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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

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A B S T R A C T

This study presents an early-stage design exploration of NRG-Foam, an innovative insulation material composed of cementitious foam doped with microencapsulated phase change materials (MPCMs). The study comprises the static part that utilizes life cycle assessment and life cycle costing assessment for getting insight into the impacts of the NRG-Foam production process and the dynamic part that identifies the trade-offs between performance characteristics of NRG-Foam using multi-objective optimization. The production of MPCMs was found to be a major contributor to environmental impacts while the addition of small amounts of reduced graphene oxide amplifies the impacts even further. The hot spot analysis pinpointed high electricity consumption as the main driver of environmental impacts. A multi-objective optimization analysis revealed trade-offs between performance characteristics, emphasizing the necessity of compromises during material development. The selection of the MPCM type was shown to be determinative of the final properties of NRG-Foam.

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 (Bayomi et al., 2021). 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 (Ürge-Vorsatz et al., 2015). 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 (Guerra et al., 2009). Specifically, heat losses through the building envelope have a major effect on the total energy demand (Najjar et al., 2019). 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 (Rodríguez-Soria et al., 2014). 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" (Communication From The Commission To The European Parliament The Council, 2020), (Felius et al., 2020).

While of primary importance for colder climates, the impact of improving envelope insulation can be much less pronounced when it comes to warmer regions (Pan et al., 2012) and could increase the risk of

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overheating (Mulville and Stravoravdis, 2016). 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 (McLeod et al., 2013). 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 (Wang et al., 2022), (Rathore and Shukla, 2019).

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 (Bozsaky, 2010). 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 (Kalnæs and Jelle, 2015) but are not yet applied as broadly as regular insulation materials within real-world construction projects (Renew).

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 (Annibaldi et al., 2021). 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 (Annibaldi et al., 2021). 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 (Abu-et al., 2019), (Füchsl et al., 2022). 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 (Aridi and Yehya, 2022), (Frigione et al., 2019). 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 (N. E. Service and P. for A. T, 2003). It was estimated that 80% of a new product's impacts are determined during the design phase (May et al., 2012). 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 (Cubberly and Bakerjian, 1989). 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 (Kravchenko et al., 2020). 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 characterization 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 (Hautier et al., 2012). For example, finite element models can be used to model thermal (e.g. (Alghamdi and Alharthi, 2017),), electrical (e.g. (Scocchi et al., 2013),) and mechanical properties of a material (e.g. (Gupta and Harsha, 2016),). Analytical models such as, e.g., the Lewis-Nielsen model could be used to obtain thermal and electrical conductivity of multi-phase materials (Pal, 2008). 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) (Ren and Toniolo, 2019). And while life cycle assessments are better suited for technologies with high technology readiness levels (TRL) (Moni et al., 2020), even at early stages they can provide some very important information such as hotspots within the production process (Clark and Macquarrie, 2008). Within the current material design process, numerical and analytical models accompany the experimental ones and together guide the further development of new materials (Hautier et al., 2012).

In this study, we focus on an early-stage design, characterization and modelling of a novel insulation material – NRG-Foam – that is currently being developed within the Horizon 2020 NRG-STORAGE project (European Commission). 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 optimization.

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. Materials and methods

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 (Pal, 2008). 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. General overview of the methodology

Fig. 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 (“openLCA.org | openLCA is a) 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 parametrized making it possible to connect them to thermal and electrical properties models and integrate them within optimization 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 Cientificas (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.

2.3. Static part: LCA and LCCA

2.3.1. Overview of the approach

For the assessment of environmental impacts, we follow general LCA guidelines outlined in ISO 14044 (ISO, 2006). 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 (Hauschild et al., 2018). 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.

2.3.2. 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 m^3 NRG-Foam and all the results shown in the report are provided for 1 m^3 NRG-Foam. We used OpenLCA software (“openLCA.org | openLCA is a) to develop the model and perform calculations.

2.3.3. 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 (Fig. 2). Since we were performing LCCA alongside LCA, each unit process also includes economic inputs and outputs – costs and revenues.

