a stakeholder disagrees with the predefined best and worst options. In this case, the values can be over-ridden and the stakeholder can indicate their own values for the best and worst options. Currently, we are working with three preference points. However, within a satellite research project, we are also conducting experiments with real-world stakeholders to determine the optimal way of collecting preference information. If the current three-point method is found

to not be flexible enough, we could provide stakeholders with the possibility of selecting more points.

When three points are provided, we can build a curve that passes through them—a so-called preference curve. The mathematical representation of a preference curve is referred to as the preference function. In order to fit a curve passing through three points, we use the Piecewise Cubic Hermite Interpolating Polynomial (PCHIP). Compared with the standard cubic spline, the PCHIP eliminates overshoots (the fitted curve never goes above the highest point), which is an important quality when dealing with preferences that should be mapped on a fixed interval. Figure 7.2 shows an illustration of a preference curve building on a hypothetical example of a construction costs objective.

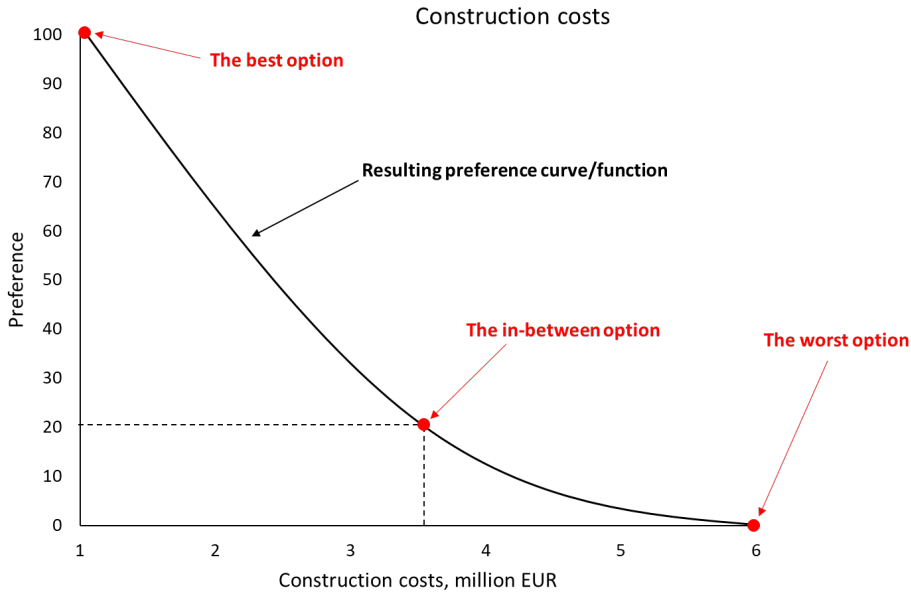


Figure 7.2: An example of obtaining a preference curve.

By means of preference functions $(p_1(f_1), p_2(f_2), \dots, p_M(f_M))$, we convert our problem into the preference form where the ultimate goal is to maximise the aggregated preference score. Our objectives can, thus, be rewritten as:

$$f_1^*(x) = p_1(f_1(x)), f_2^*(x) = p_2(f_2(x)), \dots, f_M^*(x) = p_M(f_M(x)) \quad (7.7)$$

All objectives are now measured on the preference scale, thus avoiding the issues arising from the difference in the unit of measurement between the objectives.

Step 4. Specifying weights

Stakeholders provide weights $(w_1, w_2, \dots, w_M)$ for each of the objectives. The weights should give 1 in sum. Within a collaborative design process, one might expect the weights to be spread among the objectives. However, in some cases, there might be a single stakeholder whose preferences dominate

the rest of the stakeholders (e.g., the investor). In this case, most or even all of the weight can be put towards this stakeholder and the problem will turn into a single-stakeholder one. The resulting design solution will be the one that satisfies the preferences of this single stakeholder.

Step 5. Setting up the optimisation problem

The design variables, their bounds, the objectives, and the constraints are now fed into Matlab and the optimisation problem is set up. Various algorithms and approaches can be utilised at this step. We use a genetic algorithm (GA) as it can handle complex nonlinear mixed-integer optimisation problems.

Step 6. Initial population generation

Based on the input data, the GA generates the initial population where each member of the population represents a possible design solution. For each member, we calculate the values of the objective functions in the preference form (measured on the preference scale).

Step 7. Preference aggregation and evaluation

Now, when we have preference scores for each of the objectives for all members of the population, we need to aggregate those preferences into a final score that best reflects all the individual values. This aggregated preference score is used as the final optimisation objective that the GA is trying to maximise. A straightforward and commonly accepted approach for aggregating preferences is to use the weighted mean of the individual preferences. However, this is not correct as the operations of addition and multiplication are not defined on this scale (see the information on the measurement of preferences above). Instead, aggregation should be done within the affine space to synthesise an overall preference score that provides the “best” fit of all weighted (relative) scores for all the stakeholders’ objectives. In other words, the correct way of aggregating preference scores is based on finding the aggregated preference that minimises the least-squares difference between this overall preference and each of the individual scores in the affine space (Barzilai [225]).

Therefore, our final optimisation problem can be rewritten as:

$$\min_{\mathbf{x}} -P^*(f_1^*(\mathbf{x}), f_2^*(\mathbf{x}), \dots, f_M^*(\mathbf{x}), w_1, w_2, \dots, w_M) \quad (7.8)$$

subject to

$$g_j(\mathbf{x}) \leq 0, \quad j = 1, 2, \dots, J \quad (7.9)$$

$$h_k(\mathbf{x}) = 0, \quad k = 1, 2, \dots, K \quad (7.10)$$

$$lb_i \leq x_i \leq ub_i, \quad i = 1, 2, \dots, N \quad (7.11)$$

where P^* is the aggregated preference score calculated using the PFM theory. The synthesis of the aggregated preference using the PFM theory was implemented as a solver inside of the software tool called Tetra [227]. Tetra is a standalone multi-criteria decision-making program that enables the selection of the best alternative for both single- and multi-stakeholder cases.

However, since Tetra was originally developed as a tool for decision-making, it relies on stakeholders providing a list of possible alternatives to select from and, thus, is not well-suited for use in optimisation problems where the alternatives are generated and not predefined. To overcome this, instead of the desktop version, we use a web version of Tetra ver. 3.5.1. It runs on a server and accepts data (preference scores and weights) in a special format based on XML. The calculations take place on the server and the results are provided as an XML file. In our case, the resulting file contains the aggregated preference scores for each member of the population. Tetra, thus, plays the role of an external objective function connected to the GA in Matlab.

The results are then evaluated by the GA and the algorithm checks the termination criteria. If none are satisfied, it proceeds to the next generation (Step 8). If a termination criterion is satisfied, we proceed to Step 9.

Step 8. Next generation

The GA obtains the next generation of the population by the means of survival, mutation, and crossover and iterates through Step 7.

Step 9. Selecting the best individual

When a termination criterion is satisfied, the GA selects the best individual from the population. The best individual is a representation of the optimal design solution.

Step 10. Results verification

The solution is then presented to stakeholders. If the result satisfies the stakeholders and no changes to the problem configuration are necessary, it is selected as the final design. Otherwise, the stakeholders can decide to change some parameters of the design problem or modify their inputs. For example, they might want to modify their preferences or objective weights or bring more stakeholders to the table. In that case, the process returns to the beginning and starts again.

After each iteration, the stakeholders can compare the optimal designs from each run between each other. Through that, they can obtain an understanding of how their actions are influencing the result. This can help to uncover bottlenecks and have an educational effect. The process stops when the stakeholders agree that no more changes are required.

7.3 Demonstrator case

7.3.1 Description of the Demonstrator Case Building

The demonstrator case was developed in cooperation with Heijmans (Rosmalen, the Netherlands), one of the largest design and construction contractors in the Netherlands. The selected case aims to demonstrate the application of the methodology described above and is applied to the early design stage of non-residential multi-storey building development.

The demonstrator case is based on Autodesk Revit models provided by Heijmans. As our case is concerned specifically with the early stages of project development, the building models only included three of six shearing layers: Site, Structure, and Skin (in accordance with the classification by Stewart Brand [228]). The original models were not parametrised and had a fixed gross floor area (1000 m²) and number of floors (5). In total, three complete building models were shared with us, each characterised by different sets of materials used for the façade and the structural elements:

- A concrete frame and brick façade with Rockwool insulation;
- A structural steel profile frame and hollow concrete slabs with a steel sandwich panel façade with polyisocyanurate insulation;
- A cross-laminated timber frame with a wooden joist floor and a timber frame façade with mineral wool insulation.

The models are shown in Figure 7.3. Details of the material composition for each model can be found in Appendix D.

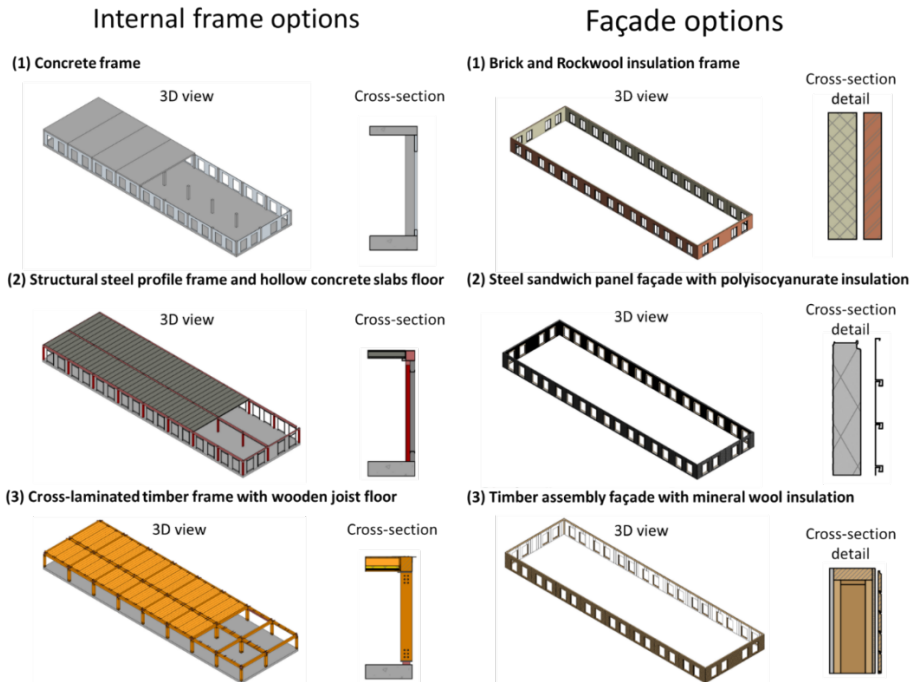


Figure 7.3: Material options for the façade and structural frame of the demonstrator case provided by Heijmans.

In order to use the models in the optimisation, they were parametrised in the following way:

- First, for each of the models, the amount of materials per floor was calculated. As each model includes two parts—a façade and a frame—

separately, in total six initial calculations were made. The materials used in Autodesk Revit models were mapped to the closest possible analogues available in the LCA software OneClick LCA [229];

- The scaling of the floor area was implemented in relation to the original total gross area:
 - a. It was assumed that the window-to-wall ratio (WWR = 0.35) and the ratio of length to width of the building (3.49) will be preserved when the floor area changes;
 - b. The total volume of materials used in the ceiling and vertical structural elements was assumed to change proportionally to the total floor area;
 - c. The total volume of materials used in walls was assumed to change proportionally to the perimeter length of the building whilst taking into account the scaling of the windows' area;
 - d. The total volume of materials used in horizontal structural elements was assumed to be proportional to the length or the width of the building (depending on the element orientation);
- To estimate the total volume of materials used in a building, first, the volume per storey was calculated based on the floor area and then the resulting value was multiplied by the number of floors;
- The resulting total volume of materials used in a building was calculated based on the floor area and the number of floors. The foundation of all building variants was assumed to be the same (500 mm thick concrete).

The material characteristics (embodied carbon emissions and prices) were obtained from the database available inside of OneClick LCA [229]. Embodied carbon emissions are based on environmental product declarations with emissions from transportation added to them. Table 7.1 provides information on all material characteristics used in the model.

Table 7.1: Characteristics of materials that were used in this study.

Material (the Full Name as it Appears in OneClick LCA)	Unit	Embodied Carbon, kg CO ₂ eq/Unit	Total Emissions from Transport, kg CO ₂ eq/Unit	Price, EUR/Unit
Ready-mix concrete, normal strength, generic, C 28/35 (4000/5000 PSI) with CEM I, 0% recycled binders (300 kg/m ³ ; 18.7 lbs/ft ³ total cement)	m ³	292.13	18.72	344.87
Ready-mix concrete, normal-strength, generic, C 40/50 (5800/7300 PSI), 0% recycled binders in cement (400 kg/m ³ /24.97 lbs/ft ³)	m ³	386.96	18.72	348
Rock wool insulation, unfaced, L = 0.035–0.04 W/mK, 40 mm, 1.2 kg/m ² , 30 kg/m ³ , Lambda = 0.035 W/(m.K), ProRox LF 970 (ROCKWOOL)	m ³	35.25	0.07	57
Wall bricks, 575 kg/m ³ (Ziegel)	m ³	138.29	1.32	115
Hot-dip galvanised structural steel, 0.45–1.5 mm, 7850 kg/m ³ (Ruukki)	m ³	20,794.65	111.24	5976.96
Structural steel profiles, generic, 90% recycled content (typical), I, H, U, L, and T sections, S235, S275 and S355	m ³	6033.17	111.24	5976.96
Hollow core concrete slab, HDF27, C 40/50, 270 mm, 344 kg/m ² , reinforcing 12,7 kg/ton (Strängbetong)	m ²	46.78	0.79	60.64
Aluminium profile, 2700.0 kg/m ³	m ³	29,289	48.60	8920
Sandwich panel with polyisocyanurate (PIR) foam and double steel siding, U = 0.21W/(m ² K), 100.9mm (Total), 0.5mm (Outer sheet), 0.4 mm (Liner sheet), 100 mm (Insulation), 12.11 kg/m ² , 120.02 kg/m ³ , SAB WB 100.1000 (SAB-profile, Tata Steel Europe)	m ²	37.2	0.20	49.92
Aluminium profiled sheets, thickness 0.7 mm, height of profile 65 mm, 2.9 kg/m ² (European Association for Panels and Profiles)	m ²	27	0.03	6.24
Cross-laminated timber, 491.65 kg/m ³ , T: 51–500 mm, max width: 2.95–4.80 m, max length: 16–20 m, X-Lam (Studiengemeinschaft Holzleimbau e.V.)	m ³	187.23	4.15	544.93
Wooden joist floor assembly, 278 mm, incl. 225 mm mineral wool insulation	m ²	36	0.45	132
Timber frame external wall assembly, incl. mineral wool insulation	m ²	65	0.73	110

7.3.2 Design Problem Specification

For the demonstrator, we assumed the following set of design variables: floor area, number of floors, set of the building's envelope materials, set of the building's internal structural frame materials, and distance from the nearest railway station (see Table 7.2).

Table 7.2: Design variables used in the demonstrator case.

Name	Bounds	Type
Floor area	700–2500 m ²	Continuous
Number of floors	2–10	Integer
Set of the building's facade materials	1—Brick and Rockwool insulation 2—Steel sandwich panel façade with polyisocyanurate insulation 3—Timber frame façade with mineral wool insulation	Categorical
Set of the building's structural frame materials	1—Concrete frame 2—Structural steel profile frame and a hollow concrete slabs floor 3—Cross-laminated timber frame with a wooden joist floor	Categorical
Distance from a railway station	0.2–15 km	Continuous

For objectives, the following were selected:

- Construction costs (EUR) (only includes the cost of materials, and all other costs (e.g., labor) were assumed to be constant);
- Embodied carbon emissions (kg CO₂eq) (based on environmental product declarations (EPDs));
- Expected profit from renting the building out (EUR/month) (based on the total floor area of the building and the rental costs per m²);
- Location (km) (characterised by the distance from the nearest railway station to a planned construction site).

The final equations used for the calculation of objectives can be found in Appendix D. It is worth mentioning that in real-world problems such a simplification of objectives is often not possible. However, as was mentioned above, the purpose of the simplified demonstrator case is to illustrate the methodology developed. In the future, we expect to work with more comprehensive building design cases where the calculations of objectives (building performance indicators) will be performed using external software tools such as EnergyPlus [230] for building energy consumption, OpenLCA [231] or Brightway2 [232] for the calculation of environmental impacts, etc. The methodology presented in this paper is universal and acts as a decision-making layer that can be built on top of any underlying calculations.

For this demonstrator, we did not include any constraints and the solution space is only limited by the design variables' boundaries. However, the model can work with both linear and non-linear constraints.

7.3.3 Optimisation Problem Specification

Given the design variables (Table 7.2) and objectives (refer to Appendix D for the equations), the optimisation problem we are dealing with is a mixed-integer nonlinear optimisation problem. To solve the optimisation problem, we used the *ga* solver in Matlab. The parameters of the solver were tweaked over time in order to ensure the desired speed-to-precision ratio. In order to decrease the running time and the number of requests sent to the server, the algorithm was set up to work in the vectorised form. The final chosen parameters of the solver are provided in Table 7.3. If a parameter is not mentioned in the table, the default value provided in Matlab was used. A relatively low value of the crossover fraction was selected in order to preserve the diversity of the population. It was also observed that this ratio results in shorter running times compared with other values.

Table 7.3: *ga* solver parameters.

Parameter	Value
Population size ('PopulationSize')	250
Max. generations ('MaxGenerations')	400
Max. stall generations ('MaxStallGenerations')	20
Function Tolerance ('FunctionTolerance')	1E-9
Vectorised form ('UseVectorized')	true
Elite population size ('EliteCount')	30
Crossover fraction ('CrossoverFraction')	0.5

As was mentioned in the Methods section, before running the main optimisation routine, we first found the minima and maxima for all of the objective functions taking into account the design variables' bounds. Table 7.4 provides those values for all objectives used in the demonstrator.

Table 7.4: *Minima and maxima of objective functions.*

Name	Minimum Value Given the Design Variables' Bounds	Maximum Value Given the Design Variables' Bounds
Embodied carbon, kg CO ₂ eq	241,950	3,992,042
Construction costs, EUR	272,675	5,636,095
Profit from rent, EUR	288,978	5,162,471
Location, km	0.2	15

Once the minima and maxima have been calculated, stakeholders construct preference curves for objectives they are interested in. For the first demonstrator case, we did not involve real stakeholders and instead provide a possible scenario of the design development. In order to illustrate the iterative nature of our method, we simulated a five-iteration design optimisation process. Thus, the optimisation model was run five times with different input parameters. For the purposes of comparison, we also ran the same optimisation but using the weighted mean of preferences instead of Tetra for the aggregation of the individual preference scores. A detailed

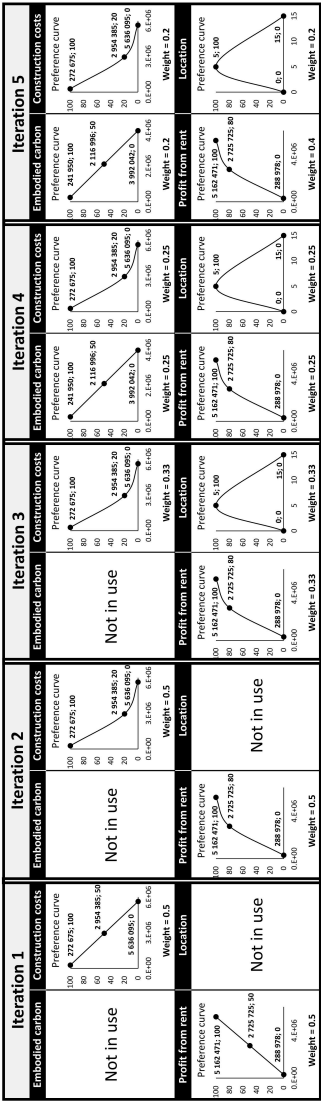
description of the parameters used in each iteration is provided in the next section.

7.3.4 Description of the Design Process Iterations used in the Study

The iterative a priori process is one of the key features of the proposed method. It makes it possible to make major changes to the problem configuration (e.g., adding or removing objectives, changing stakeholders' preferences, or modifying constraints) with relative ease and quickly see the outcome of those changes. It allows stakeholders to explore the underlying causal relationships and collaborate in real-time and has an educational effect.

We illustrate the iterative process and a possible design problem evolution on the demonstrator case. Figure 7.4 panel (a) provides a visual overview of the iterations and the corresponding input parameters used in the optimisation runs.

a) Iterations



b) Inter-iteration change of the optimal design

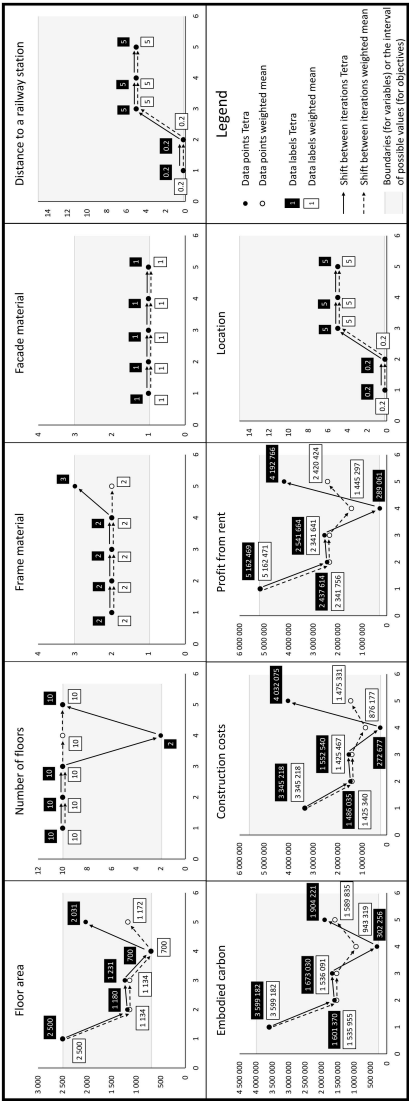


Figure 7.4: (a) Preference curves and weights for all iterations; (b) The results of optimisation runs for each iteration showing the optimal values of design variables and objectives.