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. Fig. 3 provides

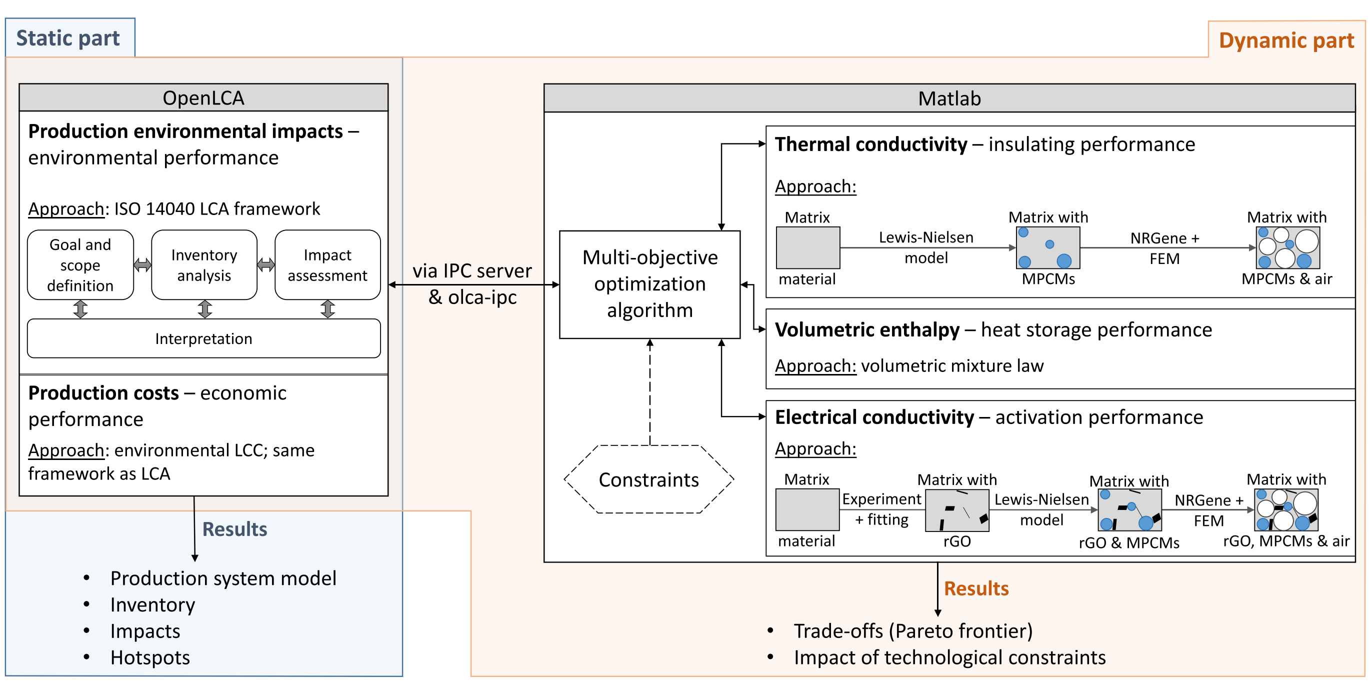

Fig. 1. Overview of the methodological approach used in this study.

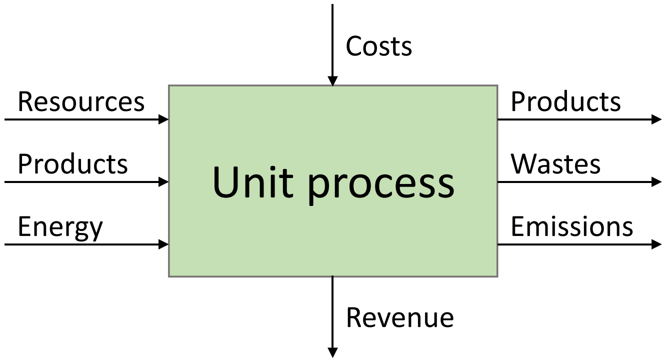

Fig. 2. A unit process with inputs and outputs.

an example of such a template for a single unit process.

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 ((Su et al., 2006; Khezri et al., 2022; Khakzad et al., 2014; Naikwadi et al., 2020; Kumar et al., 2021)) 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 ("Merck | Netherlands | Life)). Since the scope of the analysis is cradle-to-gate, there are no profits occurring and LCCA is thus limited to costs only.

2.3.4. *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 anonymized:

- For the production of inorganic coacervate (IC) shell MPCMs, the names of the chemicals used in the production process have been anonymized. 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 anonymized.

While it is not possible to disclose detailed data on those particular production processes, the reader can refer to the patent EP3070053A1 by GR (Zurutuza and Alonso, 2016) 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 (Hawlader et al., 2003; Onder et al., 2008; Wang et al., 2016). 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.

2.3.5. *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 (Home) 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 stabilizer 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.

2.3.6. *Impact assessment*

We are using ILCD 2011 Midpoint+ impact assessment method in this study (European Commission Service Site). 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

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)

Fig. 3. An example of an inventory data collection template.

- 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 S1 of the Supplementary Information file.

2.3.7. 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/m^3 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.

2.4. Dynamic part: identification of trade-offs and effect of constraints

2.4.1. Optimization problem set-up

Our case study of NRG-Foam’s early-stage development is in its essence a classical multiobjective optimization 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 optimize 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 optimization setup can be found in section S2 of the Supplementary Information file). An additional modification has been made to the standard function and during each generation, the full population has been recorded and stored. After the optimization terminated, the full list of all found solutions (final and intermediate) has been filtered out using *find_pareto_frontier* function (Sisi) 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.

2.4.2. 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 (Furuta et al., 2016); 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 (Sanfelix et al., 2019) 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 CO_2 emissions, $kg\ CO_{2\ eq}$ (environmental performance) – minimize
- Production costs, *EUR* (economic performance) – minimize
- Thermal conductivity, $W \bullet m^{-1} \bullet K^{-1}$ (insulation performance) – minimize
- Volumetric enthalpy, $J \bullet m^{-3}$ (heat storage performance) – maximize
- Electrical conductivity, $S \bullet m^{-1}$ (active application performance/activation performance) – maximize

The final optimization problem has been defined as a minimization problem. To do this, Volumetric enthalpy and Electrical conductivity objectives have been taken with the negative sign (optimization problems of maximization of an objective and minimization 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 (Kargar et al., 2018) and within the considered bounds of rGO fraction variable (0%–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 rationalizing the decision of omitting the link between rGO addition and the thermal conductivity of the paste.

2.4.3. 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 parametrized 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 ("olca-ipc." GreenDelta, 2023). 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 S2 of the Supplementary Information file.

2.4.4. 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 (Lewis and Nielsen, 1970), (Nielsen, 1974). Lewis-Nielsen model describes the thermal and electrical conductivity of a two-phase material (matrix + filler) and is defined by the following equations:

$$\frac{k}{k_1} = \frac{1 + AB\varphi_2}{1 - B\psi\varphi_2} \tag{1}$$

$$B = \frac{\frac{k_2}{k_1} - 1}{\frac{k_2}{k_1} + A} \tag{2}$$

$$\psi = 1 + \left(\frac{1 - \varphi_m}{\varphi_m^2}\right)\varphi_2 \tag{3}$$

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 $\varphi_m = 0.601$ (random loose packing).

In the second step, the addition of air bubbles has been simulated using a numerical model developed by CIMEC (Fachinotti et al., 2022). The model utilizes 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 (Fachinotti et al., 2022) 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:

$$H_{eff}(T) = \int_{T_{ref}}^{T} \rho c_{eff}(t)\, dt \tag{4}$$

where T_{ref} is an arbitrary reference temperature (we set T_{ref} at $0\,^{\circ}C$ 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 (Maxwell, 1873):

$$\rho c_{eff} = \varphi_{cem}\rho c_{cem} + \varphi_{air}\rho c_{air} + \varphi_{MPCM}\rho c_{MPCM} \tag{5}$$

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:

$$\rho c_{MCPM} = \varphi_{PCM}\rho c_{PCM} + (1 - \varphi_{PCM})\rho c_{shell} \approx \varphi_{PCM}\rho c_{PCM} \tag{6}$$

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 2.4.2., 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:

$$H_{eff}(T) = \varphi_{air}\rho c_{air}T + (1 - \varphi_{air}) * (1 - \varphi_{MPCM})\rho c_{cem}T + (1 - \varphi_{air})\varphi_{MPCM}\varphi_{PCM}\int_0^T \rho c_{PCM}(t)\, dt \tag{7}$$

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 (PureTemp)). In this study, we have calculated volumetric enthalpy at the interval of temperatures between $T_{ref} = 0$ to $T = 30\,^{\circ}C$. Section S2 of the Supplementary Information file provides the data for the heat capacities of components used in the calculations.

2.4.5. 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 generalized percolation model (Sarikhani et al., 2022). More detailed information on the experimental setup as well as the measured and fitted data can be found in section S2 of the Supplementary Information file. In the following step, the addition of MPCMs to the paste with rGO has been modelled using the Lewis-Nielsen theory (Lewis and Nielsen, 1970), (Nielsen, 1974). 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 (Fachinotti et al., 2022) (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.

2.4.6. Constraints and design space reduction

After running the optimization model with the variable bounds specified in Section 4.2. 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 S2 of the Supplementary Information file. 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.