Iteration 1

In the first iteration, we assumed that stakeholders are only interested in minimising the construction costs and maximising the profit from rent. These two objectives have an equal weight of 0.5 and the two other objectives were omitted and, thus, have no weight. The preferences are linear on the interval of values that the objective functions take.

Iteration 2

The stakeholders have made changes to their preference inputs that are now nonlinear. The requirement for Construction costs has become more strict (the preference score for the middle point decreased from 50 to 20), while for Profit from rent the change is in the opposite direction, as it has been relaxed (the preference score for the middle point increased from 50 to 80).

Iteration 3

It was decided that Location should also be considered one of the objectives. This third objective was brought in, and the preference curve was defined as being equal to 0 at the extreme points (0.2 km and 15 km) with a peak preference at 5 km. All three objectives have equal weights.

Iteration 4

A new stakeholder was involved that is interested in bringing in environmental considerations. Thus, a fourth objective—Embodied carbon emissions—has been added. The preference curve for Embodied carbon emissions was assumed to be linear and the weights of all four objectives to be equal.

Iteration 5

It was decided that the profit objective is more important than the other objectives. Thus, the weights of the objectives were modified. The weight for the Profit from rent objective was increased to 0.4 while all other objectives had an equal weight of 0.2.

7.4 Results of the Demonstrator Case

Figure 7.4 panel (b) shows how the optimum design changes at each iteration. The top row shows the optimal values of variables and the bottom row shows the corresponding values of the objective functions. Our starting design at Iteration 1 is characterised by the largest possible Profit from rent. When the preference curve for Construction costs was modified to be more strict at Iteration 2, the optimum shifted significantly and the floor area decreased from 2500 m² to 1180 m². As a consequence, the profit saw a two-fold decrease while construction costs reduced from 3.3 million EUR to 1.5 million EUR. The introduction of the third objective at Iteration 3 resulted in Distance to a railway station increasing from 0.2 km to 5 km. The floor area has seen a slight increase (by 51 m²), resulting in a minor increase in Construction costs and Profit from rent. The inclusion of Embodied carbon emissions into the model at Iteration 4 had a major effect on the optimum: the number of floors and the floor area reached their lower boundaries. In this configuration, Construction

costs reached the absolute possible minimum. Embodied carbon emissions were also close to the absolute minimum. However, while the preferences related to Construction costs and Embodied carbon emissions were well-satisfied, Profit from rent decreased from the best possible value of 5.2 million EUR/month at Iteration 1 to a near-bottom value of 0.3 million EUR/month. Increasing the weight of Profit from rent at Iteration 5 resulted in it growing to 4.2 million EUR/month. The floor area increased to 2031 m² and the number of floors moved back from 2 to 10. In addition, the optimum set of the building's structural frame materials changed from 2 (Structural steel profile frame and a hollow concrete slabs floor) to 3 (Cross-laminated timber frame with a wooden joist floor).

From the simulation results, it can be observed that the floor area is the most sensitive variable to the model parameters. The set of the building's facade materials variable, on the contrary, is not sensitive and did not change in any of the iterations. Comparing the results obtained using Tetra for handling the preferences and the aggregation using the weighted mean, it can be seen from Figure 7.4 panel (b) that the difference in the optimal design is large. While in the simplest configuration with two objectives and linear preferences at Iteration 1 the optima were exactly the same, the difference grew with each new iteration and reached its peak at the final iteration. Thus, the importance of using a correct method for handling the preferences increases with the complexity of the problem. While our demonstrator case was relatively simple, many of the real-world design optimisation problems would include even more stakeholders and objectives and using a simplistic method of preference aggregation (such as the weighted mean) can result in a suboptimal design.

7.5 Discussion

7.5.1 Limitations

The limitations of this study are related to the demonstrator case. Since the main aim of the paper was to present a novel methodology for design optimisation and decision-making, the demonstrator case was chosen to be relatively simplistic. Only a limited set of variables and objectives was used. The building model was not detailed (it was only concerned with the Site, Structure, and Skin shearing layers) and was manually parametrised in a simple manner that leaves some room for improvement. Further, the approach to the data collection was also simplified and most of the data originated from OneClick LCA. Moreover, the iterative design process and all the corresponding parameters used in the demonstrator did not involve real stakeholders and were pre-defined. Lastly, we assumed that in our case each stakeholder only provides preferences for a single objective. In real-world scenarios, there can be cases where several stakeholders have overlapping preferences for a single objective. Such cases can be handled within the PFM methodology but have not been considered yet.

Nonetheless, despite the abovementioned simplifications, we believe that the demonstrator case study developed was more than enough to illustrate the application of the proposed method. Its relative simplicity also made it easier to visualise the results. Our future work will aim to address all the limitations and apply the model to more complex real-world design projects.

7.5.2 Steps for Further Development

Our future work will focus on refining and extending the proposed methodology and applying it to more complex real-world design and construction problems. The next steps include:

- Developing the user interface and running a series of workshops with real-world stakeholders in order to obtain feedback and refine the methodology and the tool ('Preferendus');
- Validation of the methodology and the developed tool in design offices on more complex cases that include more objectives from different domains (expanding it to cover energy modelling, social aspects, circularity, resilience, ecosystem services provision, and more) and more complex stakeholder structures (e.g., stakeholders with overlapping preferences);
- In addition to whole-building design, implementing the methodology for more specific cases of design decision-making and specifically the selection of building materials. The selection of building materials is a challenging topic due to the overwhelming number of existing options, each promising specific advantages (e.g., traditional mass-market materials vs. circular materials vs. low-carbon materials vs. bio-based materials), and the selection process can be streamlined and simplified by implementing an automated preference-based decision-making system. In this context, the methodology will also be applied to a case of insulation material selection within the NRG-Storage Horizon 2020 project that this work is affiliated with;
- Integration of the methodology with parametric building design software (e.g., Rhino Grasshopper). Parametric design software allows us to seamlessly connect the building design variables to multiple different objectives such as energy consumption, environmental impacts, thermal comfort, and structural strength. Building a stakeholder-oriented layer on top of the existing parametric design functionality would allow us to properly account for stakeholders' preferences and have a fully integrated design process from preferences to the final CAD model;
- Extending the methodology to include a stalemate resolver for the automated resolution of design deadlocks where the design solution space becomes over-constrained by stakeholders and no feasible solution can be found without relaxing some of the negotiable constraints (by negotiable constraints, we mean design constraints

specified by stakeholders that can, in theory, be moved and modified during the design process such as the maximum budget, etc.);

- Developing the methodology to further allow for finding a compromise design solution using a preference-based goal attainment approach;
- As the core methodology presented in this study can be applied to preference-based optimisation (any optimisation process that should consider stakeholders' preferences) in any context, exploring the possibility of expanding the tool to be applicable in other fields such as supply chain management, asset management, etc.

7.6 Conclusions

The novel methodology presented in this study fills the existing gaps outlined in the Introduction section. We showcased a new multi-criteria optimisation and decision-making tool that better reflects the real-world design process and utilises the preference function modelling theory that resolves issues related to the measurement and aggregation of preferences found in the literature. The tool enables decision-makers to find the final design that reflects all stakeholders' concurrent preferences: the best fit for common purpose. Based on the iterative *a priori* approach, the tool has the advantage of being flexible and fast, allowing stakeholders to explore and learn about the consequences of their actions.

The application of the tool was demonstrated on a multi-storey building design optimisation case study with a focus on early stage design. The case highlighted the main difference of the tool compared with the existing solutions—the stakeholder-first approach. The preferences of stakeholders were considered as a starting point and the solution obtained reflected the preferences of all stakeholders involved. Compared to the most commonly used *a posteriori* approaches, our study expands the commonly used notion of preference, as we consider not only the weights of objectives but also the expectation levels for different numerical values of objective functions. This makes it possible to ensure that the optimum obtained has a better alignment with the predetermined expectations of stakeholders that always exist.

The flexibility and the iterative nature of the tool were showcased through a five-iteration design process where the problem configuration was adjusted between iterations. Even major changes to the configuration—such as adding an objective—were easy to execute. The combination of the fast speed of the selected *a priori* approach and the aggregation of multiple objectives into one makes the tool well-suited as a collaborative learning and exploration tool. Stakeholders can easily change the parameters and quickly see how the result changes, allowing them to learn about the underlying causal relationships.

Comparing the results obtained using the PFM methodology for preference modelling and a simple weighted mean showed major differences in optimal results between the two. While using the weighted mean could be an attractive option due to the simplicity and higher speed, our results

highlight the importance of using a correct approach to modelling stakeholders' preferences for obtaining an accurate solution.

8

PREFERENCE-BASED GOAL ATTAINMENT APPROACH FOR EQUITABLE DECISION-MAKING

In Chapter 7, a new stakeholder-focused decision-making method was introduced. While this method has been operationalised, it was found to have some significant limitations hindering its applicability in real-world decision-making: it relies on black-box proprietary software, and the results produced by it often showed a large degree of stakeholder satisfaction inequality. To address those limitations, this chapter presents a newly developed decision-making method called Preference-Based Goal Attainment (PBGA). The PBGA method is transparent and straightforward, and is focused on finding an equitable solution where no stakeholder is left behind. The method is then applied to an illustrative decision-making case focused on the selection of the optimal thermal material for a demonstrator building. The results of the illustrative decision-making case show that, under certain conditions, NRG-Panels can be an attractive thermal material providing well-balanced performance for multiple stakeholders with conflicting interests. The chapter also highlights that the strength of NRG-Panels lies in their high flexibility and customisability.

8.1 Introduction

The previous chapter has presented and demonstrated the use of an optimisation-based decision-making methodology focused on a priori incorporation of stakeholders and their preferences into the optimisation process with the aim of creating a system that better represents real-world decision-making projects. From applying the developed approach to a variety of decision-making cases later on, it was observed that the final result was often heavily skewed towards the preferences of one of the stakeholders while leaving one or several others with very low preference scores. In some cases, stakeholders were ending up on the opposite ends of the preference scale, with one of them achieving the maximum possible score of 100 while another had the minimum possible score of 0, even when their weight (or decision-making power) was the same. In the real-world setting, such a polarisation in the final outcome could create a conflict among stakeholders. Consequently, such a situation could lead to major issues for the project, causing development delays, inducing distrust and reducing stakeholders' willingness to cooperate.

The described issue of skewed satisfaction of stakeholders is not unique to the approach presented in the previous chapter, but is a characteristic of the decision-making methods that operate using integrated "collective good" metrics. While the ways of calculating the metrics vary, all such approaches focus on achieving the maximum possible "collective good", even if it happens at the inconvenience of some of the individual decision-makers. Those approaches, however, assume that the decision-making team is operating in complete unity and has a common shared goal that is prioritised over individual goals. In reality, this might not always be the case, and some stakeholders might not be willing to accept a solution that ignores or understates their individual goals.

Another major limitation of the approach introduced in the previous chapter is that it relies on proprietary black-box software. Due to this, it is not possible to validate the results and provide the stakeholders with a transparent explanation of the obtained solutions. This reduces the overall trustworthiness of the approach and could further escalate the conflicting situations where the results are skewed towards one of the stakeholders. In such cases, stakeholders who had low preference scores for the final obtained solution might question the methodology used and refuse to accept the results.

To address those issues, a new decision-making methodology has been developed called Preference-Based Goal Attainment (PBGA). This methodology is based on the same foundation of Preference Function Modelling (PFM) theory [225] introduced in the previous chapter, but is focused on obtaining an equitable solution where no stakeholder is left behind. Furthermore, the developed PBGA approach is fully transparent, and the results can be easily justified and verified, thus increasing its level of trustworthiness. The following sections describe the PBGA methodology in detail and demonstrate its application using a decision-making case related

to the selection of the optimal insulation material for a demonstrator building case.

8.2 Materials and methods

The following sections present the idea behind the PBGA approach, its mathematical formulation, technical implementation, and introduce the decision-making case that was used to illustrate its practical application.

8.2.1 Overview of the Preference-Based Goal Attainment approach

The overall idea behind the PBGA approach is illustrated in Figure 8.1.

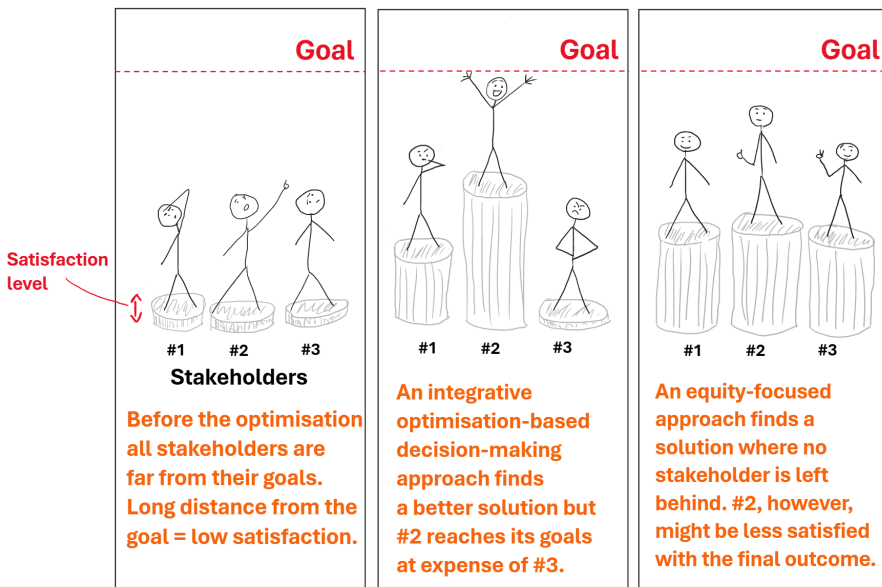


Figure 8.1: The idea behind the PBGA approach.

Traditional design decision-making processes that are still prevailing in the industry largely rely on the selection of the final design from a set of predefined alternatives and inter-stakeholder interaction based on individualistic values, where each stakeholder is seeking to maximise their personal gain. However, the design processes organised this way might result in suboptimal decisions since some possible alternatives are left out. Moreover, such design approaches are not capable of handling the ever-increasing complexity of the projects with more stakeholders being involved. The left panel in Figure 8.1 illustrates a possible suboptimal solution resulting from the traditional decision-making process.

Shifting towards a multi-stakeholder optimisation-based design process is a possible solution to the aforementioned issues. Such approaches allow to

evaluate possible solutions in an objective manner and find the best one that better satisfies the requirements of the stakeholders. However, in the case of integrative approaches focusing on the “collective good”, the final solution might be skewed and benefit one stakeholder at the expense of one or several others. This situation is illustrated in the middle panel of Figure 8.1.

PBGA is also a multi-stakeholder optimisation-based decision-making approach, but instead of “collective good”, it focuses on obtaining an equitable solution where no stakeholder is left behind. The final result of such an approach is more homogeneous and demonstrates significantly lower disparity in satisfaction levels between the stakeholders. Some stakeholders, however, might find themselves further from their goals than in the case of “collective good” decision-making methods. An outcome of the PBGA approach is illustrated in the right panel of Figure 8.1.

The following section provides a more detailed description of the PBGA approach as well as its mathematical formulation.

8.2.2 Key principles and mathematical formulation of Preference-Based Goal Attainment decision-making method

The PBGA method consists of two layers: social and technical. In the social layer, the decision-making problem is formulated, stakeholders provide their inputs, and eventually evaluate the solutions of the decision-making problem. The technical layer deals with the mathematical formulation of the decision-making problem at hand and revolves around finding an optimum solution for the decision-making problem. The layers are interconnected, and the approach is iterative in its nature. Figure 8.2 provides a schematic overview of the PBGA method.

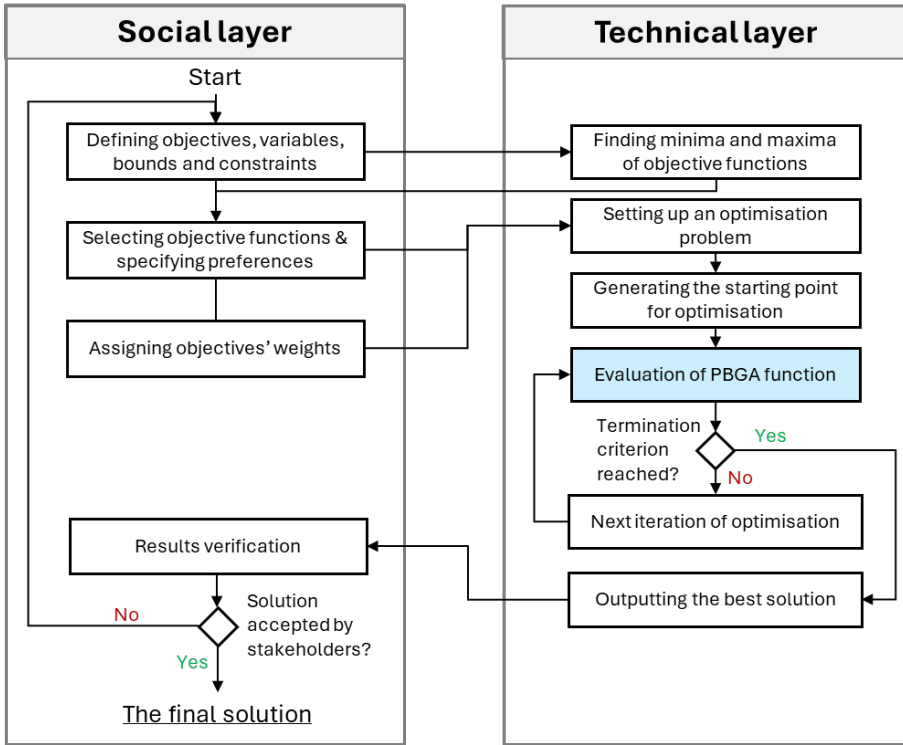


Figure 8.2: Schematic overview of the PBGA method.

The overall PBGA approach is similar to the one presented in the previous chapter. Two main differences are that the technical part has been generalised when it comes to the optimisation algorithm, and proprietary black-box software has been substituted with the PBGA function. Due to the overall similarities, the focus of this section will be only on the definition of PBGA function, while for the other parts, such as preferences modelling, the reader is referred to Chapter 7.

The PBGA method combines PFM theory [225] and goal attainment methodology (also called min-max methodology) [233], and its main goal is to find a compromise solution that minimises the maximum “dissatisfaction” with the result. In mathematical terms, this is defined as follows:

$$\text{minimise } \max_x [w_1 * (100 - P_1(f_1(x))), w_2 * (100 - P_2(f_2(x))), \dots, w_M * (100 - P_M(f_M(x)))] \quad (8.1)$$

where x is the vector of decision-making variables (or set of parameters); $f_i(x)$ are the objective functions that depend on the values of the decision-making variables; $P_i(f_i(x))$ are the preference functions for the corresponding objective functions; w_i are the weights of the objective functions. Since according to the PFM theory, the preference scale is defined from 0 to 100, the goal that each stakeholder is willing to attain is also 100, no matter the

original units of measurement of the objective. Thus, in the formulation above, the difference between 100 and a corresponding preference function is used as a measure of stakeholders' dissatisfaction with the result. In the following text, the maximum weighted distance from the goal is referred to as the PBGA score and the objective of the PBGA method is to minimise it.

In case every stakeholder has just one objective of interest, the weights of the stakeholders and the weights of the objectives are the same. However, in some cases, a stakeholder can have more than one objective. In such situations, this stakeholder is required to provide a weighing for each of their objectives. Independent of the number of objectives a stakeholder has, the weights of all their objectives should add up to one. The final weights of the objectives that are used in the PBGA method are calculated by multiplying the weights of each of the stakeholders by the weights they provided for their objectives. For example, let us consider a decision-making problem with two stakeholders with equal decision-making power (0.5 weight for each). One of the stakeholders has just one objective, and another has two, for which they provide weights of 0.3 and 0.7, respectively. The final weights of the objectives will then be $0.5 * 1 = 0.5$, $0.5 * 0.3 = 0.15$ and $0.5 * 0.7 = 0.35$.

8.2.3 Demonstrator decision-making case

For the demonstration of applying the PBGA method, let us consider the same building as used in Chapters 3-6. For the location of the building, Barcelona has been chosen in this case since, as previous chapters indicated, the climatic conditions there could ensure a better utilisation of phase change materials. For the demonstration, it is assumed that the building configuration is fixed apart from the insulation layer in the walls, and the decision-making case is focused on the selection of the optimal insulation layer configuration (Figure 8.3).

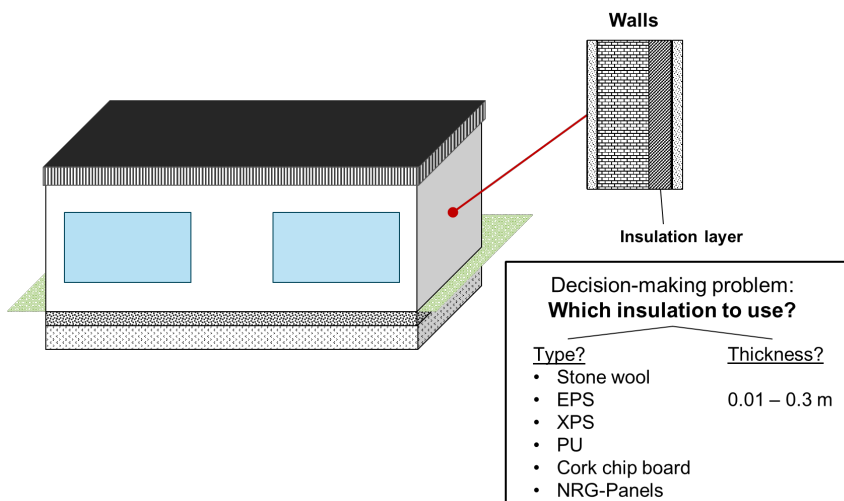


Figure 8.3: Overview of the demonstrator decision-making problem.