3. Results and discussion

3.1. Results

3.1.1. Production system model and LCA/LCCA inventory

Fig. 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.

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 1 shows the foam mix designs used for those configurations. Mix designs are the same for IC and MF shell MPCMs.

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 S3 of the Supplementary Information file. Those inventories have then been used for conducting the impact assessment. The results of the impact assessment can be found in the following section.

Table 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
Superplasticizer	0.8	1.5	2.8
Stabilizer	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

3.1.2. LCA and LCCA impact assessment and identification of hotspots

Table 2 presents the results of the impact assessment of NRG-Foam for all five configurations in absolute values and Fig. 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).

As can be seen from Table 2 and Fig. 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

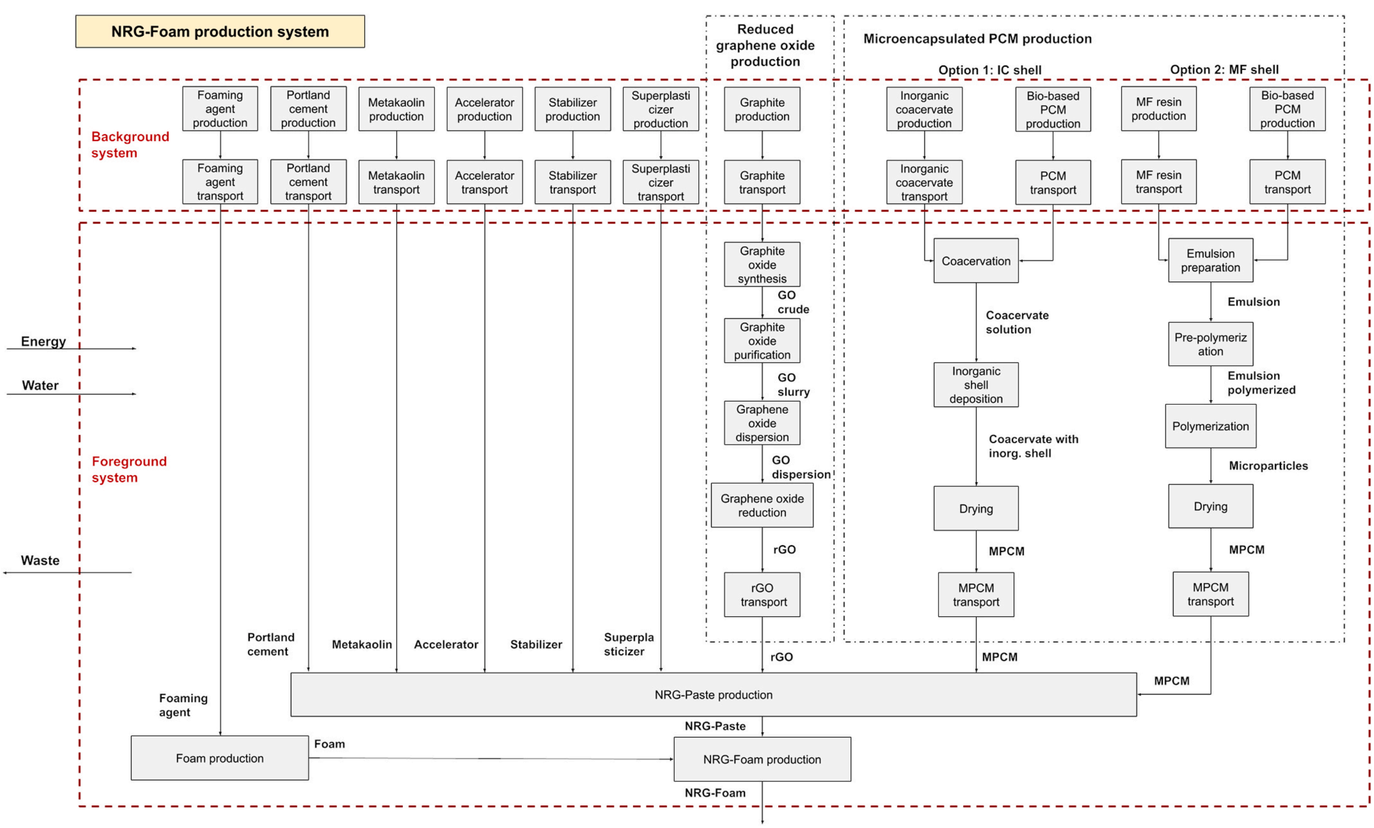

Fig. 4. NRG-Foam production system.

Table 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

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 1.8–3.1 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). Fig. 6 shows the contribution of impacts by stages for ICA foam.

As can be seen from Fig. 6, MPCM production stage is the main contributor to the overall impacts and is responsible for 66%–95% of the total impacts. A similar situation can be observed in the case of MFA foam (see Fig. 7) but the proportions are less skewed towards MPCM production: it is responsible for 39%–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.

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. Fig. 8 shows contributions for the ICA configuration and Fig. 9 – for the MFA configuration.

In Figs. 8 and 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

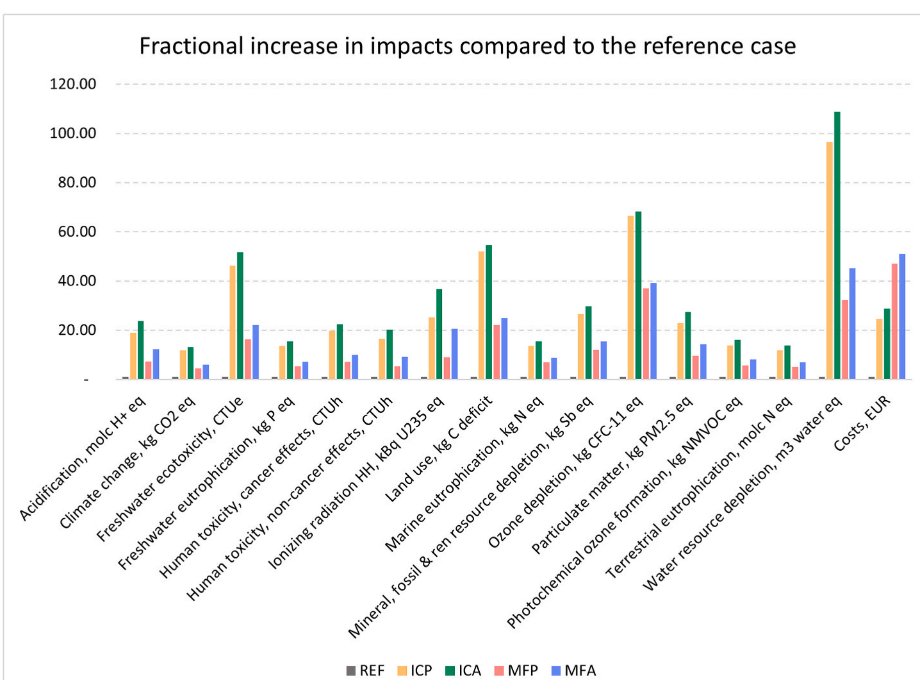

Fig. 5. The fractional increase in impacts compared to the reference case.

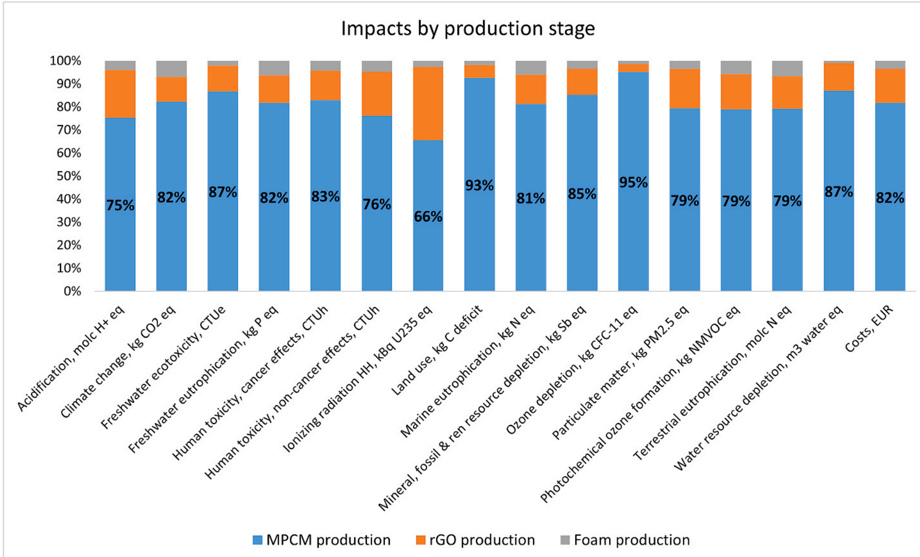

Fig. 6. Contribution of NRG-Foam production stages for ICA foam configuration.