For this decision-making problem, it is assumed that there are three stakeholders involved in the decision-making process and each of those stakeholders has a single objective of interest:

- Environmental agency – Minimisation of the lifecycle environmental costs of the building
- Building owner – Minimisation of the construction and demolition costs
- Building user – Minimisation of the energy consumption costs

Those objectives and the approach to their calculation have already been described in detail in Chapter 5. Each of the objectives is influenced by the parameters of the insulation layer. Depending on the material and thickness, the costs of the insulation layer can vary significantly, thus impacting the overall building construction costs. The physical characteristics (thermal conductivity, heat storage capacity and density) as well as the thickness of the insulation layer have a major impact on the energy consumption of the building and, consequently, the energy consumption costs that the building user bears. In the case of the lifecycle environmental costs, the differences in the insulation layer configuration impact the overall result at two different lifecycle stages: the construction stage (embodied emissions) of the insulation material and the use stage (emissions from electricity consumption for heating and cooling).

When it comes to the variable parameters of the building, it is assumed that the selection is made between some of the commonly used insulation materials (Stone wool, EPS, XPS, PU and cork chip board) as well as NRG-Panels. For the conventional insulation materials, 62 different configurations have been considered:

- Stone wool - Rockwool Fixrock Plus in 6 different thicknesses
- EPS - Valero Grafipol TR-29 SE in 18 different thicknesses
- EPS - Valero Grafipol TR-32 SE in 18 different thicknesses
- XPS - Ursa XPS F N-W E in 5 different thicknesses
- PU - Generic (no brand) in 7 different thicknesses
- Cork chip board - Socyr ICB in 8 different thicknesses

For NRG-Panels, a set of 2711 different configurations has been considered. Those generations vary in porosity, MPCM fraction, PCM material, MPCM shell material, and thickness. From those, 471 configurations have been taken from the Pareto frontiers that were obtained in Chapter 6. The remaining 2240 configurations were generated as follows. First, for each material parameter, a set of possible values has been defined:

- Porosity: 0.05, 0.2, 0.4, 0.6, 0.8, 0.95
- MPCM fraction: 0.01, 0.2, 0.4, 0.6
- PCM type: PT18, PT20, PT23, PT25, PT37
- MPCM shell: melamine-formaldehyde shell or inorganic coacervate shell

- Thickness: 0.01 m, 0.02 m, 0.03 m, 0.04 m, 0.05 m, 0.06 m, 0.07 m, 0.08 m, 0.09 m, 0.1 m, 0.15 m, 0.2 m, 0.25 m, 0.3 m

Next, NRG-Panels with every possible combination of those pre-selected values have been defined. Finally, the obtained set of configurations has been filtered to remove NRG-Panels configurations that are not feasible due to the foam stability constraint (refer to Chapter 2 for the information on the stability constraint).

For the calculation of the building construction costs objective, the overall costs were divided into fixed costs, including everything except for the insulation layer and variable costs (insulation). In the case of conventional insulation materials, the prices of different material configurations were obtained from the “Generador de Precios. España” (Price generator. Spain) developed and maintained by CYPE Ingenieros [234]. This resource provides a database of construction material prices for Spain, including various insulation material options. To obtain the total variable costs, the price per square meter obtained from the database has been multiplied by the overall area covered by insulation (68 m²). For NRG-Panels, life cycle cost assessment (LCCA) has been performed as described in Chapter 4. Since LCCA of NRG-Panels only included material costs, it is not directly compatible with market prices of conventional insulation materials. In order to enable the comparison, it has been assumed that material costs account for 60% of the market price of the material (the value has been selected based on the personal communication with industry professionals). Based on this assumption, the estimated market price of NRG-Panels has been obtained by dividing the LCCA results by 0.6.

To estimate the energy consumption of the demonstrator building with different insulation layer options, building energy simulations were performed in EnergyPlus. The overall approach to energy simulations is described in Chapters 4 and 5. The necessary physical parameters of the conventional insulation materials were obtained from the same source as the prices and from the producers' datasheets. In case of missing data (e.g. no exact heat capacity provided), a typical value for this kind of material has been assumed. In most analysed cases, however, the necessary information could be found in the datasheets. For NRG-Panels, the effective parameters of the panels were calculated as described in the methodology section of Chapter 5.

The weather data for energy simulations has been downloaded from the EnergyPlus weather data portal [127]. More specifically, TMY for the Barcelona airport weather station has been used. This weather file has then been modified to account for the effects of climate change using the CCWorldWeatherGen tool [166] and the 2050 climate projection as described in Chapter 6. Compared to Chapters 4-6, a different weather data source has been used. This has been done due to some observed inconsistencies in the weather data obtained from the EU's weather data source [154]. Furthermore, the outcomes of the decision-making problem when using the new weather data source have proven to be more illustrative. And since the main goal of

this chapter is to introduce and demonstrate the newly developed PBGA method, it has been decided that it will be beneficial to select a case that provides a clearer illustration of the method.

The overall electricity consumption costs were calculated based on the yearly electricity consumption estimated using EnergyPlus and the price of electricity in Spain for private sector users obtained from Eurostat (0.26 EUR/kWh) [155]. The costs were corrected for inflation using the 10-year average inflation rate in Spain of 2.1% [156] and assuming a building lifetime of 60 years.

The lifecycle environmental costs objective has been calculated using the same upscaled life cycle assessment (LCA) approach as described in Chapter 4. Embodied emissions of conventional insulation materials were obtained from the ecoinvent database. Environmental costs of electricity use for heating and cooling were calculated by multiplying the yearly electricity consumption obtained from energy simulations, the building lifetime of 60 years and the environmental costs of 1 kWh of electricity Spanish energy mix obtained from the ecoinvent database.

All of the conventional insulation materials' characteristics that were used for calculations in this chapter can be found in Appendix E.

8.3 Results and discussion

As the schematic of the PBGA approach presented in Figure 8.2 shows, for stakeholders to provide their preferences, first, the minimum and maximum values of each selected objective have to be found. In the demonstrator case described above, those were found to be as follows:

- Environmental costs: 2.24×10^4 – 2.94×10^4 EUR
- Energy consumption costs: 6.72×10^4 – 7.84×10^4 EUR
- Construction and demolition costs: 0.68×10^5 – 2.00×10^5 EUR

Using those intervals, the preference curves for the objectives were defined as shown in . The stakeholders and, consequently, their objectives were assumed to have equal weights of 1/3.

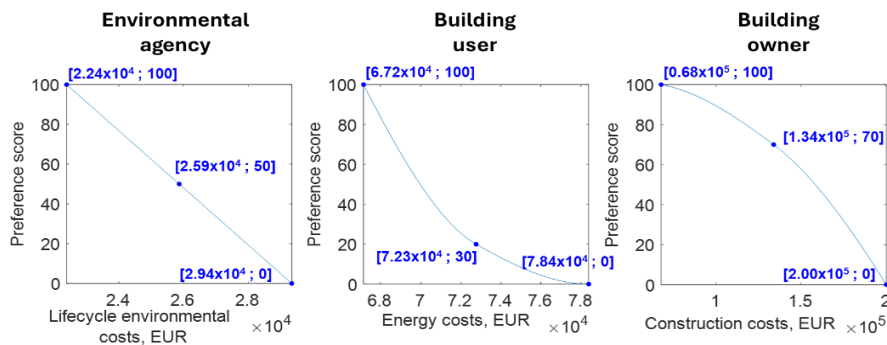


Figure 8.4: Preference curves for the selected decision-making objectives.

Based on the defined preference curves and applying the PBGA method, the insulation solution that provides the best compromise among the stakeholders has been found to be NRG-Panels with the following configuration:

- Porosity of 0.6
- MPCM fraction of 0.4
- MPCM with a melting temperature of 18 °C and melamine-formaldehyde shell
- Panel thickness of 15 cm

This configuration of NRG-Panels had a PBGA score of 7.6, while the closest conventional insulation material was PU panels with a thickness of 4 cm and had a PBGA score of 10.6. Figure 8.5 provides the comparison between those two solutions and the associated preference scores for each of the stakeholders.

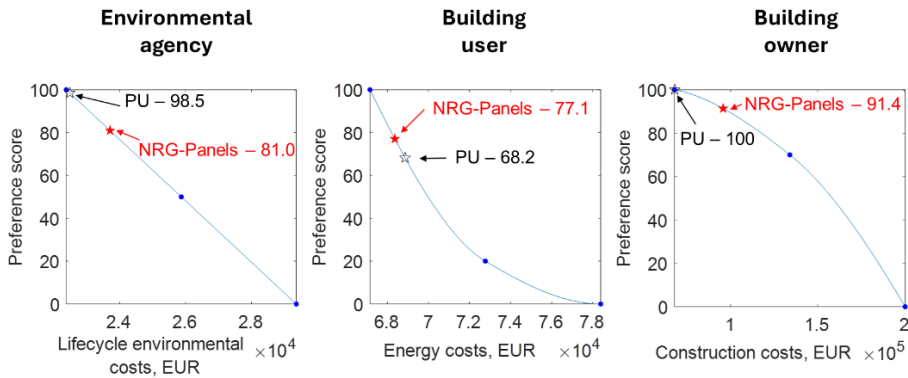


Figure 8.5: The comparison of the preference scores between the final selected solution (NRG-Panels) and the conventional insulation material with the closest PBGA score (PU panels).

Figure 8.5 provides a clear demonstration of the PBGA method's operating principles. The solution with a 4 cm thick PU insulation layer is not balanced: while it satisfies the preferences of the environmental agency and the building owner almost perfectly, the building user finds themselves much further from their goal. Such a discrepancy in the results might potentially result in a conflicting situation, as the building user might refuse to accept such an outcome. On the other hand, in the case of NRG-Panels with the configuration provided above, the resulting preference scores of all stakeholders are significantly more homogeneous. As a result, no stakeholder should feel greatly disadvantaged by the outcome compared to others. This solution is thus more equitable than in the case of PU insulation.

While Figure 8.5 above provides the comparison between the best-scoring options across NRG-Panels configurations and conventional insulation materials, it is also possible to compare them at a more general level. Figure

8.6 shows all analysed configurations of NRG-Panels alongside all analysed conventional insulation materials.

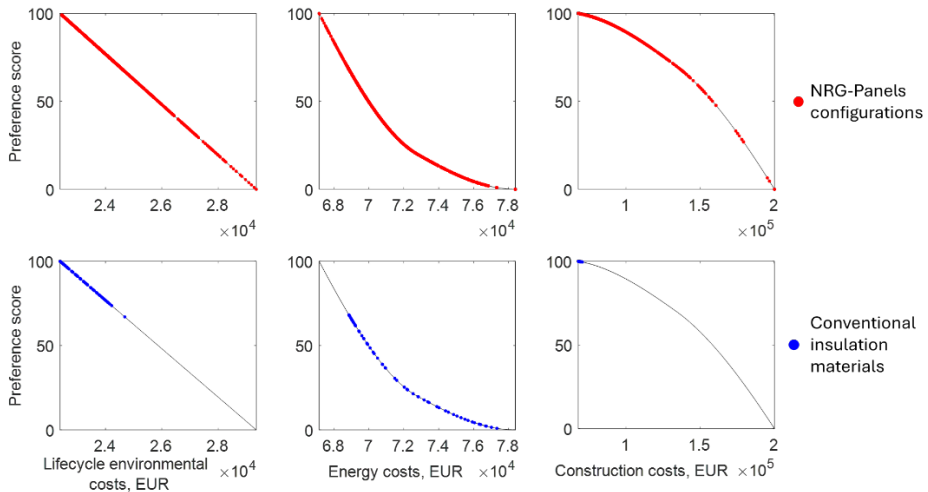


Figure 8.6: Comparison between all the analysed NRG-Panels' configurations and all of the conventional insulation materials.

As can be seen from Figure 8.6, NRG-Panels cover a significantly broader range when it comes to their performance from the perspective of each of the stakeholders. No matter which objective is considered, there is always a possible NRG-Panels configuration that would provide the best possible preference score (however, as pointed out before, there are trade-offs between the analysed objectives and thus the ideal solution is not achievable). Conventional insulation materials assessed in this chapter generally demonstrate good performance from the perspective of the environmental agency and building owner: the preference scores for the corresponding objectives are close to 100 for all materials. In contrast, when it comes to energy costs, conventional insulation materials cannot achieve the same level of performance as NRG-Panels. Due to this, in the demonstrator case analysed, if a conventional insulation material is chosen as the final solution, it will always leave the building user in a disadvantageous position with a significantly lower satisfaction level compared to the other two stakeholders.

The results highlight some important qualities of NRG-Panels and their advantages compared to conventional insulation materials. First of all, due to energy-storing qualities, NRG-Panels could overperform conventional insulation materials in suitable climatic conditions. Secondly, due to the high degree of flexibility and customisability, it is possible to find a configuration of NRG-Panels that would provide a balanced compromise solution that would look attractive to all stakeholders.

8.4 Limitations and future work

This chapter provided an introduction to the PBGA method and demonstrated its application using a simplified decision-making case that did not involve actual stakeholders in the process. The social layer of the PBGA approach and the interaction between the social layer and the technical layer thus require further investigation and refinement. As the next step in the development, the methodology should be applied to a real-world project and involve actual stakeholders. There has already been work done in this direction with the master's thesis by Himanshu Patel that applied the PBGA method to the development project of the Co-Creation Center (CCC) in the Green Village of TU Delft [235]. As part of this study, the stakeholders involved in the CCC project provided their inputs for setting up a decision-making problem as well as reflections regarding the practical use of the PBGA method and the results obtained. However, that work had some limitations as well. First of all, the PBGA method has been implemented post-factum when the project was already completed. Due to this, no real decisions could be made, and the study has only provided a reflection on what other possible solutions were there and how different the final outcome of the project would have been had the PBGA methodology been applied. Consequently, the stakeholders originally involved in the project did not have enough time to contribute and had little stake in the study. Furthermore, from the standpoint of NRG-Panels development, the thesis had a different focus and did not specifically address the questions related to thermal insulation. Nevertheless, this work provided valuable insight and collected important feedback from the stakeholders related to the usage of the PBGA method. In the future, the PBGA method should be applied to real-world projects under development, where it could be used to facilitate actual decisions.

As for NRG-Panels' competitiveness with the existing insulation materials, the results obtained in this as well as in the preceding chapters show that it can be a viable option, and it has its niche. While in colder regions it might not be as attractive, it is best suited for warm climates where heat-storing properties become a valuable advantage over conventional insulation materials. Improved heat storage capacity, however, comes at the cost of increased embodied carbon emissions and manufacturing costs. While NRG-Panels were chosen as a final solution in the demonstrator case presented in this chapter, the results show that the material is mostly attractive for the building user but not as much from the perspective of other stakeholders. If we imagine a situation where the building user is not involved in the decision-making process, either NRG-Panels will not be chosen as the final solution at all or the chosen configuration will include no MPCM - a configuration that is not that different from ordinary aerated concrete. In order to make NRG-Panels more universally competitive, further development is needed to reduce the embodied emissions and costs of the material. And since a major part of the environmental and economic costs of NRG-Panels comes from MPCM particles, improving their production process should be the main priority of future research and development.

8.5 Conclusions

This chapter has presented a newly developed decision-making approach called Preference-Based Goal Attainment and demonstrated its application on an example decision-making problem focusing on the selection of the optimal insulating solution for a demonstrator building. This novel decision-making approach combines preference measurement theory with the goal attainment method and enables finding a compromise solution among stakeholders with contradicting goals. Through its formulation, the PBGA approach allows to curtail possible conflicting situations by focusing on minimising the maximum dissatisfaction with the final outcome across all the stakeholders, thus providing a more equitable solution compared to “collective good” decision-making methods. Furthermore, the approach has been shown to be transparent, straightforward, and easy to implement. Those qualities make it easy to explain the PBGA approach to the stakeholders and to justify the obtained results, improving its trustworthiness, especially compared to the black-box methods such as the one introduced in the previous chapter.

From the standpoint of NRG-Panels development, the application of the PBGA approach showed that, at least in certain cases, NRG-Panels could be a viable alternative to conventional insulation materials. However, since the TRL level of NRG-Panels is still far behind the market materials, the current results have a large degree of uncertainty. Further research and development are necessary, but the results obtained in this thesis show that there is potential for the utilisation of NRG-Panels as a thermal performance improvement solution under suitable climatic conditions.

9

CONCLUSIONS AND RECOMMENDATIONS

9.1 Conclusions

This PhD dissertation contributes to the broad field of thermal material research and revolves around the development of a novel thermal material called NRG-Foam. The dissertation presents an in-depth cross-TRL investigation of NRG-Foam, including modelling, assessment, improvement, and optimisation of the material and its functional, environmental and economic performance. While NRG-Foam is the main focus point of this PhD thesis (alongside NRG-Panels produced from NRG-Foam), it also goes beyond a single material and addresses a wide range of overarching topics related to the modelling and simulation of phase change materials (PCM), material design optimisation, thermal resilience, as well as stakeholder involvement and decision-making in construction projects. From this perspective, the results of this work are expected to be of interest to a diverse group of stakeholders across academia, industry, and legislative bodies. The following sections provide a brief overview of the findings for each thematic section of the dissertation.

9.1.1 Material level

The first part of the dissertation provides an in-depth look into the properties of NRG-Foam and its components. The key outcomes of the material level chapter are summarised below.

- The overall impacts of NRG-Foam production are largely driven by the impacts of microencapsulated phase change material (MPCM) and, more specifically, by the electricity use within MPCM production. Electricity consumption is also the main hotspot within the overall production process of NRG-Foam, and reducing energy intensity must be the main focus when it comes to improvement and upscaling of the NRG-Foam manufacturing process.
- Even a small addition of reduced graphene oxide (rGO) has a major impact on the overall impacts of NRG-Foam production. Similarly to MPCM production, high impacts of rGO production are also caused by the energy intensity of the manufacturing processes.
- MPCM with inorganic coacervate (IC) shell exhibits higher environmental impacts compared to melamine-formaldehyde (MF) MPCM due to higher energy requirements. On the other hand, IC MPCM particles are cheaper to manufacture as the IC shell is composed of widely available and inexpensive raw materials.
- Multiple trade-offs between the performance characteristics of NRG-Foam can be observed. An especially important aspect of those trade-offs is that the improvement of the heat storage capacity of

NRG-Foam would inevitably negatively impact its insulating properties and lead to an increase in environmental impacts and costs. Consequently, practical implementation of NRG-Foam would require a careful and case-specific balancing of its insulating and energy-storing properties. It, however, is not possible to predict how those material-level trade-offs would translate into the building-level performance, and the analysis of NRG-Foam needs to advance to the building level to gain this insight.

- Some configurations of NRG-Foam are infeasible and cannot be produced due to the foam stability limitations. The foam stability is limited by the fraction of MPCM and porosity: the higher the load of MPCM is, the lower the maximum porosity that can be achieved without causing the foam to collapse and vice versa. This constraint significantly reduces the range of available NRG-Foam configurations, making the configurations with the highest possible electrical conductivity and heat capacity unachievable.

9.1.2 Building level

Guided by the results of the material-level assessments and optimisation of NRG-Foam, the analysis moves to the building level. This part of the dissertation begins with exploring the current state-of-the-art in PCM modelling in the context of building energy simulation software and uncovers existing limitations and issues. Following that, it proceeds with upscaled assessments of NRG-Foam, NRG-Panels, as well as building-level assessments and performance comparisons with the conventional materials. Based on the observations that the analysed configuration of NRG-Panels might have been suboptimal for the given case, the dissertation continues with the optimisation of the NRG-Panels configuration in the context of the demonstrator building. Finally, guided by the conclusion that NRG-Panels require different climatic conditions to best utilise their energy-storing properties, the building-level part of the thesis focuses on identifying the geographical areas that have the highest potential for NRG-Panels application. The key outcomes and observations from this part of the dissertation are as follows.

- Currently existing comprehensive PCM models that take the effects of PCM hysteresis into account have multiple limitations and issues. A major consequence of those observations is that it is not possible to know to what extent the result of the simulation is determined by the actual performance of PCM and to what extent they are impacted by the choice of the PCM model and associated limitations. In such a situation, in order to ensure the consistency of the results, a better option might be using a simplified approach to PCM modelling that does not take PCM hysteresis into account. Consequently, such an approach has also been used throughout the rest of the dissertation.

- Implementation of the upscaling scenarios resulted in a major reduction in environmental impacts and costs of MPCM, NRG-Foam and NRG-Panels. The upscaled assessments show a more homogeneous distribution of impacts across different processes, with cement, MPCM slurry and foaming agent being dominant contributors in the upscaling results. Those main contributors could be considered to be new hotspots and should be the focus of further improvements for the production process of NRG-Panels.
- Between the two analysed encapsulation options, NRG-Panels produced using the IC shell have slightly higher environmental costs but significantly lower economic costs. Nevertheless, both panel variations based on IC shell MPCM and on MF shell MPCM were shown to be comparable with the conventional insulation materials when it comes to their environmental and economic costs.
- The comparison of NRG-Panels and EPS in the context of a demonstrator building showed that while their performance was comparable, a building with EPS demonstrated lower environmental and economic costs. Most of the difference came from the use stage, where a building with NRG-Panels consumed more electricity for heating and cooling compared to a building with EPS. This comparison, however, was based on one particular configuration of NRG-Panels representing the panels that were manufactured and installed in physical demonstrator buildings in Sofia. The design of those physically manufactured panels was not optimised for the demonstrator buildings, but to a large degree was a result of technological and time constraints. It can thus be concluded that the configuration of NRG-Panels could be further fine-tuned to ensure the best possible performance for the given demonstrator building and climatic conditions.
- Following the previous findings, the configuration of NRG-Panels has been optimised for the Sofia demonstrator building case using three objectives: environmental costs, costs of electricity for heating and cooling, and construction and demolition costs. All three obtained configurations demonstrated better building-level performance than the as-built configuration and EPS. However, in all the cases, the obtained optimal configuration of NRG-Panels has been characterised by having the maximum possible porosity and, depending on whether the stability constraint is taken into account or not, an insignificant amount of total embedded MPCM or no embedded MPCM at all. Such a material cannot be considered to be a dual-purpose material and instead acts mostly as an insulator with negligible heat storage capacity, technologically very similar to aerated concrete. Consequently, such a material would hardly qualify

as a novel development. This insulation-dominant configuration, however, is to a large extent a result of cold climatic conditions in Sofia with a long heating season. On the other hand, in warmer climates, the situation might be different since heat storage capacity would become a more desirable property. Under such conditions, the optimal configuration of NRG-Panels is expected to shift towards a real dual-purpose material.