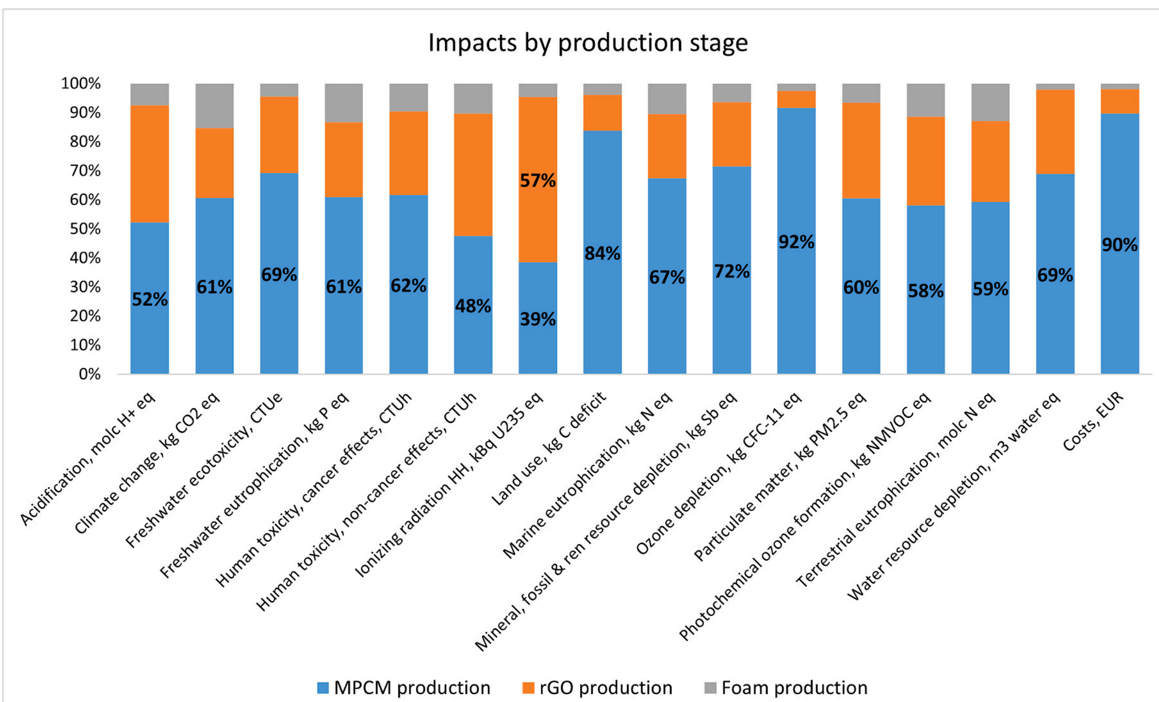

Fig. 7. Contribution of NRG-Foam production stages for MFA foam configuration.

- 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.

Figs. 8 and 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 Figs. 6 and 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

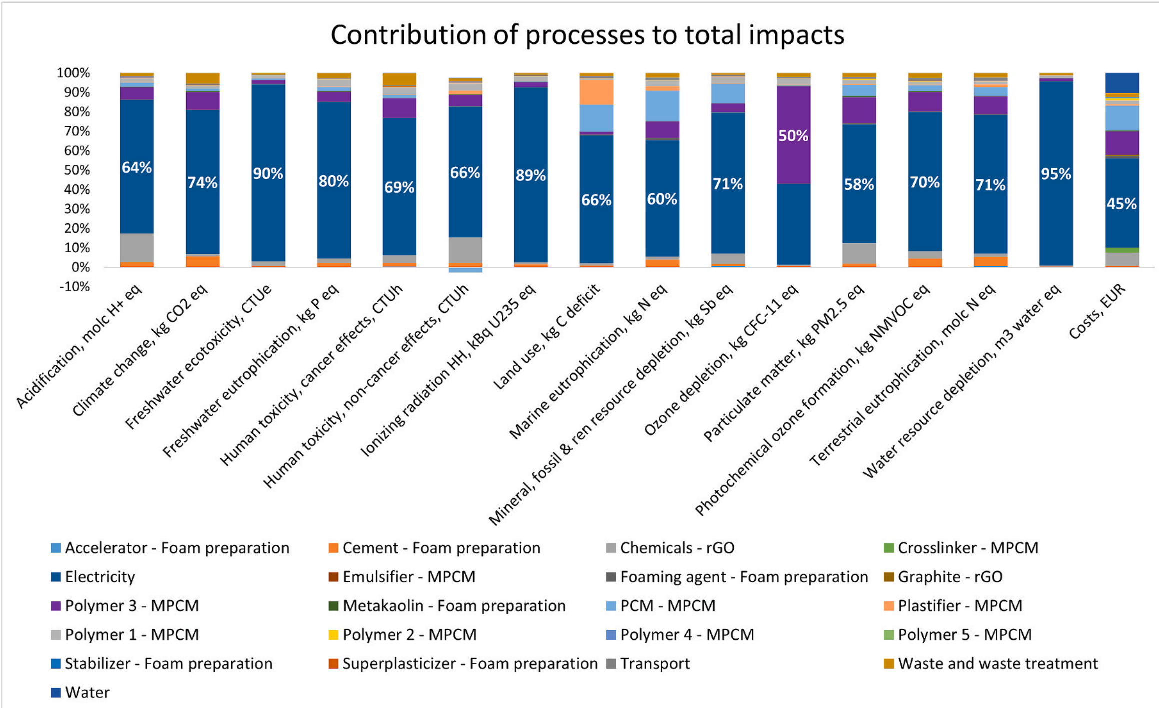

Fig. 8. Contribution of NRG-Foam production processes for ICA foam configuration.

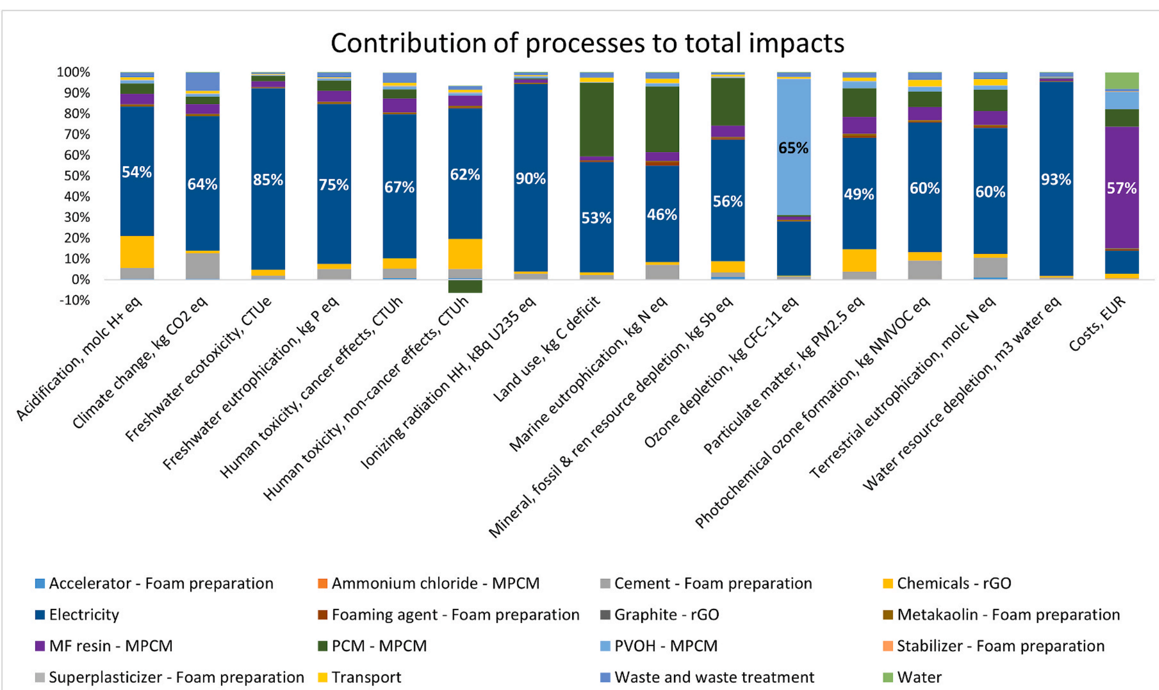

Fig. 9. Contribution of NRG-Foam production processes for MFA foam configuration.

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.

3.1.3. *Optimization 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. Fig. 10 shows all possible projections of the five-dimension Pareto frontier obtained.