- The optimisation of NRG-Panels in the context of different climatic conditions resulted in multiple important outcomes for the future development of the material. First of all, similarly to the material level optimisations in Chapter 2, the building level multi-objective optimisations uncovered a number of trade-offs. No matter the location analysed, at least two of the three analysed objectives were in a trade-off state and, in many cases, all of them were. This emphasises the importance of careful optimisation of NRG-Panels parameters for each particular case, as well as the need for the tools to resolve possible conflicts between stakeholders who are interested in contradicting objectives.

While increasing the fraction of MPCM and, consequently, the heat storage capacity of NRG-Panels has been shown to be beneficial for reducing building energy consumption under some climatic conditions, those benefits were not large enough to offset the increased embedded emissions from MPCM production. Consequently, more research and development is required to reduce the embedded impacts of NRG-Panels and to make them more universally attractive.

The results of climate-dependent optimisation of NRG-Panels have also emphasised that when optimising thermal materials, it is important to take the effects of climate change into account since the configuration that is optimal for the current climate might become suboptimal in the future. To ensure thermal resilience of the built environment, thermal performance solutions for both new buildings and buildings requiring renovation should be selected with future climatic conditions in mind.

Finally, all things considered, the most promising area for NRG-Panels application is the one characterised by the hot-summer Mediterranean (Csa) climate. In multiple locations falling under those climatic conditions, the configuration of NRG-Panels optimised for the minimisation of building energy consumption outperforms EPS. Furthermore, this optimal configuration also incorporates a significant fraction of embedded MPCM, indicating that NRG-Panels

act as a heat-storing material and not only as an insulator, like in colder climatic conditions.

9.1.3 Construction project level

The construction project part of the dissertation is focused on the development of a decision-making and conflict resolution method that integrates the subjective preferences of stakeholders into the decision-making process. The summary of the construction project level developments and outcomes is provided below.

- A new multi-criteria design optimisation and decision-making method has been developed and operationalised. This method is focused on a priori inclusion of stakeholders and their subjective preferences into the decision-making process, thus reflecting the real-world dynamics of construction projects' design rooms. The application of this newly developed method has been demonstrated using an illustrative case based on a real-world construction project.
- Based on the observations from using the method introduced above, it has been concluded that it has some intrinsic limitations: the resulting solution has often been skewed, leading to large preference satisfaction inequality among stakeholders. Furthermore, due to the reliance on the black-box proprietary software, it was not possible to validate the results and to justify them to stakeholders. To address those major limitations, a new decision-making methodology called preference-based goal attainment (PBGA) has been developed. This methodology focuses on finding an equitable compromise solution to decision-making problems while also being transparent and straightforward in its implementation. Such an approach allows for minimising possible conflicting situations in the construction projects involving multiple stakeholders with contradicting interests and objectives.
- The newly developed PBGA methodology has been applied to a decision-making case focused on the selection of the thermal material solution for a demonstrator building involving three stakeholders with conflicting interests. It has been shown that, at least under some circumstances, NRG-Panels could be a good compromise option for improved building thermal performance, providing a balanced solution acceptable for a wide range of stakeholders' interests. Further, the obtained results suggest that the strength of NRG-Panels lies in their flexibility, allowing for fine-tuning of their performance profile for a specific construction project case. Those findings indicate that NRG-Panels have potential as a feasible market product for improving the thermal performance of buildings.

9.2 Recommendations for future research

This dissertation uses a multi-disciplinary approach and covers a broad scope of research and development topics. Inevitably, this also leads to a relatively large number of limitations that could not be addressed within the limited time available. Those limitations form a basis for future research directions that are outlined in Sections 9.2.1 to 9.2.3. In addition to those directions that are focused on NRG-Foam and NRG-Panels, Section 9.2.4 also introduces wide-ranging research and development topics related to PCM in general.

9.2.1 Material level

- **Analyse the influence of different types of PCM and encapsulation methods on the performance of NRG-Foam.**

Within this work, only a limited number of PCM types and encapsulation techniques have been analysed. However, even with those few options, some obstacles for the production of NRG-Foam have been observed. For example, it was not possible to manufacture NRG-Foam that had an organic PCM core and IC shell due to the collapse of the foam. More research and testing is thus needed to assess the compatibility of different types of PCM and encapsulation with NRG-Foam. Furthermore, in addition to testing the compatibility, it is also necessary to analyse the impact of various MPCM particles on the performance of NRG-Foam, including not only functional but also environmental and economic aspects. Among multiple possible options, there might be some MPCM variations that have not been considered yet but that would result in better stability and performance of NRG-Foam and, consequently, of NRG-Panels as well as of a building including those panels. Furthermore, currently, the environmental and economic data on PCM and MPCM production is extremely limited in the academic literature and almost non-existent in the publicly available sources such as databases, producers' datasheets, and environmental product declarations. Conducting environmental and cost assessments of various kinds of PCM and MPCM production (especially based on the primary data) is thus not only necessary for finding the best option for use in NRG-Foam but also beneficial for the research and development of PCM in general.

9.2.2 Building level

- **Conducting detailed regionalised studies of NRG-Panels' performance and applicability**

The work presented in this thesis, and especially environmental and cost assessments, was generally based on the generalised data obtained from various databases. This approach is feasible to obtain a general insight into the performance of the material at the early development stages when no specifics about the target market are known yet. However, when it becomes necessary to assess the applicability potential of NRG-Panels in a particular market, this calls for the use of more detailed and region-specific data. Chapter 6 has indicated a general area where NRG-Panels have better applicability potential that covers multiple countries and regions. A further investigation into the potential of NRG-Panels should focus on making detailed assessments of their performance in the context of those regions. The regionalised assessments should rely on environmental and cost data specific to those regions, obtained from producers, country-specific environmental product declarations, and national databases. Basing such an analysis on generic data could lead to misguided decisions critical for the real-world application of NRG-Panels.

- **Assessing NRG-Panels' performance in the context of different building configurations**

This dissertation has relied on a single specific demonstrator building case for assessing the performance of NRG-Panels. This building configuration was selected due to its simplicity and compact size, making it possible to physically construct four of such buildings within the existing space, budget, and time constraints. The performance of NRG-Panels, however, could be very different in the context of other building cases. Depending on the building size and geometry, envelope configuration, the parameters of the HVAC system, occupants' behaviour, and other building-specific parameters, NRG-Panels might provide larger or lower energy savings. Furthermore, depending on the case, the optimal configuration of NRG-Panels could change as well. It is therefore important to continue this line of research and extend the work with more building cases. As the number of possible building configurations is essentially infinite, future work could focus on the most common building archetypes using, for example, reference building models developed by the U.S. Department of Energy for commercial buildings [236] and building typologies from the TABULA project for residential buildings [237].

- **Improving the recycling of NRG-Foam and recovery of components**

The building-level assessments presented in this dissertation include the end of life (EoL) stage of NRG-Panels as well as the benefits beyond EoL based on the work by Klemczak et al. [147]. As it has been discussed in Chapter 4, however, the resulting substitution rates when recycled waste NRG-Foam is used as cement replacement in mortars were relatively low at 0.2. As a consequence, the benefits beyond EoL were found to be limited. Moreover, while MPCM particles are responsible for a large share of the total production impacts of NRG-Panels, no experiments have been conducted so far aiming at recovering PCM material from the panels after their EoL. Future work related to the recycling of NRG-Panels is necessary, with the main focus on increasing the substitution rates of raw materials by the products of NRG-Panels' recycling, as well as on the possible recovery and reuse of PCM.

- **Assessing the functional durability of NRG-Panels**

An important aspect of NRG-Panels that was not addressed in this dissertation is the functional durability and longevity of the panels. As with any other material, NRG-Panels will physically degrade over time, causing their functional properties to deteriorate. Since NRG-Panels are a complex and dynamic dual-purpose material, this change in properties becomes even more complex and unpredictable compared to conventional materials. At some point, the functional performance will become unacceptable, and the panels will need to be replaced. The rate of functional degradation is thus the key factor in estimating the expected lifetime of NRG-Panels and, consequently, their overall lifecycle environmental impacts and costs as well as their competitiveness compared to other thermal performance materials. While long-term durability studies were not originally a part of the NRG-STORAGE project, taking into account their importance for the future development of NRG-Panels, the author of this dissertation has initiated additional accelerated ageing experiments. The experiments were performed by the project partner Silesian University of Technology using a climate ageing chamber. Within the experiment, a number of test panels in different configurations were subjected to 700 heating-cooling cycles. The temperatures and timing were set up in a way that ensures complete melting and solidification of the embedded PCM. Afterwards, the panels that underwent the cycling and the reference panels that were not subjected to ageing were compared. The thermal and mechanical properties of the sample panels were analysed, and their macro- and microstructures were imaged. The tests were divided between multiple project partners, including TU Delft, where the author of this work obtained SEM images and CT scans of non-aged and aged samples. While many results have already been produced, no particular conclusions have been reached yet. Future work should focus on finalising the necessary tests, processing the experimental data, and extracting practical ramifications for NRG-Panels' durability and lifetime.

While not included in this dissertation, the results are expected to be published in the future in a journal paper preliminary titled “A resistance of MPCM-enriched cementitious foam to accelerated ageing”.

- **Expanding the assessment and optimisation of NRG-Panels for a more exhaustive mapping of their performance**

This work has mainly focused on three main performance aspects of NRG-Panels: thermal, environmental and economic. While those characteristics are arguably the most important ones for analysing the building-level performance of NRG-Panels, there are numerous additional performance aspects that should also be taken into account. Those include mechanical performance, fire resistance performance, acoustic performance, water absorption and vapour penetrability performance. All those characteristics depend on the configuration of NRG-Panels and, as a consequence, are interconnected. It is thus important not only to assess all sides of NRG-Panels' performance separately but also to combine them within a single multi-objective optimisation. This optimisation-based approach would allow to identify trade-offs as well as to optimise NRG-Panels' performance in a more holistic manner.

- **Dynamic modelling, assessment and optimisation of NRG-Panels using high-resolution hourly data**

Evaluations of the environmental and economic impacts of electricity consumption for heating and cooling were performed in this dissertation using averaged long-term data. For the environmental impacts, the estimations were based on the environmental data for the long-time average electricity mix for the specific energy market and for the costs, based on the average yearly price of electricity obtained from the Eurostat database. In reality, however, the environmental impacts and costs of 1 kWh of electricity are not fixed, and the overall operational impacts over the period of time depend not only on the total amount of electricity consumed, but also on the hourly structure of this consumption. In case of environmental impacts, the energy generation mix is changing from hour to hour, depending on the structure of the demand and supply. In addition to this, there are also some seasonal variations, weather-induced variations, network constraints, and other factors, all of which could influence the environmental impacts of electricity generation during the given hour. As for the costs of electricity, they could also vary hourly if the building user has a dynamic pricing contract. In this case, the price of the energy for users is generally connected to the market price of electricity, which, in turn, is influenced by many of the same factors as the hourly environmental impacts. For a building containing PCM, the analysis of the electricity use impacts with high temporal resolution becomes especially important due to the dynamic nature of PCM that could cause major shifts in the electricity demand profile. The environmental and

economic impacts of those shifts can only be estimated when high-resolution hourly or even sub-hourly data is used. Consequently, for a PCM-embedded material like NRG-Panels, it is of great importance to take those effects into account since they could potentially result in additional benefits compared to the conventional thermal materials. Furthermore, from the standpoint of a material designer, if the hourly dynamic is taken into account, the optimal configuration of NRG-Panels that results in the minimal environmental and/or economic impacts could be significantly different compared to when evaluations are made using long-term average data.

In addition to static environmental and cost assessments, when an hourly consumption profile is considered, it becomes possible to utilise the techniques for the active control of building energy consumption. For example, the structure of energy generation (which can be used to estimate the environmental impacts) and hourly prices of electricity are generally known a day in advance. Using the forecasted weather data, the hourly electricity costs and environmental impacts, occupancy and other factors, it is possible to optimise the hourly electricity consumption for HVAC while taking the full advantage of the dynamic properties of PCM. In the case of NRG-Panels, such an active control could result in better utilisation of PCM heat capacity and reduce the overall environmental impacts and costs of building operation.

9.2.3 Construction project level

- **Developing the PBGA approach into a practical decision-making tool and its application for real-world decision-making support**

Chapter 8 of this dissertation has introduced a new equity-focused decision-making approach called preference-based goal attainment (PBGA). While the approach has been operationalised and its application has been demonstrated on an illustrative decision-making case, it is currently far from being a practical tool ready for real-world application. The key part of turning the PBGA approach into a decision-making tool would be the development of a user interface. This interface should include functionality for stakeholders' preferences elicitation as well as for the review and evaluation of the results. Furthermore, the tool should reflect the iterative nature of the decision-making process and allow stakeholders to quickly modify the inputs and move to the next iteration. Finally, the tool could also provide decision-makers with some additional information that might be helpful for making an informed decision, such as sensitivity analysis of the results to the changes in stakeholders' inputs. All of the described tool developments and improvements will require cooperating with actual stakeholders in order to test the functionality as well as to collect and implement feedback, ideally in the context of an ongoing real-world decision-making case.

- **Explore alternative business models for NRG-Panels**

As it has been shown throughout this dissertation, NRG-Panels is a complex material with a large number of design variables. Consequently, the number of possible unique material configurations is extremely large, with each configuration characterised by a specific performance profile. If NRG-Panels are to be manufactured as a conventional prefabricated material with a limited set of available configurations, it will not be possible to provide an optimal material for each particular building case. However, as this dissertation highlighted, the strength of NRG-Panels is in the flexibility of their properties that could be fine-tuned for a particular case. From this perspective, instead of turning NRG-Panels into a fixed-configuration material, it might be beneficial to explore the possibility of using alternative business models. A possible alternative option could be a thermal-performance-as-a-service business model. In this case, the service provider is not just a material manufacturer but is responsible for ensuring the best possible thermal performance of a building. Provided with a specific construction project case, the service provider optimises the configuration of the material, manufactures the panels in the optimal configuration, installs them, monitors them and could also be responsible for their maintenance and end-of-life treatment. Such a business model, while not easy to operationalise, could result in significantly better building performance compared to conventional materials.

9.2.4 Research and development directions beyond NRG-Foam and NRG-Panels

- **Developing a smart self-sensing thermal performance material on the basis of NRG-Foam**

As it was touched upon in Chapter 2 of this dissertation, within the original scope of the NRG-STORAGE project, two ways of NRG-Foam use were considered: passive and active. For the active application, an electrically conductive filler (reduced graphene oxide) has been added to the cementitious matrix, thus allowing for melting PCM on demand by resistive heating. While some experiments were conducted to investigate the feasibility of such an active approach, it has been proven to be challenging to implement in reality. First of all, to make the material conductive enough for melting PCM by applying voltage to NRG-Foam, very large amounts of conductive filler were required. The increased fraction of the conductive filler results in a significant increase in costs and environmental impacts of NRG-Foam and also influences its properties and manufacturability. Furthermore, the energy and time required for resistive melting made the usefulness of the approach questionable. However, in addition to the possibility of resistive heating, making a material electrically conductive

creates a new opportunity: self-sensing. Self-sensing techniques are commonly applied for monitoring the mechanical condition of structural materials but to the author's knowledge, self-sensing has never been applied to a thermal performance material. In this context, by attaching sensors to the material and monitoring its electrical resistivity, it could be possible to track its long-term performance (thermal and mechanical) as well as the current state (e.g., the phase of PCM). The monitoring of real-time material state could potentially be used as one of the inputs in active predictive control of a building's HVAC system for reduced costs and environmental impacts. The long-term monitoring of changes in properties, in turn, could make it possible to detect performance issues and signal when an intervention is needed. For example, it could be possible to detect when the insulating or energy-storing properties have deteriorated and building maintenance is required. This possibility is also well-aligned with the thermal-performance-as-a-service business model described in the previous subchapter.

- **Conduct an in-depth investigation into the weather data inconsistencies and their impact on the assessments of building energy performance.**

Weather data is an essential input for building energy simulations alongside the building configuration data. Consequently, the selection of the weather data and its quality could have a major impact on the results of building energy simulation and, hence, on the decisions informed by those simulation results. Throughout this dissertation, a number of different weather data sources have been used, and the comparison between them suggested that there might be some issues when it comes to the reliability of the data. Those issues include gaps in the data or data that contradict physical laws (for example, when local horizontal solar irradiation exceeds the extraterrestrial solar irradiation during some hours). Furthermore, different data sources often showed unusually large differences between the same weather parameters for the same location, especially solar irradiation. This could potentially be caused by the differences in the approaches for the processing of meteorological observation data and the subsequent transformation of the multi-year data into a singular typical meteorological year (TMY) data file. The observed inconsistencies raise questions about the overall reliability of the available weather data, the existing procedures of data quality checks, the certainty of the building energy simulation results, and, consequently, the correctness of the decisions that were made based on building energy simulations. In the case of PCM and materials containing PCM, those issues might have an even greater impact since, due to the intrinsically dynamic and nonlinear nature of such materials, their modelling is very sensitive to short-term variations in weather conditions and, consequently, to the quality of the weather data. It is thus essential for future research to explore the abovementioned weather data issues in detail to ensure the reliability of

building energy simulations and to facilitate the practical application of PCM materials in the construction sector.

- **Advancing the modelling of PCM in the context of building energy simulations**

As Chapter 3 of this dissertation showed, modelling of PCM in full-building energy simulations has a long way to go. The simplified models are straightforward and stable, but are incapable of reflecting the real-world behaviour of PCM. On the other hand, currently existing comprehensive PCM models all have some inherent limitations and issues impacting the reliability of the simulation results. The development of PCM into a practical construction material, therefore, to a large extent relies on the further advancement of PCM modelling. The issues in the existing models should be addressed and the models should be validated against the real-world experiments, preferably on a building scale and not in a laboratory using a small sample. Furthermore, either the existing PCM models in building simulation software should be updated to include the aspects of PCM behaviour that are currently not accounted for (such as supercooling) or new models should be developed as a replacement.

Another aspect of PCM modelling that needs further development is the changes in PCM properties from pure PCM to encapsulated PCM and then from encapsulated PCM to being embedded into the final construction material. When pure PCM is encapsulated, depending on the encapsulation process used, the final melting and solidification temperatures of MPCM particles could be significantly different from those of the original PCM. The same applies to the situation when MPCM particles are embedded within another material: melting temperature, hysteresis degree, and other properties could change again. The final building performance is then dependent on the adjusted effective PCM properties and not on the properties of raw PCM listed in the producers' datasheets. Not accounting for those effects could lead to misleading conclusions and suboptimal decisions regarding the choice of the optimal PCM for a specific building case. It is therefore necessary to develop methodologies for the translation of PCM properties from raw material to the building-level and add this functionality to building energy simulation software.

- **Developing energy-storing material with dynamically-adjustable properties**

The properties of PCM, such as melting and solidification temperatures, depend on a variety of factors such as the presence of impurities, physical conditions, external fields, the thermal history, and the rates of heating and cooling. Usually, those factors are looked at as being uncontrollable variables that cannot be regulated. However, it is also possible to turn the situation

around and instead focus on the active control of the factors that impact the final properties of PCM for improved building performance. For example, let us consider a building that has a PCM layer in its envelope. If it were possible to adjust the melting and solidification temperature (and possibly other properties) dynamically by, for example, changing the pressure, applying external fields, or adding chemical admixtures. PCM performance could be fine-tuned to better account for the ever-changing conditions. Depending on how long the intervention takes, the properties could be varied hourly to adjust for the weather and energy market conditions, weekly to reflect the building occupation patterns, monthly to account for seasonal effects, or yearly to take the long-term market and climate changes. The effects of different interventions on PCM properties, however, are currently not well-studied, and the practical feasibility of such a dynamic PCM material requires further extensive investigation.

APPENDIX A

CHAPTER 2: EARLY-STAGE ANALYSIS AND OPTIMISATION OF A NOVEL THERMAL PERFORMANCE MATERIAL BASED ON MPCM-DOPED CEMENTITIOUS FOAM

A



A1. Costs used for LCCA calculations

Table A1 below shows the costs that were used for calculations of LCCA impacts.

Table A1. Product costs.

IC shell MPCM production		
Product	Price	Unit
Distilled water	0.4	EUR/l
Polymer 1	10	EUR/kg
Polymer 2	20	EUR/kg
Emulsifier	43.8	EUR/l
PCM	14.2	EUR/kg
Crosslinker	84	EUR/kg
Plasticiser	3	EUR/kg
Polymer 4	2.89	EUR/kg
Polymer 5	5.25	EUR/kg
Polymer 3	20	EUR/kg
Electricity	0.25	EUR/kWh
MF shell MPCM production		
Product	Price	Unit
Distilled water	0.4	EUR/l
PCM	14.2	EUR/kg
PVOH	370	EUR/kg
MF resin	200	EUR/l
Ammonium chloride	70.6	EUR/kg
Electricity	0.25	EUR/kWh

Table A1. Product costs (continued).

rGO production		
Product	Price	Unit
Graphite	19.49	EUR/kg
Chemical 3	0.44	EUR/kg
Chemical 2	11.46	EUR/kg
Deionised water	0.2	EUR/l
Chemical 1	9.97	EUR/l
Electricity	0.31	EUR/kWh
Acidic waste disposal	220	EUR/l
Foam production		
Product	Price	Unit
Cement	0.1	EUR/kg
Metakaolin	0.4	EUR/kg
Accelerator	2.25	EUR/kg
Stabiliser	2.25	EUR/kg
Superplasticiser	2.25	EUR/kg
Foaming agent	18.45	EUR/kg
Electricity	0.3	EUR/kWh

A2. Details of the modelling approach used in the dynamic part of the study

A2.1. Parameters used for finding a Pareto frontier using gamultiobj Matlab function

Table A2. Parameters of gamultiobj algorithm.

Parameter	Value
Population size	50
Crossover fraction	0.8
Number of elite members	2
Maximum number of iterations	400
Function tolerance	1E-4

Each objective function has also been optimised separately and the results of those optimisation runs have been passed to gamultiobj function as the initial population.

A2.2. Physical parameters of the components used for the calculations and modelling in this study

Table A3. Densities of the components.

Component	Name used in the model	Density, kg/m ³
Cement	d_{cem}	3100
Metakaolin	d_{met}	1450
Accelerator	d_{acc}	1300
Superplasticiser	d_{sup}	1060
Stabiliser	d_{sta}	1300
MPCMs	d_{mpcm}	780
Water	d_{wat}	1000
rGO	d_{rgo}	1900
Foam (water + foaming agent + air)	d_f	70

Table A4. Thermal conductivities of components.

Component	Thermal conductivity, $W \cdot m^{-1} \cdot K^{-1}$
Air	0.025
Cement paste	0.5
MF MPCMs	0.11
IC MPCMs	0.23

Table A5. Volumetric heat capacities of components.

Component	Volumetric heat capacity, $J \cdot K^{-1} \cdot m^{-3}$
Air	1225
Cement paste	1284000

Table A6. Electrical conductivities of components.

Component	Thermal conductivity, $S \cdot m^{-1}$
Air	1.2E-12
Cement paste	2.61E-09
MF MPCMs	1E-3
IC MPCMs	1E-4
rGO	1E-02

A2.3. Details of the modelling of environmental and cost objectives

As it was mentioned in the methodology section, the production system in the dynamic part of this study has been slightly modified and rGO has been added into the paste mix as a dry powder rather than slurry. Thus, an additional process has been added to the system for converting rGO slurry to powder. Table below provides inputs and outputs of this process:

Table A7. Inputs and outputs of the rGO drying process.

Input	Amount
rGO slurry	1 l
Electricity	1.4 kWh
Output	Amount
Dry rGO	10 g
Water vapour	1 kg

It has been assumed that the mass fractions of the components in the base cement paste (only paste without MPCMs, rGO or foam) are remaining the same for all possible configurations of the foam. Those fractions are presented in Table A8 below.

Table A8. Mass fractions of components in cementitious paste.

Component	Name used in the model	Mass fraction
Cement	f_{cem}	0.620
Metakaolin	f_{met}	0.102
Accelerator	f_{acc}	0.014
Superplasticiser	f_{sup}	0.004
Stabiliser	f_{sta}	0.021
Water (for water-to-binder ratio)	f_{wat}	0.238

The model in OpenLCA has been parametrised to take all the amounts of components as inputs. In total, 11 parameters have been created:

- Total mass of accelerator - m_1
- Total mass of foaming agent - m_2
- Total mass of cement - m_3
- Total mass of MC MPCMs - m_4
- Total mass of IC MPCMs - m_5
- Total mass of metakaolin - m_6
- Total mass of rGO - m_7
- Total mass of stabiliser - m_8
- Total mass of superplasticiser - m_9
- Total mass of water (including water for w/b ratio and water for foam preparation) - m_{10}
- Total mass of waste water (assuming all water for w/b ratio is remaining in the foam while all water used for foam preparation is ending up in waste) - m_{11}

Those input parameters depend on the optimisation variables that are denoted as:

- x_1 – Volumetric MPCMs fraction
- x_2 – Porosity of the foam
- x_3 – mass fraction of rGO
- x_4 – type of MPCMs (0 – IC, 1 – MF)

The procedure of obtaining the values of parameters $m_1 - m_{11}$ is as follows. Taking the target volume of NRG-Foam of 1 m^3 , the total volume of the foam

can be found as $v_f = 1 * x_2$. Mass of the foam is equal to $m_f = v_f * d_f$, where d_f is the density of the foam. From here, $m_2 = m_f * 0.02$ since 2% of foaming agent is required to produce the foam. Consequently, $m_{11} = m_f - m_2$.

The volume of MPCMs can be found as $v_{mpcm} = x_1 * (1 - x_2) * 1$ and the mass is, consequently, $m_{mpcm} = v_{mpcm} * d_{mpcm}$ where d_{mpcm} is the density of MPCMs. Depending on the value of x_4 , m_{mpcm} is being assigned to either m_4 or m_5 : if $x_4 = 0$ then $m_4 = m_{mpcm}$ and $m_5 = 0$; if $x_4 = 1$ then $m_5 = m_{mpcm}$ and $m_4 = 0$.

Remaining volume is cementitious paste with rGO and is equal to $v_{prgo} = 1 - v_f - v_{mpcm}$. The density of the cementitious paste without rGO can be calculated as:

$$d_p = 1 / \left(\frac{f_{cem}}{d_{cem}} + \frac{f_{met}}{d_{met}} + \frac{f_{acc}}{d_{acc}} + \frac{f_{sup}}{d_{sup}} + \frac{f_{sta}}{d_{sta}} + \frac{f_{wat}}{d_{wat}} \right) \quad (A1)$$

From there, the mass of paste with rGO can be found as:

$$m_p = \frac{v_{prgo}}{\frac{1}{d_p} + \frac{x_3}{d_{rgo} * (1 - x_3)}} \quad (A2)$$

Consequently, the total mass of rGO can be found as:

$$m_7 = m_p * \frac{x_3}{1 - x_3} \quad (A3)$$

The weights of individual components of paste depend on their fractions and the total weight of the paste: $m_1 = f_{acc} * m_p$, $m_3 = f_{cem} * m_p$, $m_6 = f_{met} * m_p$, $m_8 = f_{sta} * m_p$, $m_9 = f_{sup} * m_p$

And finally, the total mass of water is equal to $m_{10} = m_{11} + f_{wat} * m_p$.

A2.4. Experimental measurements of electrical conductivity and the fitting using generalised percolation model

Sample Preparation:

Four distinct samples with varying amounts of reduced graphene oxide (rGO) (0 wt%, 1 wt%, 1.5 wt%, and 2 wt%) were prepared. The preparation process involved mixing ordinary Portland cement (OPC) with rGO for 1 minute at 300 rpm. Subsequently, a mixture of water and superplasticiser (Powerflow 3195;

2 wt %) was added and further mixed for 1.5 minutes at 750 rpm. The water-to-cement ratio was fixed at $w/c=0.4$. Finally, the resulting paste was poured into molds to obtain discs with a height (h) of 0.5 cm and a diameter (d) of 1.5 cm. The molds were then sealed and left at room temperature for 24 hours. Afterward, the specimens were demolded and immersed in water for a curing period of 7 days. Table A9 shows experimental as well as modelled values of electrical conductivity of cementitious paste at different fractions of rGO added.

Experimental Method:

The electrical conductivity of the specimens were measured using a broadband dielectric spectrometer (Novocontrol Alpha-A+) operating in the frequency range of 10^1 - 10^6 Hz. For the measurements, disk-shaped samples with a thickness of 2 mm were placed between parallel gold-plated electrodes with a diameter of 10 mm. To prevent any moisture absorption from the surrounding atmosphere, the samples were maintained under a constant nitrogen flux throughout the measurements. Moreover, prior to data acquisition, the samples were kept inside the instrument at a temperature of 315 K for a duration of 10 minutes. Subsequently, isothermal frequency scans were performed, with the temperature increments of 5 K within the range of 285-315 K. The sample temperature was controlled ensuring a stability better than ± 0.1 K.

Table A9. Experimental and modelled electrical conductivity of cementitious foam depending on the fraction of rGO added.

rGO load by weight, %	Measured electrical conductivity, S/cm	Modelled electrical conductivity, S/cm
0	2.61E-09	2.61E-09
1	8.48E-08	9.18E-08
1.5	1.56E-06	1.42E-06
2	4.19E-06	4.39E-06
3		1.51E-05
4		3.25E-05
5		5.63E-05

The modelled data has been obtained by fitting the experimental data using the generalised percolation framework [87]. Within this framework, the effective conductivity of the composite Y_{eff} material can be found using Threshold-Adjusted Generalized Percolation (TAGP) equation:

$$(2\phi_c - \phi) \frac{Y_m^{\frac{1}{s}} - Y_{eff}^{\frac{1}{s}}}{Y_m^{\frac{1}{s}} + Y_{eff}^{\frac{1}{s}}} + \phi \frac{Y_{f^*}^{\frac{1}{t}} - Y_{eff}^{\frac{1}{t}}}{Y_{f^*}^{\frac{1}{t}} + Y_{eff}^{\frac{1}{t}}} = 0 \quad (A4)$$

where ϕ_c is the percolation threshold, ϕ is the fraction of the filler, Y_m is the conductivity of the matrix, $Y_{f^*} = Y_{eff}(2\phi_c)$ is the conductivity in super-critical

region, s is pre-percolation exponent and t is the post-percolation exponent. The values of s and t have been set according to the recommendations provided in [87] ($s = 0.73, t = 2$). The conductivity of the matrix is known ($2.61\text{e-}9$). In order to fit the experimental data, we have set s, t and Y_m and found the values of Y_{f^*} and ϕ_c resulting in the lowest squared cumulative difference between the fitted data and Y_{eff} obtained from Eq. A4. The resulting values of $Y_{f^*} = 2.32 * 10^{-6}$ and $\phi_c = 0.7\%$ were found to be in good agreement with similar cases shown in [87].

A2.5. Foam stability constraint

Table A10 presents the data on the stability of foam at different fractions of MPCMs in cementitious foam.

Table A10. Maximum achievable porosities at different fractions of MPCMs in paste.

Volumetric fraction of MPCMs in paste	Maximum achievable porosity
0.05	0.92
0.1	0.88
0.2	0.86
0.3	0.8
0.4	0.6

A3. Inventories for five different NRG-Foam configurations

Tables A11-A15 below present the inventories for five NRG-Foam configurations analysed in this study. As it was mentioned in the Methodology section, some of the data related to the production of MPCMs and rGO cannot be disclosed since those production processes are commercial know-how of the corresponding project partners. Due to that, some fields in the tables below are empty. Further, some of the rows in the tables are highlighted in orange. Those are the processes that were cut off due to the lack of data.

Table A11. Inventory for the REF configuration of NRG-Foam.

Inputs			
Product	Process	Amount	Unit
Cement, Portland	market for cement, Portland cement, Portland Cutoff, S - Europe without Switzerland	139.29	kg
Tap water	market for tap water tap water Cutoff, S - Europe without Switzerland	113.80	kg
Electricity, low voltage	market for electricity, low voltage electricity, low voltage Cutoff, S - DE	67.92	MJ
Metakaolin	Metakaolin production	22.93	kg
Stabiliser	Stabiliser dummy	4.69	kg
Calcium nitrate	market for calcium nitrate calcium nitrate Cutoff, S - RER	3.25	kg
Foaming agent	market for foaming agent foaming agent Cutoff, S - GLO	1.23	kg
Polycarboxylates, 40% active substance	market for polycarboxylates, 40% active substance polycarboxylates, 40% active substance Cutoff, S - RER	0.81	kg
Outputs			
Product	Process	Amount	Unit
NRG-Foam	Reference	1	m3
Wastewater, average	market for wastewater, average wastewater, average Cutoff, S - Europe without Switzerland	0.06	m3

Table A12. Inventory for the ICP configuration of NRG-Foam.

Inputs			
Product	Process	Amount	Unit
Electricity, low voltage	market for electricity, low voltage electricity, low voltage Cutoff, S - IT	11945.5	MJ
Water, deionised	market for water, deionised water, deionised Cutoff, S - Europe without Switzerland	407.273	kg
Cement, Portland	market for cement, Portland cement, Portland Cutoff, S - Europe without Switzerland	123.959	kg
Tap water	market for tap water tap water Cutoff, S - Europe without Switzerland	107.906	kg
Electricity, low voltage	market for electricity, low voltage electricity, low voltage Cutoff, S - DE	67.922	MJ
Metakaolin	Metakaolin production	20.412	kg
Fatty acid	market for fatty acid fatty acid Cutoff, S - GLO	18.474	kg
Transport, freight, lorry, unspecified	market for transport, freight, lorry, unspecified transport, freight, lorry, unspecified Cutoff, S - RER	17.943	t*km
Polymer 3 - MPCM production		12.342	kg
Stabiliser	Stabiliser dummy	4.184	kg
Polymer 1 - MPCM production		3.702	kg
Calcium nitrate	market for calcium nitrate calcium nitrate Cutoff, S - RER	2.882	kg
Plastifier - MPCM production		1.727	kg
Polycarboxylates, 40% active substance	market for polycarboxylates, 40% active substance polycarboxylates, 40% active substance Cutoff, S - RER	1.498	kg
Polymer 4 - MPCM production		1.481	kg
Soda ash, dense	market for soda ash, dense soda ash, dense Cutoff, S - GLO	1.481	kg
Polymer 2 - MPCM production		1.234	kg
Foaming agent	market for foaming agent foaming agent Cutoff, S - GLO	1.230	kg
Crosslinker - MPCM production		0.593	kg

Table A12. Inventory for the ICP configuration of NRG-Foam (continued).

Emulsifier - MPCM production		0.036	kg
Outputs			
Product	Process	Amount	Unit
NRG-Foam	Reference	1	m3
Wastewater, average	market for wastewater, average wastewater, average Cutoff, S - Europe without Switzerland	0.060	m3
Hazardous waste, for incineration	treatment of hazardous waste, hazardous waste incineration, with energy recovery hazardous waste, for incineration Cutoff, S - Europe without Switzerland	15.949	kg

Table A13. Inventory for the ICA configuration of NRG-Foam.

Inputs			
Product	Process	Amount	Unit
Electricity, low voltage	market for electricity, low voltage electricity, low voltage Cutoff, S - IT	11612.6	MJ
Electricity, low voltage	market for electricity, low voltage electricity, low voltage Cutoff, S - ES	1333.889	MJ
Water, deionised	market for water, deionised water, deionised Cutoff, S - Europe without Switzerland	634.730	kg
Cement, Portland	market for cement, Portland cement, Portland Cutoff, S - Europe without Switzerland	120.504	kg
Transport, freight, lorry, unspecified	market for transport, freight, lorry, unspecified transport, freight, lorry, unspecified Cutoff, S - RER	82.844	t*km
Lime, hydrated, loose weight	market for lime, hydrated, loose weight lime, hydrated, loose weight Cutoff, S - RoW	72.689	kg
Chemical 3 - rGO production			
Electricity, low voltage	market for electricity, low voltage electricity, low voltage Cutoff, S - DE	67.922	MJ
Tap water	market for tap water tap water Cutoff, S - Europe without Switzerland	60.275	kg
Metakaolin	Metakaolin production	19.843	kg
Fatty acid	market for fatty acid fatty acid Cutoff, S - GLO	17.959	kg
Polymer 3 - MPCM production		11.998	kg

Table A13. Inventory for the ICA configuration of NRG-Foam (continued).

Stabiliser	Stabiliser dummy	4.067	kg
Polymer 1 - MPCM production		3.599	kg
Polycarboxylates, 40% active substance	market for polycarboxylates, 40% active substance polycarboxylates, 40% active substance Cutoff, S - RER	2.812	kg
Calcium nitrate	market for calcium nitrate calcium nitrate Cutoff, S - RER	2.802	kg
Plastifier - MPCM production		1.679	kg
Chemical 2 - rGO production			
Polymer 4 - MPCM production		1.439	kg
Soda ash, dense	market for soda ash, dense soda ash, dense Cutoff, S - GLO	1.439	kg
Foaming agent	market for foaming agent foaming agent Cutoff, S - GLO	1.206	kg
Polymer 2 - MPCM production		1.200	kg
Chemical 1 - rGO production			
Crosslinker - MPCM production		0.577	kg
Graphite	market for graphite graphite Cutoff, S - GLO	0.523	kg
Emulsifier - MPCM production		0.035	kg
Outputs			
Product	Process	Amount	Unit
NRG-Foam	Reference	1	m3
Wastewater, average	market for wastewater, average wastewater, average Cutoff, S - Europe without Switzerland	0.283	m3
Hazardous waste, for incineration	market for hazardous waste, for incineration hazardous waste, for incineration Cutoff, S - Europe without Switzerland	15.50484	kg

Table A14. Inventory for the MFP configuration of NRG-Foam.

Inputs			
Product	Process	Amount	Unit
Electricity, low voltage	market for electricity, low voltage electricity, low voltage Cutoff, S - IT	3952.528	MJ
Water, deionised	market for water, deionised water, deionised Cutoff, S - Europe without Switzerland	582.566	kg
Cement, Portland	market for cement, Portland cement, Portland Cutoff, S - Europe without Switzerland	123.959	kg
Tap water	market for tap water tap water Cutoff, S - Europe without Switzerland	107.906	kg
Electricity, low voltage	market for electricity, low voltage electricity, low voltage Cutoff, S - DE	67.922	MJ
Fatty acid	market for fatty acid fatty acid Cutoff, S - GLO	21.375	kg
Metakaolin	Metakaolin production	20.412	kg
Transport, freight, lorry, unspecified	market for transport, freight, lorry, unspecified transport, freight, lorry, unspecified Cutoff, S - RER	17.943	t*km
Melamine formaldehyde resin	market for melamine formaldehyde resin melamine formaldehyde resin Cutoff, S - RER	6.029	kg
Isobutanol	market for isobutanol isobutanol Cutoff, S - RER	4.366	kg
Stabiliser	Stabiliser dummy	4.184	kg
Calcium nitrate	market for calcium nitrate calcium nitrate Cutoff, S - RER	2.882	kg
Polycarboxylates, 40% active substance	market for polycarboxylates, 40% active substance polycarboxylates, 40% active substance Cutoff, S - RER	1.498	kg
Foaming agent	market for foaming agent foaming agent Cutoff, S - GLO	1.230	kg
Polyvinylalcohol, at plant/kg/RER U	polyvinylalcohol, at plant - RER	0.802	kg
Ammonium chloride	market for ammonium chloride ammonium chloride Cutoff, S - GLO	0.107	kg
Outputs			
Product	Process	Amount	Unit
NRG-Foam	Reference	1	m3
Wastewater, average	market for wastewater, average wastewater, average Cutoff, S - Europe without Switzerland	0.060	m3
Hazardous waste, for incineration	market for hazardous waste, for incineration hazardous waste, for incineration Cutoff, S - Europe without Switzerland	4.388	kg

Table A15. Inventory for the MFA configuration of NRG-Foam.

Inputs			
Product	Process	Amount	Unit
Electricity, low voltage	market for electricity, low voltage electricity, low voltage Cutoff, S - IT	3842.359	MJ
Electricity, low voltage	market for electricity, low voltage electricity, low voltage Cutoff, S - ES	1333.889	MJ
Water, deionised	market for water, deionised water, deionised Cutoff, S - Europe without Switzerland	805.137	kg
Cement, Portland	market for cement, Portland cement, Portland Cutoff, S - Europe without Switzerland	120.504	kg
Transport, freight, lorry, unspecified	market for transport, freight, lorry, unspecified transport, freight, lorry, unspecified Cutoff, S - RER	82.844	t*km
Lime, hydrated, loose weight	market for lime, hydrated, loose weight lime, hydrated, loose weight Cutoff, S - RoW	72.689	kg
Chemical 3 - rGO production			
Electricity, low voltage	market for electricity, low voltage electricity, low voltage Cutoff, S - DE	67.922	MJ
Tap water	market for tap water tap water Cutoff, S - Europe without Switzerland	60.275	kg
Fatty acid	market for fatty acid fatty acid Cutoff, S - GLO	20.779	kg
Metakaolin	Metakaolin production	19.843	kg
Melamine formaldehyde resin	market for melamine formaldehyde resin melamine formaldehyde resin Cutoff, S - RER	5.861	kg
Isobutanol	market for isobutanol isobutanol Cutoff, S - RER	4.244	kg
Stabiliser	Stabiliser dummy	4.067	kg
Polycarboxylates, 40% active substance	market for polycarboxylates, 40% active substance polycarboxylates, 40% active substance Cutoff, S - RER	2.812	kg
Calcium nitrate	market for calcium nitrate calcium nitrate Cutoff, S - RER	2.802	kg
Chemical 2 - rGO production			
Foaming agent	market for foaming agent foaming agent Cutoff, S - GLO	1.206	kg
Chemical 1 - rGO production			
Polyvinylalcohol, at plant/kg/RER U	polyvinylalcohol, at plant - RER	0.779	kg

Table A15. Inventory for the MFA configuration of NRG-Foam (continued).

Graphite	market for graphite graphite Cutoff, S - GLO	0.523	kg
Ammonium chloride	market for ammonium chloride ammonium chloride Cutoff, S - GLO	0.104	kg
Outputs			
Product	Process	Amount	Unit
NRG-Foam	Reference	1	m3
Wastewater, average	market for wastewater, average wastewater, average Cutoff, S - Europe without Switzerland	0.283	m3
Hazardous waste, for incineration	market for hazardous waste, for incineration hazardous waste, for incineration Cutoff, S - Europe without Switzerland	4.26608	kg

In addition, Metakaolin production has been modelled separately since there was no data for it in ecoinvent. The modelling has been based on the information provided in a paper by Heath et al. [238]. Table A16 shows the inputs and outputs in the metakaolin production process. Transport distance for metakaolin has been assumed to be 300 km (not included below but added in the overall NRG-Foam production process).

Table A16. Metakaolin production inputs and outputs.

Inputs			
Flow	Provider	Amount	Unit
heat, district or industrial, natural gas	heat production, natural gas, at industrial furnace low-NOx >100kW heat, district or industrial, natural gas Cutoff, S - Europe without Switzerland	2.5	MJ
kaolin	market for kaolin kaolin Cutoff, S - GLO	1.16	kg
Outputs			
Flow	Provider	Amount	Unit
Metakaolin		1	kg

APPENDIX B

CHAPTER 4: PROTOTYPE-LEVEL ASSESSMENT OF NRG-FOAM AND NRG- PANELS IN THE CONTEXT OF A DEMONSTRATOR BUILDING

B1. Bill of materials for demonstration buildings

Table B1: Bill of materials for the demonstrator buildings.