The optimization problem has been set up as a minimization problem. Two maximization objectives – Electrical conductivity and Volumetric enthalpy – were converted into minimization objectives by adding the negative sign to them. Thus, the utopia point in all plots within Fig. 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

Fig. 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 characterized 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 optimization. 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

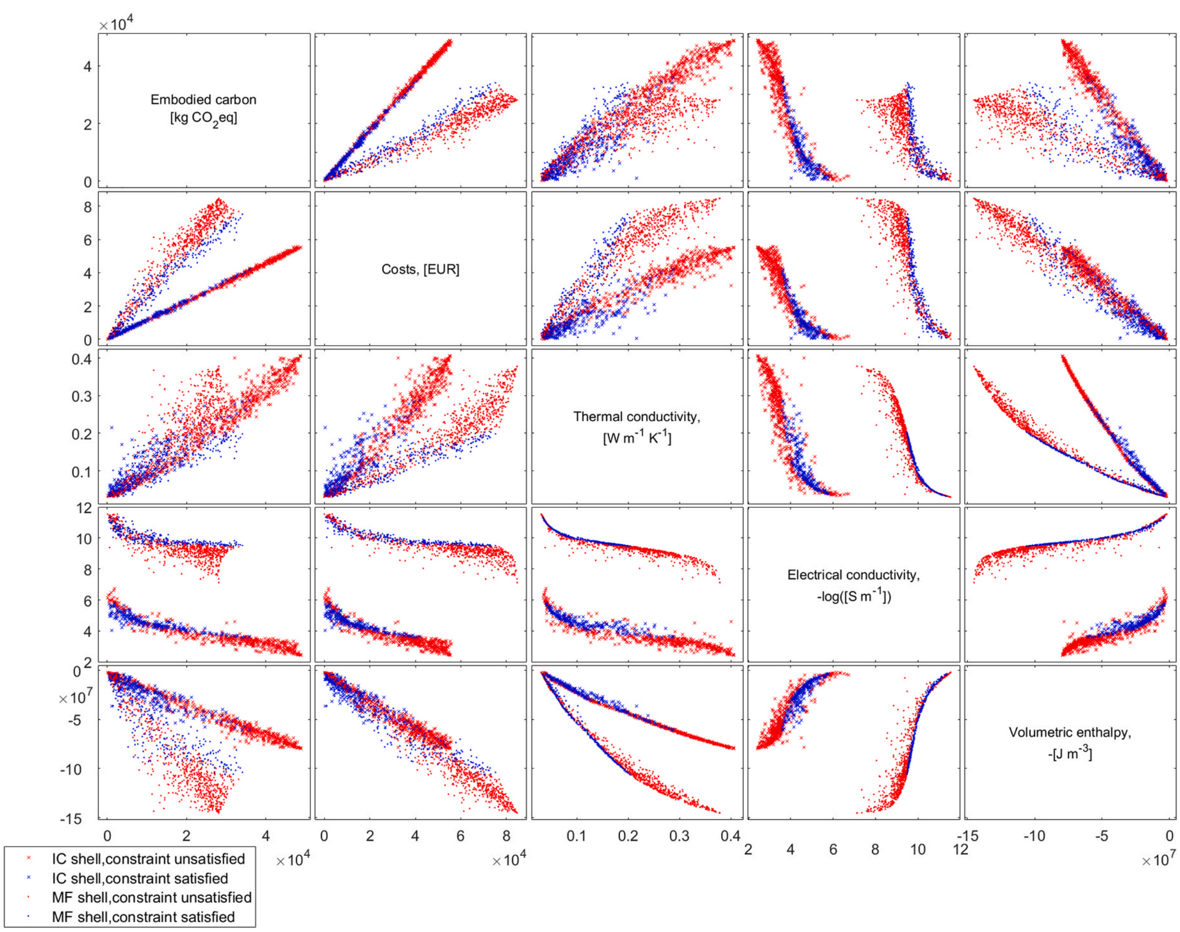

Fig. 10. Two-dimensional projections of five-dimension Pareto frontier. The data points in blue represent the points on the Pareto frontier that satisfy the functional constraint described in Section 4.6 and points in red that do not satisfy this constraint. Solutions with MF shell MPCMs are represented 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. (For interpretation of the references to colour in this figure legend, the reader is referred to the Web version of this article.)

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.

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 optimization 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.

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 optimized 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 (Bauer, 1986), (Wei, 2017). 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. (Cao et al., 2019),), others concluded that the benefits are negligible (e.g. (Khalili et al., 2023),). 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 summarize, 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 optimization on the building level. The general approach would be similar to the dynamic part of this study but the optimization will be performed on building-level objectives instead of material-level ones. This would allow us to optimize the material design in the context of a building, identify building-level trade-offs and provide further guidance for the material development process.

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%–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 optimization 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.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

Some of the data used in the study is confidential and cannot be shared. Non-confidential data can be provided on request.

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Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.dibe.2023.100243.

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