Location	Layer	Market name (Brand + Product name)	Volume, per 1 building		Price per unit
Floor	Reinforced concrete slab		39.0	m ²	6.4
	Concrete	C30/37 (B35)	6.1	m ³	51
	Waterproof tarp		40.0	m ²	1.02
	XPS insulation	Gias Grafit XPS	42.0	m ²	18.22
	Bituminous hydro insulation	Tehnobit FLEX P 4.0	106.5	m ²	3.56
Roof	Roof hydro insulation #1	Vedasprint	50.0	m ²	9.18
	Wooden boarding		5.0	m ³	430
	Light mineral wool between beams	Saint Gobain Isover Unirol Profi	45.0	m ²	10.2
	Plasterboard coating		40.0	m ²	6.63
	Steel cladding		84.0	m ¹	6.12
	Internal wooden structure for ceilings		50.0	m ²	4.08
	Gutter		9.0	m ¹	7.14
	Anchor	Hilti-HST-M12x235/140	22.0	pieces	2.55
	Wood screws	TBS 8x240	14.0	pieces	0.51
Wall	Sheetrock	KNAUF Finitura	110.0	m ²	6.12
	Brick	WIENERBERGER Porotherm Light Plus	14.0	m ³	41.66
	Mortar	Globus 23/Rofix 150	70.0	m ²	2.04
	Glue for insulation	Rofix W50	68.0	m ²	13.26
	EPS insulation	Rofix 80F			
	Fasteners	Rofix Rocket 80			
	Reinforcing mesh	Rofix P 50	68.0	m ²	9.9
	Putty	Rofix W50			
	Primer	Rofix Putzgrund Premium	68.0	m ²	5.87
	Plaster	Rofix Sisi - Putz			

Table B1(continued): Bill of materials for the demonstrator buildings.

	Window	REHAU Sinego	10.9	m ²	77.52
	Door	Rehau	1.0	pieces	-
Structural frame	Concrete	C25/30 (B30)	1.5	m ³	99.45
	Reinforcement	Steel B500B	654.5	kg	0.9
	Formwork	Doka	27.0	m ²	24.48
Foundation	Gravel		27.0	m ³	19.13
	Concrete	C25/30 (B30)	14.6	m ³	48.45
	Reinforcement	Steel B500B	35.5	kg	0.9
	Formwork	Doka	45.0	m ²	24.48

B2. Kiva foundation parameters for demonstrator buildings modelling

Table B2: Parameters of Kiva foundation used in the building energy simulations.

Parameter	Value
Initial Indoor Air Temperature	15 °C
Interior Vertical Insulation Depth	0.2 m
Wall Height Above Grade	0.1 m
Wall Depth Below Slab	0.8 m
Soil Conductivity	1.73 W/m-K
Soil Density	1842 kg/m ³
Soil Specific Heat	500 J/kg-K
Ground Solar Absorptivity	0.9
Ground Thermal Absorptivity	0.9
Ground Surface Roughness	0.012
Far-Field Width	40 m
Deep-Ground Boundary Condition	ZeroFlux
Deep-Ground Depth	40 m
Minimum Cell Dimension	0.02
Maximum Cell Growth Coefficient	1.5
Simulation Timestep	Timestep

B3. Inventories for the production of MPCM, NRG-Panels and demonstrator buildings

Table B3: Inventory of MF MPCM production.

Inputs			
Product	Process	Amount	Unit
MF-Resin	MF-resin (50% “market for formaldehyde formaldehyde Cutoff, S - RER” and 50% “market for melamine melamine Cutoff, S - GLO”)	0.21	kg
Isobutanol	market for isobutanol isobutanol Cutoff, S	0.15	kg
PCM (FAME)	treatment of waste cooking oil, purified, esterification fatty acid methyl ester Cutoff, S	0.75	kg
Water	market for water, deionised water, deionised Cutoff, S	2.83	kg
PVA	polyvinylalcohol, at plant - RER (based on the data from LC-Inventories.ch - Photovoltaics)	0.03	kg
Electricity	market for electricity, low voltage electricity, low voltage Cutoff, S	5.07	MJ
Transport	market for transport, freight, lorry, unspecified transport, freight, lorry, unspecified Cutoff, S	0.23	t*km
Ammonium chloride	market for ammonium chloride ammonium chloride Cutoff, S	0.00	kg
Outputs			
Product	Process	Amount	Unit
MF MPCM slurry	Reference	3.98	kg
From which solid MPCM		1.00	kg

Table B4: Inventory of IC MPCM production.

Inputs			
Product	Process	Amount	Unit
Water	market for water, deionised water, deionised Cutoff, S	6.85	kg
PCM (FAME)	treatment of waste cooking oil, purified, esterification fatty acid methyl ester Cutoff, S	0.68	kg
Gelatine	Modelled based on Ma et al. [145]	0.11	kg
Electricity	market for electricity, low voltage electricity, low voltage Cutoff, S	7.12	MJ
Crosslinker		0.02	kg
Polymer 2		0.04	kg
Plasticiser		0.05	kg
Emulsifier		0.00	kg
Transport	market for transport, freight, lorry, unspecified transport, freight, lorry, unspecified Cutoff, S	0.21	t*km
Shell material		0.05	kg
Soda ash	market for soda ash, dense soda ash, dense Cutoff, S	0.05	kg
Outputs			
Product	Process	Amount	Unit
IC MPCM slurry	Reference	6.66	kg
From which solid MPCM		1.00	kg

Table B5: Inventory of NRG-Panels production.

Inputs				
Product	Process	Amount (MF MPCM)	Amount (IC MPCM)	Unit
MPCM Slurry (equiv. to 10.19 kg of dry MPCM)	Input from upscaled LCA of MPCM	42.71	71.51	kg
Cement CEM III/C	market for cement, blast furnace slag 81-95% cement, blast furnace slag 81-95% Cutoff, S	143.69	143.69	kg
Stabiliser	No dataset available, not included	4.84	4.84	kg
Accelerator	market for calcium nitrate calcium nitrate Cutoff, S	3.35	3.35	kg
Foaming agent	market for foaming agent foaming agent Cutoff, S	1.27	1.27	kg
Metakaolin	Metakaolin production (modelled based on Heath et al. [238])	23.65	23.65	kg
Superplasticiser	market for polycarboxylates, 40% active substance polycarboxylates, 40% active substance Cutoff, S	0.83	0.83	kg
Tap water	market for tap water tap water Cutoff, S	85.42	64.06	kg
Electricity	market for electricity, low voltage electricity, low voltage Cutoff, S	0.88	0.88	MJ
Rainwater	market for water, harvested from rainwater water, harvested from rainwater Cutoff, S	13.16	13.16	kg
Electricity PV	electricity production, photovoltaic, 3kWp slanted-roof installation, single-Si, panel, mounted electricity, low voltage Cutoff, S	2.46	2.46	MJ
Reinforcement mesh	market for glass fibre reinforced plastic, polyester resin, hand lay-up glass fibre reinforced plastic, polyester resin, hand lay-up Cutoff, S	3.30	3.30	kg
Steel	market for steel, low-alloyed steel, low-alloyed Cutoff, S	2.40	2.40	kg
Outputs				
Product	Process	Amount (MF MPCM)	Amount (IC MPCM)	Unit
MPCM Panels	Reference	1	1	m3
Waste cement slurry	market for hazardous waste, for underground deposit hazardous waste, for underground deposit Cutoff, S	1.096491	1.10	kg

Table B5 (continued): Inventory of NRG-Panels production.

Waste water	market for wastewater, average wastewater, average Cutoff, S	0.076125	0.08	m3
Waste steel	treatment of scrap steel, inert material landfill scrap steel Cutoff, S	2.40	2.40	kg

Table B6: Inventory of EPS building production.

Inputs				
Product	Process	Amount	Unit	
Wooden boarding	market for sawnwood, board, hardwood, dried (u=10%), planed sawnwood, board, hardwood, dried (u=10%), planed Cutoff, S - Europe without Switzerland	5.8	m3	
Concrete	concrete slab production concrete slab Cutoff, S - RoW	7.8	m3	
Door	market for door, outer, wood-glass door, outer, wood-glass Cutoff, S - GLO	2.0256	m2	
Brick	market for clay brick clay brick Cutoff, S - GLO	8036	kg	
Mortar	market for lime mortar lime mortar Cutoff, S - GLO	3069.6	kg	
Light mineral wool between beams (roof)	market for glass wool mat, uncoated, Saint-Gobain ISOVER SA glass wool mat, uncoated, Saint-Gobain ISOVER SA Cutoff, S - CH	170.1	kg	
Structural frame	market for concrete, 25MPa concrete, 25MPa Cutoff, S - RoW	16.1	m3	
Plasterboard	market for gypsum plasterboard gypsum plasterboard Cutoff, S - GLO	576	kg	
EPS insulation	market for polystyrene foam slab polystyrene foam slab Cutoff, S - GLO	108.8	kg	
Steel reinforcement for concrete	market for reinforcing steel reinforcing steel Cutoff, S - GLO	690	kg	
Concrete	market for concrete, 35MPa concrete, 35MPa Cutoff, S - RoW	6.1	m3	
Windows	market for glazing, triple, U<0.5 W/m2K glazing, triple, U<0.5 W/m2K Cutoff, S - GLO	10.9	m2	
Steel cladding (roof)	market for steel, low-alloyed steel, low-alloyed Cutoff, S - GLO	294.84	kg	
Gravel	market for gravel, crushed gravel, crushed Cutoff, S - RoW	41850	kg	
Waterproof layer (roof and ceiling)	market for packaging film, low density polyethylene packaging film, low density polyethylene Cutoff, S - GLO	48	kg	
Bitumen	market for bitumen adhesive compound, cold bitumen adhesive compound, cold Cutoff, S - GLO	860.75	kg	

Table B6 (continued): Inventory of EPS building production.

XPS insulation (floor)	market for polystyrene, extruded polystyrene, extruded Cutoff, S - GLO	142.8	kg
Transport	transport, freight, lorry, all sizes, EURO6 to generic market for transport, freight, lorry, unspecified transport, freight, lorry, unspecified Cutoff, S - RER	2595.42	t*km
Powder coating of roof cladding steel	powder coating, steel powder coat, steel Cutoff, S - RER	8.4	m2
Lime	market for lime, hydraulic lime, hydraulic Cutoff, S - RER	42.9	kg
Tap water	market for tap water tap water Cutoff, S - Europe without Switzerland	816.4356	kg
Diesel fuel for machinery	market for diesel, burned in building machine diesel, burned in building machine Cutoff, S - GLO	24355.32	MJ
Electricity	market for electricity, low voltage electricity, low voltage Cutoff, S - BG	676911.5	MJ
Outputs			
Product	Process	Amount	Unit
Waste concrete	market for waste concrete, not reinforced waste concrete, not reinforced Cutoff, S - Europe without Switzerland	72000	kg
Waste gravel	treatment of waste concrete gravel, collection for final disposal waste concrete gravel Cutoff, S - RoW	41850	kg
Waste brick	market for waste brick waste brick Cutoff, S - Europe without Switzerland	8036	kg
Waste cement	market for waste cement in concrete and mortar waste cement in concrete and mortar Cutoff, S - Europe without Switzerland	3112.5	kg
Waste bitumen	market for waste bitumen waste bitumen Cutoff, S - Europe without Switzerland	860.75	kg
Waste reinforcement steel	market for waste reinforcement steel waste reinforcement steel Cutoff, S - RoW	984.84	kg
Waste plasterboard	market for waste gypsum plasterboard waste gypsum plasterboard Cutoff, S - GLO	576	kg
Waste XPS and EPS	market for waste polystyrene isolation, flame-retardant waste polystyrene isolation, flame-retardant Cutoff, S - Europe without Switzerland	251.6	kg
Waste mineral wool	market for waste mineral wool waste mineral wool Cutoff, S - Europe without Switzerland	170.1	kg

Table B6 (continued): Inventory of EPS building production.

Waste glass	market for waste glass waste glass Cutoff, S - BG	459.39	kg
Waste waterproof layers	market group for waste polyethylene waste polyethylene Cutoff, S - Europe without Switzerland	48	kg

Table B7: Inventory of NRG building production.

Inputs			
Product	Process	Amount	Unit
Wooden boarding	market for sawnwood, board, hardwood, dried (u=10%), planed sawnwood, board, hardwood, dried (u=10%), planed Cutoff, S - Europe without Switzerland	5.8	m3
Concrete	concrete slab production concrete slab Cutoff, S - RoW	7.8	m3
Door	market for door, outer, wood-glass door, outer, wood-glass Cutoff, S - GLO	2.0256	m2
Brick	market for clay brick clay brick Cutoff, S - GLO	8036	kg
Mortar	market for lime mortar lime mortar Cutoff, S - GLO	3069.6	kg
Light mineral wool between beams (roof)	market for glass wool mat, uncoated, Saint-Gobain ISOVER SA glass wool mat, uncoated, Saint-Gobain ISOVER SA Cutoff, S - CH	170.1	kg
Structural frame	market for concrete, 25MPa concrete, 25MPa Cutoff, S - RoW	16.1	m3
Plasterboard	market for gypsum plasterboard gypsum plasterboard Cutoff, S - GLO	576	kg
NRG-Panels production	Result from the upscaled LCA	68	m2
Steel reinforcement for concrete	market for reinforcing steel reinforcing steel Cutoff, S - GLO	690	kg
Concrete	market for concrete, 35MPa concrete, 35MPa Cutoff, S - RoW	6.1	m3
Windows	market for glazing, triple, U<0.5 W/m2K glazing, triple, U<0.5 W/m2K Cutoff, S - GLO	10.9	m2
Steel cladding (roof)	market for steel, low-alloyed steel, low-alloyed Cutoff, S - GLO	294.84	kg
Gravel	market for gravel, crushed gravel, crushed Cutoff, S - RoW	41850	kg

Table B7 (continued): Inventory of NRG building production.

Waterproof layer (roof and ceiling)	market for packaging film, low density polyethylene packaging film, low density polyethylene Cutoff, S - GLO	48	kg
Bitumen	market for bitumen adhesive compound, cold bitumen adhesive compound, cold Cutoff, S - GLO	860.75	kg
XPS insulation (floor)	market for polystyrene, extruded polystyrene, extruded Cutoff, S - GLO	142.8	kg
Transport	transport, freight, lorry, all sizes, EURO6 to generic market for transport, freight, lorry, unspecified transport, freight, lorry, unspecified Cutoff, S - RER	2595.42	t*km
Powder coating of roof cladding steel	powder coating, steel powder coat, steel Cutoff, S - RER	8.4	m2
Lime	market for lime, hydraulic lime, hydraulic Cutoff, S - RER	42.9	kg
Tap water	market for tap water tap water Cutoff, S - Europe without Switzerland	816.4356	kg
Diesel fuel for machinery	market for diesel, burned in building machine diesel, burned in building machine Cutoff, S - GLO	24355.32	MJ
Electricity	market for electricity, low voltage electricity, low voltage Cutoff, S - BG	723404.6	MJ
Electricity	market group for electricity, low voltage electricity, low voltage Cutoff, S - Europe without Switzerland	421.056	MJ
Outputs			
Product	Process	Amount	Unit
Waste concrete	market for waste concrete, not reinforced waste concrete, not reinforced Cutoff, S - Europe without Switzerland	72000	kg
Waste gravel	treatment of waste concrete gravel, collection for final disposal waste concrete gravel Cutoff, S - RoW	41850	kg
Waste cement	market for waste cement in concrete and mortar waste cement in concrete and mortar Cutoff, S - Europe without Switzerland	3928.5	kg
Waste plastic	market for waste plastic, mixture waste plastic, mixture Cutoff, S - BG	22.44	kg
Waste brick	market for waste brick waste brick Cutoff, S - Europe without Switzerland	8036	kg
Waste bitumen	market for waste bitumen waste bitumen Cutoff, S - Europe without Switzerland	860.75	kg
Waste reinforcement steel	market for waste reinforcement steel waste reinforcement steel Cutoff, S - RoW	984.84	kg
Waste plasterboard	market for waste gypsum plasterboard waste gypsum plasterboard Cutoff, S - GLO	576	kg

Table B7 (continued): Inventory of NRG building production.

Waste XPS	market for waste polystyrene isolation, flame-retardant waste polystyrene isolation, flame-retardant Cutoff, S - Europe without Switzerland	142.8	kg
Waste mineral wool	market for waste mineral wool waste mineral wool Cutoff, S - Europe without Switzerland	170.1	kg
Waste glass	market for waste glass waste glass Cutoff, S - BG	459.39	kg
Waste waterproof layers	market group for waste polyethylene waste polyethylene Cutoff, S - Europe without Switzerland	48	kg

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B4. Absolute values of environmental impacts for MPCM, NRG-Panels and demonstrator buildings

Table B8: Absolute values of environmental impacts of MF MPCM production.

Impact category	Environmental impact by contributor								Total environmental impact
	MF-Resin	Electricity	Isobutanol	PVA	PCM (FAME)	Transport	Ammonium chloride	Water	
Agricultural land occupation, m ² a	2.20E-02	3.02E-02	1.99E-02	9.33E-03	4.63E-03	2.22E-04	2.21E-04	4.17E-05	8.66E-02
Climate change, kg CO ₂ eq	7.90E-01	5.31E-01	3.56E-01	2.54E-01	2.05E-01	2.95E-02	5.90E-03	1.23E-03	2.17E+00
Fossil depletion, kg oil eq	3.31E-01	1.65E-01	2.47E-01	1.45E-01	1.21E-01	1.08E-02	1.56E-03	3.35E-04	1.02E+00
Freshwater ecotoxicity, kg 1,4-DB eq	2.06E-02	3.42E-02	6.76E-03	8.18E-03	4.08E-03	2.15E-04	2.10E-04	4.66E-05	7.43E-02
Freshwater eutrophication, kg P eq	2.04E-04	1.38E-04	1.03E-04	8.76E-05	5.01E-05	2.02E-06	1.81E-06	4.55E-07	5.88E-04
Human toxicity, kg 1,4-DB eq	2.42E-01	1.42E-01	9.37E-02	9.24E-02	5.11E-02	8.59E-03	2.21E-03	5.37E-04	6.32E-01
Ionising radiation, kBq U235 eq	2.79E-02	7.36E-02	5.23E-02	3.99E-02	1.23E-02	2.36E-03	3.51E-04	1.40E-04	2.09E-01
Marine ecotoxicity, kg 1,4-DB eq	1.78E-02	3.00E-02	6.18E-03	7.37E-03	3.28E-03	2.89E-04	1.88E-04	4.25E-05	6.51E-02
Marine eutrophication, kg N eq	3.39E-04	7.75E-05	5.02E-05	4.84E-05	3.84E-05	6.76E-06	1.78E-05	2.94E-07	5.78E-04
Metal depletion, kg Fe eq	5.12E-02	2.34E-02	1.47E-02	1.92E-02	1.00E-02	1.17E-03	5.32E-04	1.26E-04	1.20E-01
Natural land transformation, m ²	1.99E-04	7.11E-05	7.89E-05	5.44E-05	6.13E-05	1.17E-05	1.18E-06	2.07E-07	4.78E-04
Ozone depletion, kg CFC-11 eq	6.64E-08	6.37E-08	4.00E-08	8.12E-08	2.89E-08	5.52E-09	3.45E-10	6.94E-10	2.87E-07
Particulate matter formation, kg PM ₁₀ eq	1.44E-03	6.33E-04	4.45E-04	3.70E-04	3.29E-04	6.83E-05	1.02E-05	3.38E-06	3.30E-03
Photochemical oxidant formation, kg NMVOC	2.39E-03	1.22E-03	1.45E-03	8.67E-04	5.86E-04	1.90E-04	1.50E-05	3.69E-06	6.73E-03
Terrestrial acidification, kg SO ₂ eq	3.78E-03	2.00E-03	1.30E-03	9.31E-04	7.10E-04	1.28E-04	2.37E-05	8.94E-06	8.88E-03
Terrestrial ecotoxicity, kg 1,4-DB eq	7.13E-05	4.15E-05	1.33E-05	3.19E-05	4.64E-05	1.48E-05	6.80E-07	1.91E-07	2.20E-04

Table B8 (continued): Absolute values of environmental impacts of MF MPCM production.

Urban land occupation, m2a	1.75E-03	4.19E-03	8.92E-04	8.54E-04	3.17E-03	2.04E-03	2.37E-05	1.08E-05	1.29E-02
Water depletion, m3	-1.11E+00	-7.17E+00	-1.04E+00	-1.05E+00	-6.11E-01	-2.69E-02	-1.74E-02	-3.18E-03	-1.10E+01

Table B9: Absolute values of environmental impacts of IC MPCM production.

Impact category	Contributor											Total environmental impact
	Electricity	Plasticiser	Gelatine	Polymer 2	PCM (FAME)	Soda ash	Shell material	Transport	Water	Crosslinker	Emulsifier	
Agricultural land occupation, m2a	4.25E-02	1.95E-01	2.88E-02	8.28E-02	4.20E-03	2.14E-03	5.24E-03	2.01E-04	1.01E-04	-	-	3.66E-01
Climate change, kg CO2 eq	7.45E-01	1.29E-01	2.29E-01	1.47E-01	1.86E-01	5.67E-02	2.22E-02	2.68E-02	2.97E-03	-	-	1.64E+00
Fossil depletion, kg oil eq	2.31E-01	3.62E-02	7.05E-02	4.50E-02	1.10E-01	1.49E-02	5.43E-03	9.77E-03	8.10E-04	-	-	5.53E-01
Freshwater ecotoxicity, kg 1,4-DB eq	4.81E-02	3.69E-03	1.18E-02	3.31E-03	3.71E-03	2.03E-03	1.85E-03	1.95E-04	1.13E-04	-	-	8.08E-02
Freshwater eutrophication, kg P eq	1.94E-04	4.00E-05	1.83E-04	5.21E-05	4.55E-05	1.73E-05	1.28E-05	1.83E-06	1.10E-06	-	-	5.72E-04
Human toxicity, kg 1,4-DB eq	1.99E-01	3.58E-02	2.07E-01	5.52E-02	4.64E-02	2.07E-02	1.65E-02	7.79E-03	1.30E-03	-	-	6.15E-01
Ionising radiation, kBq U235 eq	1.03E-01	9.41E-03	8.04E-02	1.45E-02	1.12E-02	3.38E-03	1.99E-03	2.14E-03	3.39E-04	-	-	2.40E-01
Marine ecotoxicity, kg 1,4-DB eq	4.21E-02	2.79E-03	1.14E-02	3.05E-03	2.98E-03	1.81E-03	1.68E-03	2.63E-04	1.03E-04	-	-	7.15E-02
Marine eutrophication, kg N eq	1.09E-04	1.24E-03	6.71E-04	3.11E-05	3.48E-05	1.45E-04	1.47E-05	6.14E-06	7.13E-06	-	-	2.27E-03
Metal depletion, kg Fe eq	3.28E-02	7.90E-03	2.58E-02	6.80E-03	9.09E-03	5.19E-03	4.91E-03	1.07E-03	3.05E-04	-	-	9.80E-02
Natural land transformation, m2	9.99E-05	2.01E-05	3.94E-05	2.84E-05	5.56E-05	1.14E-05	3.88E-06	1.06E-05	5.00E-07	-	-	2.82E-04
Ozone depletion, kg CFC-11 eq	8.95E-08	2.75E-08	1.07E-07	2.39E-08	2.63E-08	2.60E-09	1.26E-09	5.01E-09	1.68E-09	-	-	2.96E-07
Particulate matter formation, kg PM10 eq	8.89E-04	3.36E-04	5.26E-04	3.40E-04	2.99E-04	9.79E-05	7.16E-05	6.20E-05	8.17E-06	-	-	2.74E-03

Table B9 (continued): Absolute values of environmental impacts of IC MPCM production.

Photochemical oxidant formation, kg NMVOC	1.72E-03	4.27E-04	7.28E-04	4.66E-04	5.32E-04	1.47E-04	8.08E-05	1.73E-04	8.93E-06	-	-	4.49E-03
Terrestrial acidification, kg SO2 eq	2.81E-03	1.36E-03	1.51E-03	6.38E-04	6.45E-04	2.25E-04	2.67E-04	1.16E-04	2.16E-05	-	-	7.95E-03
Terrestrial ecotoxicity, kg 1,4-DB eq	5.83E-05	4.22E-03	2.87E-03	2.16E-05	4.22E-05	5.82E-06	3.41E-06	1.34E-05	4.62E-07	-	-	7.25E-03
Urban land occupation, m2a	5.89E-03	3.25E-03	2.24E-03	8.08E-04	2.88E-03	2.61E-04	1.95E-04	1.85E-03	2.61E-05	-	-	1.81E-02
Water depletion, m3	1.01E+01	4.53E-01	1.98E+00	5.99E-01	5.54E-01	1.67E-01	7.41E-02	2.44E-02	7.69E-03	-	-	-1.52E+01

Table B10: Absolute values of environmental impacts of NRG-Panels with MF MPCM.

Impact category	Contributor																	Total
	Cement III/C	MF MPCM	Slurry	Foaming agent	Reinforcement mesh	Metakaolin	Steel	Accelerator	Superplasticiser	Waste cement slurry	Electricity PV	Electricity	Waste water	Waste steel	Tap water	Rainwater	Stabiliser	
Agricultural land occupation, m2a	1.53E+00	9.61E-01	2.58E+00	7.53E-01	2.83E-01	1.35E-01	2.00E-01	2.63E-02	1.21E-01	3.16E-03	4.84E-03	1.15E-03	6.66E-04	1.41E-03	5.52E-05		6.60E+00	
Climate change, kg CO2 eq	3.74E+01	2.75E+01	3.20E+00	1.27E+01	1.01E+01	4.62E+00	5.32E+00	9.17E-01	2.26E-01	7.41E-02	1.26E-01	3.66E-02	1.24E-02	2.77E-02	3.20E-03		1.02E+02	
Fossil depletion, kg oil eq	8.25E+00	1.25E+01	3.40E-01	4.50E+00	3.41E+00	1.13E+00	1.35E+00	4.23E-01	6.01E-02	2.00E-02	3.18E-02	8.21E-03	8.40E-03	7.55E-03	6.64E-04		3.20E+01	
Freshwater ecotoxicity, kg 1,4-DB eq	6.93E-01	8.27E-01	1.40E-01	2.74E-01	1.31E-01	2.46E-01	2.82E-01	3.06E-02	6.04E-03	2.08E-02	9.03E-03	1.87E-03	9.19E-05	7.38E-04	6.89E-05		2.66E+00	
Freshwater eutrophication, kg P eq	1.08E-02	6.59E-03	5.35E-04	3.06E-03	2.41E-03	2.24E-03	1.03E-03	2.30E-04	9.58E-05	4.66E-05	1.89E-04	8.51E-05	1.17E-06	2.04E-05	8.09E-07		2.74E-02	
Human toxicity, kg 1,4-DB eq	1.11E+01	8.00E+00	9.42E-01	6.85E+00	2.18E+00	2.32E+00	1.97E+00	2.87E-01	8.02E-02	8.25E-02	1.22E-01	2.15E-02	1.61E-03	2.04E-02	9.08E-04		3.40E+01	
Ionising radiation, kBq U235 eq	4.83E+00	2.57E+00	7.94E-02	9.02E-01	8.26E-01	2.07E-01	2.28E-01	8.78E-02	8.08E-03	7.07E-03	2.34E-02	5.02E-03	1.57E-03	1.01E-02	1.33E-04		9.79E+00	
Marine ecotoxicity, kg 1,4-DB eq	6.49E-01	7.40E-01	6.21E-02	2.50E-01	1.20E-01	2.38E-01	2.55E-01	2.78E-02	5.90E-03	1.86E-02	8.09E-03	1.71E-03	8.76E-05	6.93E-04	6.64E-05		2.38E+00	
Marine eutrophication, kg N eq	6.17E-03	7.16E-03	1.68E-02	3.83E-03	1.22E-03	1.47E-03	1.45E-03	1.25E-04	4.95E-05	2.93E-05	4.77E-05	1.57E-03	4.53E-06	9.26E-06	6.29E-07		3.99E-02	
Metal depletion, kg Fe eq	1.57E+00	1.46E+00	1.53E-01	9.33E-01	2.25E-01	6.29E+00	7.89E-01	7.67E-02	1.83E-01	2.31E-02	4.89E-03	1.04E-02	5.97E-04	4.89E-03	1.34E-03		1.17E+01	
Natural land transformation, m2	7.64E-03	6.78E-03	3.75E-03	3.03E-03	2.06E-03	5.27E-04	9.42E-04	1.56E-04	3.37E-05	1.29E-05	7.74E-06	1.84E-05	-9.63E-05	3.98E-06	6.33E-06		2.49E-02	
Ozone depletion, kg CFC-11 eq	2.59E-06	3.86E-06	2.01E-07	1.14E-06	1.12E-06	2.28E-07	4.17E-07	1.34E-07	1.25E-08	7.15E-09	3.06E-09	2.61E-09	4.05E-09	1.71E-09	1.95E-10		9.71E-06	
Particulate matter formation, kg PM10 eq	5.80E-02	4.51E-02	6.32E-03	2.51E-02	1.32E-02	1.67E-02	7.32E-03	1.24E-03	7.72E-04	2.13E-04	8.51E-05	1.36E-04	4.24E-05	6.37E-05	8.49E-06		1.74E-01	
Photochemical oxidant formation, kg NMVOC	1.10E-01	9.91E-02	9.37E-03	7.74E-02	1.99E-02	2.13E-02	9.67E-03	2.39E-03	1.13E-03	2.96E-04	1.73E-04	1.75E-04	1.32E-04	9.40E-05	1.38E-05		3.51E-01	
Terrestrial acidification, kg SO2 eq	1.50E-01	1.13E-01	1.48E-02	5.58E-02	2.83E-02	1.64E-02	2.86E-02	2.82E-03	7.57E-04	4.39E-04	2.47E-04	3.30E-04	9.02E-05	1.20E-04	1.03E-05		4.13E-01	
Terrestrial ecotoxicity, kg 1,4-DB eq	3.93E-03	4.46E-03	4.87E-01	8.48E-03	3.69E-04	3.92E-04	4.14E-04	5.59E-05	4.17E-05	1.16E-04	8.62E-06	2.26E-05	1.33E-06	2.81E-06	2.83E-07		5.05E-01	
Urban land occupation, m2a	5.66E-01	4.28E-01	1.77E-02	7.89E-02	1.57E-02	2.13E-02	2.45E-02	3.97E-03	2.74E-03	1.31E-04	6.40E-04	2.19E-03	2.99E-04	2.14E-04	1.63E-03		1.16E+00	
Water depletion, m3	1.39E+02	1.22E+02	3.43E+00	3.60E+01	3.18E+01	2.96E+01	8.48E+00	-2.63E+00	-3.51E-01	1.02E+00	-5.07E-01	-2.51E-01	-1.18E-02	-1.45E-01	-7.22E-03		3.76E+02	

Table B11: Absolute values of environmental impacts of NRG-Panels with IC MPCM.

Impact category	Contributor													Total
	Cement III/C	IC MPCM	Slurry	Foaming agent	Reinforcement mesh	Metakaolin	Steel	Accelerator	Supplementary cementitious	Waste cement slurry	Electricity PV	Electricity	Waste water	Stabiliser
Agricultural land occupation, m2a	1.53E+00	3.92E+00	2.58E+00	7.53E-01	2.83E-01	1.35E-01	2.00E-01	2.63E-02	1.21E-01	3.16E-03	4.84E-03	1.15E-03	6.66E-04	9.56E+00
Climate change, kg CO2 eq	3.74E+01	2.36E+01	3.20E+00	1.27E+01	1.01E+01	4.62E+00	5.32E+00	9.17E-01	2.26E-01	7.41E-02	1.26E-01	3.66E-02	1.24E-02	9.83E+01
Fossil depletion, kg oil eq	8.25E+00	8.17E+00	3.40E-01	4.50E+00	3.41E+00	1.13E+00	1.35E+00	4.23E-01	6.01E-02	2.00E-02	3.18E-02	8.21E-03	8.40E-03	2.77E+01
Freshwater ecotoxicity, kg 1,4-DB eq	6.93E-01	8.53E-01	6.45E-02	2.74E-01	1.31E-01	2.46E-01	2.82E-01	3.06E-02	6.04E-03	2.08E-02	9.03E-03	1.87E-03	9.19E-05	2.61E+00
Freshwater eutrophication, kg P eq	1.08E-02	6.36E-03	5.35E-04	3.06E-03	2.41E-03	2.24E-03	1.03E-03	2.30E-04	9.59E-05	4.66E-05	1.89E-04	8.51E-05	1.17E-06	2.71E-02
Human toxicity, kg 1,4-DB eq	1.11E+01	8.36E+00	8.83E-01	6.85E+00	2.18E+00	2.32E+00	1.97E+00	2.87E-01	8.02E-02	8.25E-02	1.22E-01	2.15E-02	1.61E-03	3.43E+01
Ionising radiation, kBq U235 eq	4.83E+00	2.99E+00	7.94E-02	9.02E-01	8.26E-01	2.07E-01	2.28E-01	8.78E-02	8.08E-03	7.07E-03	2.34E-02	5.02E-03	1.57E-03	1.02E+01
Marine ecotoxicity, kg 1,4-DB eq	6.49E-01	7.79E-01	5.65E-02	2.50E-01	1.20E-01	2.38E-01	2.55E-01	2.78E-02	5.90E-03	1.86E-02	8.09E-03	1.71E-03	8.76E-05	2.41E+00
Marine eutrophication, kg N eq	6.17E-03	2.58E-02	1.68E-02	3.83E-03	1.22E-03	1.47E-03	1.45E-03	1.25E-04	4.95E-05	2.93E-05	4.77E-05	1.57E-05	4.53E-06	5.86E-02
Metal depletion, kg Fe eq	1.57E+00	1.29E+00	1.53E-01	9.33E-01	2.25E-01	6.29E+00	7.89E-01	7.67E-02	1.83E-01	2.31E-02	4.89E-03	1.04E-02	5.97E-04	1.15E+01
Natural land transformation, m2	7.64E-03	5.66E-03	3.75E-03	3.03E-03	2.06E-03	5.27E-04	9.42E-04	1.56E-04	3.37E-05	1.29E-05	7.74E-06	1.84E-05	2.99E-06	2.37E-02
Ozone depletion, kg CFC-11 eq	2.59E-06	4.36E-06	2.01E-07	1.14E-06	1.12E-06	2.28E-07	4.17E-07	1.34E-07	1.25E-08	7.15E-09	3.05E-09	2.61E-09	4.05E-09	1.02E-05
Particulate matter formation, kg PM10 eq	5.80E-02	4.44E-02	6.32E-03	2.51E-02	1.32E-02	1.67E-02	7.32E-03	1.24E-03	7.72E-04	2.13E-04	8.51E-05	1.36E-04	4.24E-05	1.74E-01
Photochemical oxidant formation, kg NMVOC	1.10E-01	9.10E-02	9.37E-03	7.74E-02	1.99E-02	2.13E-02	9.67E-03	2.39E-03	1.13E-03	2.96E-04	1.73E-04	1.75E-04	1.32E-04	3.43E-01
Terrestrial acidification, kg SO2 eq	1.50E-01	1.12E-01	1.48E-02	5.58E-02	2.83E-02	1.64E-02	2.86E-02	2.82E-03	7.57E-04	4.39E-04	2.47E-04	3.30E-04	9.02E-05	4.11E-01
Terrestrial ecotoxicity, kg 1,4-DB eq	3.93E-03	8.12E-02	3.77E-03	8.48E-03	3.69E-04	3.92E-04	4.14E-04	5.59E-05	4.17E-05	1.16E-04	8.62E-06	2.26E-05	1.33E-06	9.88E-02
Urban land occupation, m2a	5.66E-01	6.71E-01	1.77E-02	7.89E-02	1.57E-02	2.13E-02	2.45E-02	3.97E-03	2.74E-03	-1.31E-04	6.40E-04	2.19E-03	2.99E-04	1.41E+00
Water depletion, m3	1.39E+02	1.56E+02	3.43E+00	3.60E+01	3.18E+01	2.96E+01	8.48E+00	2.63E+00	-3.51E-01	-5.07E-01	-2.51E-01	-1.18E-02	-1.08E-01	4.09E+02

APPENDIX C

CHAPTER 6: CLIMATE-DEPENDENT DESIGN
OF NRG-PANELS AND IDENTIFICATION OF
FAVORABLE LOCATIONS FOR NRG-PANELS
APPLICATION

C1. Heating and cooling demands used for the comparison of the thermal performance of NRG-Panels and EPS

Table C1. Heating and cooling demand of the demonstrator building in different climatic conditions under the current climate.

City	Electricity demand for the building with EPS, kWh/year		Electricity demand for the building with NRG-Panels (unconstrained case), kWh/year		Electricity demand for the building with NRG-Panels (constrained case), kWh/year	
	Heating	Cooling	Heating	Cooling	Heating	Cooling
Adana	272.8	4127.9	154.5	4113.4	158.8	4111.8
Amsterdam	1256.4	706.0	1165.3	744.4	1230.1	719.2
Ankara	1082.4	1972.2	997.9	2022.8	1059.1	1989.0
Antalya	328.3	2551.2	332.7	2451.9	340.7	2450.3
Athens	337.8	3043.9	108.7	3174.8	112.5	3171.5
Barcelona	279.7	1113.5	278.7	1022.5	307.3	1033.5
Belgrade	1085.5	2331.8	1092.1	2281.7	1063.1	2346.2
Berlin	1458.8	1500.6	1353.0	1539.2	1428.9	1514.4
Bern	1865.4	750.4	1730.3	795.6	1827.7	766.2
Birmingham	1592.9	286.4	1475.4	316.5	1560.1	296.6
Bratislava	1103.0	1848.9	1013.6	1884.7	1077.1	1861.4
Brussels	1001.1	865.6	916.9	908.3	976.8	880.0
Bucharest	1226.9	2127.8	1138.7	2162.5	1200.5	2140.5
Budapest	1365.9	1946.4	1275.9	1980.6	1341.1	1958.0
Bursa	1433.7	1316.8	1339.4	1370.3	1407.2	1334.6
Chisinau	2175.7	2005.9	2046.1	2033.7	2138.5	2016.4
Copenhagen	2588.4	332.2	2436.2	364.7	2544.6	341.4
Diyarbakir	476.1	3638.4	471.9	3617.0	462.0	3650.3
Dublin	985.1	396.1	896.8	431.6	960.1	408.3
Gaziantep	506.0	3321.3	572.9	3205.3	492.5	3335.0
Hamburg	2021.7	980.6	1902.3	1016.4	1986.9	993.4
Helsinki	4304.9	317.3	4101.0	342.7	4246.7	326.8
Istanbul	487.7	2170.2	617.5	1964.1	566.0	2078.2
Izmir	357.5	3135.2	425.0	2966.8	572.7	2886.6
Kayseri	1491.7	1828.3	1385.4	1879.4	1461.4	1844.9
Kharkiv	2862.6	1934.2	2712.7	1962.2	2820.7	1944.3
Konya	731.7	2047.1	696.5	2041.6	709.3	2063.6
Kyiv	1963.4	1552.8	1848.7	1593.3	1931.7	1566.7

Table C1 (continued). Heating and cooling demand of the demonstrator building in different climatic conditions under the current climate.

Lisbon	113.7	1338.7	131.1	1262.0	145.9	1247.9
Ljubljana	1567.8	1410.6	1461.0	1442.7	1537.1	1422.4
London	1325.3	587.8	1230.3	619.8	1297.1	600.2
Madrid	300.7	2244.7	358.4	2120.9	352.9	2180.7
Milan	863.4	2714.9	789.9	2744.4	842.9	2725.6
Minsk	3311.0	919.9	3136.7	951.9	3262.3	930.8
Munich	1562.0	745.3	1447.7	783.9	1530.3	758.8
Odesa	1828.3	1215.3	1710.1	1248.6	1794.6	1226.7
Oslo	2781.5	838.4	2629.6	863.9	2738.6	847.4
Paris	1279.2	990.7	1237.8	977.9	1253.4	1006.7
Podgorica	718.0	2117.0	649.6	2151.2	698.8	2129.1
Prague	1750.6	1077.2	1634.9	1117.8	1717.2	1091.5
Pristina	985.6	1542.0	889.6	1572.7	958.2	1553.4
Riga	3204.1	1104.6	3040.6	1137.8	3156.0	1117.0
Rome	400.3	2269.6	429.2	2132.8	531.1	2058.2
Sarajevo	1863.5	1099.9	1738.4	1135.8	1827.6	1113.0
Skopje	853.5	1622.4	821.5	1620.1	831.9	1638.8
Sofia	1861.5	782.2	1730.6	817.8	1824.1	795.1
Stockholm	2644.6	633.6	2495.1	662.6	2602.2	644.3
Tallinn	3130.8	579.8	2964.3	613.2	3082.6	591.6
Tirana	489.4	2139.7	586.2	2006.9	472.2	2156.4
Vienna	1214.4	1192.7	1118.1	1227.6	1186.7	1205.1
Vilnius	2678.6	798.3	2531.9	831.9	2635.5	810.5
Warsaw	1991.3	1148.8	1875.9	1179.9	1958.2	1159.4
Zagreb	1337.7	1898.5	1248.8	1940.4	1312.4	1913.6

Table C2. Heating and cooling demand of the demonstrator building in different climatic conditions under future climatic projections.

City	Electricity demand for the building with EPS, kWh/year		Electricity demand for the building with NRG-Panels (unconstrained case), kWh/year		Electricity demand for the building with NRG-Panels (constrained case), kWh/year	
	Heating	Cooling	Heating	Cooling	Heating	Cooling
Athens 2050	123.3	4738.9	53.3	4779.5	52.7	4779.9
Athens 2080	56.1	5748.9	26.5	5759.7	26.5	5759.9
Barcelona 2050	139.5	3072.0	100.0	3090.2	103.0	3087.2
Barcelona 2080	56.0	4028.0	80.2	3985.3	81.0	3984.7
Berlin 2050	1086.5	2435.2	1002.8	2465.3	1063.5	2445.6
Berlin 2080	865.7	2961.8	794.0	2984.9	845.8	2970.0
Istanbul 2050	248.2	3366.3	361.0	3169.6	336.1	3241.9
Istanbul 2080	145.7	4186.4	168.8	4113.5	184.0	4130.6
Lisbon 2050	36.3	2479.6	73.1	2262.7	73.3	2262.5
Lisbon 2080	20.5	3237.2	34.8	3020.2	34.7	3020.3
Madrid 2050	198.3	3486.9	191.0	3406.7	227.5	3396.7
Madrid 2080	144.9	4333.5	115.5	4294.8	144.5	4283.4
Paris 2050	1039.6	1848.9	1090.2	1737.3	1019.4	1862.7
Paris 2080	857.3	2451.0	951.0	2292.2	840.9	2462.8
Podgorica 2050	400.5	3614.2	358.4	3633.3	388.9	3620.8
Podgorica 2080	287.3	4386.0	254.8	4395.3	278.7	4389.5
Sofia 2050	1343.2	1881.5	1241.3	1908.4	1315.0	1892.4
Sofia 2080	1107.2	2542.5	1023.8	2564.4	1085.0	2551.3
Tirana 2050	240.1	3459.8	298.8	3357.1	245.5	3455.3
Tirana 2080	145.3	4248.9	142.7	4218.8	175.1	4216.3

C2. Optimal EPS configurations for minimising building energy consumption

Table C3. Optimal thickness of EPS panels for minimising the demonstrator building energy consumption under the current climate.

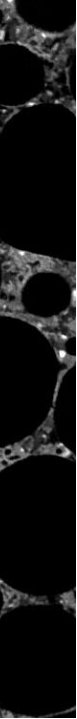
City	Thickness, m
Adana	0.04
Amsterdam	0.30
Ankara	0.30
Antalya	0.06
Athens	0.02
Barcelona	0.11
Belgrade	0.30
Berlin	0.30
Bern	0.30
Birmingham	0.30
Bratislava	0.30
Brussels	0.30
Bucharest	0.30
Budapest	0.30
Bursa	0.30
Chisinau	0.30
Copenhagen	0.30
Diyarbakir	0.30
Dublin	0.30
Gaziantep	0.30
Hamburg	0.30
Helsinki	0.30
Istanbul	0.30
Izmir	0.15
Kayseri	0.30
Kharkiv	0.30
Konya	0.30
Kyiv	0.30
Lisbon	0.02
Ljubljana	0.30
London	0.30
Madrid	0.20

Table C3 (continued). Optimal thickness of EPS panels for minimising the demonstrator building energy consumption under the current climate.

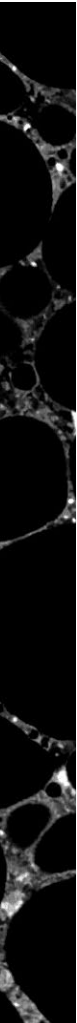
Milan	0.30
Minsk	0.30
Munich	0.30
Odesa	0.30
Oslo	0.30
Paris	0.30
Podgorica	0.30
Prague	0.30
Pristina	0.30
Riga	0.30
Rome	0.10
Sarajevo	0.30
Skopje	0.30
Sofia	0.30
Stockholm	0.30
Tallinn	0.30
Tirana	0.30
Vienna	0.30
Vilnius	0.30
Warsaw	0.30
Zagreb	0.30

Table C4. Optimal thickness of EPS panels for minimising the demonstrator building energy consumption under future climatic projections.

City	Thickness, m
Athens 2050	0.02
Athens 2080	0.03
Barcelona 2050	0.02
Barcelona 2080	0.02
Berlin 2050	0.30
Berlin 2080	0.30
Istanbul 2050	0.30
Istanbul 2080	0.30
Lisbon 2050	0.01
Lisbon 2080	0.01
Madrid 2050	0.10
Madrid 2080	0.08
Paris 2050	0.30
Paris 2080	0.30
Podgorica 2050	0.30
Podgorica 2080	0.30
Sofia 2050	0.30
Sofia 2080	0.30
Tirana 2050	0.28
Tirana 2080	0.25



C



APPENDIX D

CHAPTER 7: BEST FIT FOR COMMON
PURPOSE: A MULTI-STAKEHOLDER
DESIGN OPTIMISATION METHODOLOGY
FOR CONSTRUCTION MANAGEMENT

D1. Material Composition of Frame and Façade Options

The table below shows the material composition of all the structural frame and façade options used in this study. The values provided are for a single floor with a floor area of 1000 m². As was mentioned above, the foundation was assumed to be the same for all design variants; so, it is provided separately in the table as well. Note that the units are different for different materials.

Table D1. Material composition of structural frame and façade options.

Material	Unit	Frame				Façade		
		Foundation	1— Concrete Frame	2—Structural Steel Profile Frame and a Hollow Concrete Slabs Floor	3—Cross- Laminated Timber Frame with a Wooden Joist Floor	1—Brick and Rockwool Insulation	2—Steel Sandwich Panel Façade with Polyisocyanurate Insulation	3—Timber Frame Façade with Mineral Wool Insulation
Ready-mix concrete, normal strength, generic, C 28/35 (4000/5000 PSI) with CEM I, 0% recycled binders (300 kg/m ³ ; 18.7 lbs/ft ³ total cement)	m ³	0	329.1	0	0	0	0	0
Ready-mix concrete, normal-strength, generic, C 40/50 (5800/7300 PSI), 0% recycled binders in cement (400 kg/m ³ /24.97 lbs/ft ³)	m ³	500.0	14.7	0	0	0	0	0
Rock wool insulation, unfaced, L = 0.035–0.04 W/mK, 40 mm, 1.2 kg/m ² , 30 kg/m ³ , Lambda = 0.035 W/(m.K), ProRox LF 970 (ROCKWOOL)	m ³	0	0	0	0	58.2	0	0
Wall bricks, 575 kg/m ³ (Ziegel)	m ³	0	0	0	0	36.4	0	0
Hot-dip galvanised structural steel, 0.45–1.5 mm, 7850 kg/m ³ (Ruukki)	m ³	0	0	1.2	0	0	0	0
Structural steel profiles, generic, 90% recycled content (typical), I, H, U, L, and T sections, S235, S275 and S355	m ³	0	0	6.0	3.6	0	0	0
Hollow core concrete slab, HDF27, C 40/50, 270 mm, 344 kg/m ² , reinforcing 12,7 kg/ton (Strängbetong)	m ²	0	0	945.0	0	0	0	0

Table D1 (continued). Material composition of structural frame and façade options.

Aluminium profile, 2700.0 kg/m3	m ³	0	0	0	0	0	0	0	0
Sandwich panel with polyisocyanurate (PIR) foam and double steel siding, U = 0.21W/(m2K), 100.9 mm (Total), 0.5 mm (Outer sheet), 0.4 mm (Liner sheet), 100 mm (Insulation), 12.11 kg/m2, 120.02 kg/m3, SAB Steel Europe)	m ²	0	0	0	0	0	0	363.9	0
Aluminium profiled sheets, thickness 0.7 mm, height of profile 65 mm, 2.9 kg/m2 (European Association for Panels and Profiles)	m ²	0	0	0	0	0	0	363.9	0
Cross-laminated timber, 491.65 kg/m3, T:51–500 mm, max width: 2.95–4.80 m, max length: 16–20 m, X-Lam (Studiengemeinschaft Holzleimbau e.V.)	m ³	0	0	0	0	88.9	0	0	3.1
Wooden joist floor assembly, 278 mm, incl. 225 mm mineral wool insulation	m ²	0	0	0	0	688.1	0	0	0
Timber frame external wall assembly, incl. mineral wool insulation	m ²	0	0	0	0	0	0	0	363.9

D2. Equations for Calculating the Volume of Materials Used in the Model

The material composition of the building influences two of the objectives—Embodied carbon emissions and Construction costs. As mentioned in Section 7.3.1., the model was parameterised in order to make it suitable for use in optimisation. The amount of materials used in the design will, thus, depend on four variables: Floor area a , Number of floors n , Set of the building's structural frame materials m_1 , and Set of the building's facade materials m_2 . The calculations were conducted in matrix form. The total number of unique materials used in our design optimisation problem was 13 (see Table 7.1) and that was the length of the material vector that was used as a basis in the problem. For example, the vector $v = [1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1]$ includes 1 m³ of “Ready-mix concrete, normal strength, generic, C 28/35 (4000/5000 PSI) with CEM I, 0% recycled binders (300 kg/m³; 18.7 lbs/ft³ total cement)” and 1 m² of “Timber frame external wall assembly, incl. mineral wool insulation”. Note that since the data provided in EPDs can be measured using different units, the vector contains both values measured in m² and m³.

As was mentioned in Section 7.3.1., the original models that were shared with us were not parameterised and the original gross floor area of those building designs was fixed at 1000 m². In further equations, it is denoted as a_0 . The proportions of the floor area were assumed to be constant (the length-to-width ratio of the building is equal to 3.49). The equations provided below are sometimes defined through the length of the building that—given the fixed proportions—can be defined as:

$$s = \sqrt{a/3.49}$$

Independently of the design option, the foundation was always assumed to be the same 0.5 m thick concrete slab. Thus, the vector representing the material composition related to the foundation can be defined as:

$$f = [0, a * 0.5, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0]$$

The amount of materials used in the internal frame construction was defined as:

$$M_1 = \left\{ \begin{array}{l} \left[\begin{array}{l} (18.8 * s - 27.2) * 0.1 + \\ a * 0.3, 27 * 3.4 * 0.16 * \frac{a}{a_0}, \\ 0,0,0,0,0,0,0,0,0,0 \end{array} \right], \text{when } m_1 = 1 \\ \\ \left[\begin{array}{l} 0,0,0,0, \\ 27 * 0.046 * \frac{a}{a_0}, \\ 27 * 0.011 * \sqrt{\left(\frac{a}{a_0}\right)} + \\ \left(s - 3 * 0.3 * \sqrt{\left(\frac{a}{a_0}\right)}\right) * 0.009 * 2 * \frac{a}{a_0} + \\ \left(3.49 * s - 9 * 0.3 * \sqrt{\left(\frac{a}{a_0}\right)}\right) * 0.023 * 3 * \frac{a}{a_0} + \\ \left(3.49 * s - 9 * 0.3 * \sqrt{\left(\frac{a}{a_0}\right)}\right) * 0.0016 * 4 * \frac{a}{a_0} + \\ 40 * 2 * 0.009 + \\ 40 * 2 * 0.0027 * \sqrt{(0.2 * s)}, \\ \left(s - 0.85 * \sqrt{\left(\frac{a}{a_0}\right)}\right) * \left(3.49 * s - 0.3 * \sqrt{\left(\frac{a}{a_0}\right)}\right), \\ 0,0,0,0,0,0,0,0,0,0 \end{array} \right], \text{when } m_1 = 2 \\ \\ \left[\begin{array}{l} (2 * 27 * 0.021 + 2 * 4 * 0.02 + 2 * 14 * 0.025 + 2 * 7 * 0.037 + 2 * 2 * 0.018) * \frac{a}{a_0} + \\ 2 * 27 * 0.001 * \sqrt{\left(\frac{a}{a_0}\right)} + \\ (6 * 16 * 0.0001 + 6 * 8 * 0.002) * \frac{a}{a_0} + \\ 4 * (3.49 * s - 6) * 0.004, 0,0,0,0, \\ (4 * 0.483 + 16 * 0.727 + 7 * 1.087) * \frac{a}{a_0} + \\ (9 * 0.2 * (s - 1.1) + 2 * (3.49 * s - 2.92) * 0.2 + 0.3 * (3.49 * s - 3.2)) * \frac{a}{a_0}, \\ \left(3.49 * s^2 - 9 * s * \sqrt{\left(\frac{a}{a_0}\right)} - 2 * 3.49 * s * \sqrt{\left(\frac{a}{a_0}\right)} - 0.7 * 3.49 * s * \sqrt{\left(\frac{a}{a_0}\right)}\right), \\ 0 \end{array} \right], \text{when } m_1 = 3 \end{array} \right.$$

The amount of materials used in the façade was defined as:

$$M_2 = \begin{cases} \begin{bmatrix} 0,0, \\ 21.5 * s * 0.16, \\ 21.5 * s * 0.1, \\ 0,0,0,0,0,0,0,0 \end{bmatrix}, & \text{when } m_2 = 1 \\ \begin{bmatrix} 0,0,0,0,0,0, \\ 4 * 0.005 * \frac{a}{a_0} + \\ 82 * 0.002 * \frac{a}{a_0}, \\ 21.5 * s, \\ 21.5 * s, \\ 0,0,0 \end{bmatrix}, & \text{when } m_2 = 2 \\ \begin{bmatrix} 0,0,0,0,0,0,0,0,0, \\ 4 * 0.786 * \sqrt{\left(\frac{a}{a_0}\right)}, \\ 0, \\ 21.5 * s \end{bmatrix}, & \text{when } m_2 = 3 \end{cases}$$

D3. Calculation of the Objectives

D3.1. Embodied Carbon Emissions

The vector of values for embodied carbon emissions can be represented as (the values are also provided in Table 7.1):

$$e_e = [292.13, 386.96, 35.25, 138.29, 20794.65, 6033.17, 46.78, 29289, 37.2, 27, 187.23, 36, 65]$$

In addition to the values provided in EPDs, we also included the transportation emissions. Those were taken directly from OneClick LCA and converted into the same units as the corresponding values from EPDs. The vector of transportation emissions can be written as:

$$e_t = [18.72, 18.72, 0.069, 1.32, 111.24, 111.24, 0.79, 48.60, 0.20, 0.03, 4.14, 0.45, 0.73]$$

The overall emissions vector is a sum of the embodied carbon emissions obtained from EPDs and the transportation emissions:

$$e = e_e + e_t$$

The embodied carbon emissions can be calculated as follows:

$$E = n * (M_1^T \cdot e + M_2^T \cdot e) + f^T \cdot e$$

D3.2. Construction Costs

The vector of values for costs can be represented as (the values are also provided in Table 7.1):

$c = [344.87, 348, 57, 115, 5976.96, 5976.96, 60.64, 8920, 49.92, 6.24, 544.93, 132, 110]$

The construction costs can be calculated as follows:

$$C = n * (M_1^T \cdot c + M_2^T \cdot c) + f^T \cdot c$$

D3.3. Profit from Rent

Expected profit from rent was assumed to be dependent on the total area of the building and the distance to the railway station (denoted as *dist*). The objective for the expected profit from rent was defined as follows:

$$P = a * n * (2 * 10^{-7} * d^2 - 0.58 * 10^{-2} * d + 206.5)$$

The part in brackets is based on the average prices for the office space for the four biggest cities in the Netherlands (Amsterdam, Rotterdam, the Hague, and Utrecht) [239] and a study on the influence of the distance to a railway station on real estate prices [240].

D3.4. Location Objective

Location is simply the distance to the railway station:

$$L = d$$

APPENDIX E

CHAPTER 8: PREFERENCE-BASED GOAL ATTAINMENT APPROACH FOR EQUITABLE DECISION-MAKING

E1. Insulation material data used for the calculation of the objectives

Table E1: Parameters of insulation materials used for the calculations in Chapter 8.

Type	Brand	Name	Thickness, m	Thermal conductivity, W/mK	Density, kg/m ³	Heat capacity, J/kgK	Price, EUR/m ³	Env. Price, EUR/m ²	ecoinvent dataset
Rock wool	Rockwool	Fixrock Plus	0.04	0.033	50	1030	11.65	0.68	market for stone wool stone wool Cutoff, S - GLO
Rock wool	Rockwool	Fixrock Plus	0.05	0.033	50	1030	13.97	0.85	
Rock wool	Rockwool	Fixrock Plus	0.06	0.033	50	1030	16.31	1.02	
Rock wool	Rockwool	Fixrock Plus	0.08	0.033	50	1030	21.86	1.35	
Rock wool	Rockwool	Fixrock Plus	0.1	0.033	50	1030	26.44	1.69	
Rock wool	Rockwool	Fixrock Plus	0.12	0.033	50	1030	31.00	2.03	
EPS	Valero	Grafipol TR-29 SE	0.03	0.029	20	1260	6.10	0.39	market for polystyrene foam slab for perimeter insulation polystyrene foam slab for perimeter insulation Cutoff, S - GLO
EPS	Valero	Grafipol TR-29 SE	0.04	0.029	20	1260	7.99	0.52	
EPS	Valero	Grafipol TR-29 SE	0.05	0.029	20	1260	9.88	0.66	
EPS	Valero	Grafipol TR-29 SE	0.06	0.029	20	1260	11.74	0.79	
EPS	Valero	Grafipol TR-29 SE	0.07	0.029	20	1260	13.63	0.92	
EPS	Valero	Grafipol TR-29 SE	0.08	0.029	20	1260	15.51	1.05	
EPS	Valero	Grafipol TR-29 SE	0.09	0.029	20	1260	17.38	1.18	
EPS	Valero	Grafipol TR-29 SE	0.1	0.029	20	1260	19.27	1.31	
EPS	Valero	Grafipol TR-29 SE	0.11	0.029	20	1260	21.16	1.44	
EPS	Valero	Grafipol TR-29 SE	0.12	0.029	20	1260	23.05	1.57	
EPS	Valero	Grafipol TR-29 SE	0.13	0.029	20	1260	24.94	1.71	
EPS	Valero	Grafipol TR-29 SE	0.14	0.029	20	1260	26.81	1.84	
EPS	Valero	Grafipol TR-29 SE	0.15	0.029	20	1260	28.68	1.97	
EPS	Valero	Grafipol TR-29 SE	0.16	0.029	20	1260	30.57	2.10	
EPS	Valero	Grafipol TR-29 SE	0.17	0.029	20	1260	32.46	2.23	

Table E1 (continued): Parameters of insulation materials used for the calculations in Chapter 8.

EPS	Valero	Grafipol TR-29 SE	0.18	0.029	20	1260	34.33	2.36	
EPS	Valero	Grafipol TR-29 SE	0.19	0.029	20	1260	36.22	2.49	
EPS	Valero	Grafipol TR-29 SE	0.2	0.029	20	1260	38.11	2.62	
EPS	Valero	Grafipol TR-32 SE	0.03	0.032	20	1260	4.23	0.39	
EPS	Valero	Grafipol TR-32 SE	0.04	0.032	20	1260	5.45	0.52	
EPS	Valero	Grafipol TR-32 SE	0.05	0.032	20	1260	6.72	0.66	
EPS	Valero	Grafipol TR-32 SE	0.06	0.032	20	1260	7.97	0.79	
EPS	Valero	Grafipol TR-32 SE	0.07	0.032	20	1260	9.23	0.92	
EPS	Valero	Grafipol TR-32 SE	0.08	0.032	20	1260	10.50	1.05	
EPS	Valero	Grafipol TR-32 SE	0.09	0.032	20	1260	11.72	1.18	
EPS	Valero	Grafipol TR-32 SE	0.1	0.032	20	1260	13.01	1.31	
EPS	Valero	Grafipol TR-32 SE	0.11	0.032	20	1260	14.23	1.44	
EPS	Valero	Grafipol TR-32 SE	0.12	0.032	20	1260	15.50	1.57	
EPS	Valero	Grafipol TR-32 SE	0.13	0.032	20	1260	16.75	1.71	
EPS	Valero	Grafipol TR-32 SE	0.14	0.032	20	1260	18.00	1.84	
EPS	Valero	Grafipol TR-32 SE	0.15	0.032	20	1260	19.27	1.97	
EPS	Valero	Grafipol TR-32 SE	0.16	0.032	20	1260	20.51	2.10	
EPS	Valero	Grafipol TR-32 SE	0.17	0.032	20	1260	21.75	2.23	
EPS	Valero	Grafipol TR-32 SE	0.18	0.032	20	1260	23.03	2.36	
EPS	Valero	Grafipol TR-32 SE	0.19	0.032	20	1260	24.26	2.49	
EPS	Valero	Grafipol TR-32 SE	0.2	0.032	20	1260	25.53	2.62	
XPS	Ursa	Ursa XPS F N-W E	0.04	0.032	30	1450	7.04	1.16	market for polystyrene, extruded polystyrene, extruded Cutoff, S - GLO
XPS	Ursa	Ursa XPS F N-W E	0.05	0.032	30	1450	8.69	1.45	
XPS	Ursa	Ursa XPS F N-W E	0.06	0.032	30	1450	10.35	1.74	
XPS	Ursa	Ursa XPS F N-W E	0.08	0.032	30	1450	13.65	2.32	
XPS	Ursa	Ursa XPS F N-W E	0.1	0.032	30	1450	17.90	2.90	

Table E1 (continued): Parameters of insulation materials used for the calculations in Chapter 8.

PU	NA	NA	0.02	0.035	40	1450	2.36	1.02	market for polyurethane, rigid foam polyurethane, rigid foam Cutoff, S - RER
PU	NA	NA	0.03	0.035	40	1450	3.13	1.53	
PU	NA	NA	0.04	0.035	40	1450	4.16	2.03	
PU	NA	NA	0.05	0.035	40	1450	5.10	2.54	
PU	NA	NA	0.06	0.035	40	1450	5.58	3.05	
PU	NA	NA	0.07	0.035	40	1450	6.05	3.56	
PU	NA	NA	0.08	0.035	40	1450	6.52	4.07	
Cork chip board	Socyr	ICB	0.01	0.04	115	1700	7.77	2.82	market for cork slab cork slab Cutoff, S - RER
Cork chip board	Socyr	ICB	0.02	0.04	115	1700	10.17	5.64	
Cork chip board	Socyr	ICB	0.03	0.04	115	1700	14.01	8.45	
Cork chip board	Socyr	ICB	0.04	0.04	115	1700	18.10	11.27	
Cork chip board	Socyr	ICB	0.05	0.04	115	1700	22.20	14.09	
Cork chip board	Socyr	ICB	0.06	0.04	115	1700	26.46	16.91	
Cork chip board	Socyr	ICB	0.08	0.04	115	1700	35.29	22.55	
Cork chip board	Socyr	ICB	0.1	0.04	115	1700	43.49	28.18	

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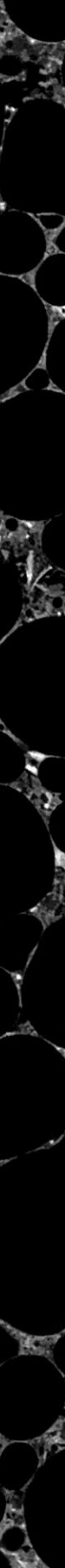
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CURRICULUM VITÆ

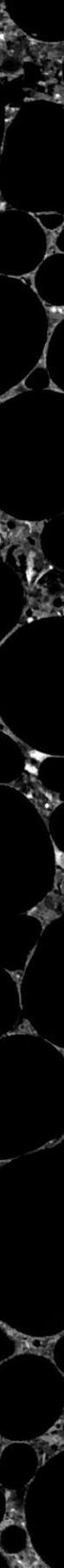
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LIST OF PUBLICATIONS

Published

1. **Zhilyaev, D.**, Binnekamp, R., Wolfert, A.M.R., 2022. Best Fit for Common Purpose: A Multi-Stakeholder Design Optimization Methodology for Construction Management. *Buildings* 12, 527. <https://doi.org/10.3390/buildings12050527>
2. **Zhilyaev, D.**, Fachinotti, V.D., Zanoni, F., Ortega, A., Goracci, G., Mankel, C., Koenders, E.A.B., Jonkers, H.M., 2023. Early-stage analysis of a novel insulation material based on MPCM-doped cementitious foam: Modelling of properties, identification of production process hotspots and exploration of performance trade-offs. *Developments in the Built Environment* 16, 100243. <https://doi.org/10.1016/j.dibe.2023.100243>
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