LCA modelling of Cement and Lime-based Construction Materials Systems

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Accepted doctoral thesis by Luciano Sambataro

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Fix your course on a star and you will navigate any storm.
Leonardo da Vinci

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Darmstadt, 14 Mai 2024

Luciano Sambataro

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Rather than coming to an end, the journey is just beginning.

Abstract

Lime-based construction material systems have observed the evolution of mankind throughout the last millennials. Some of them are still present today. They have witnessed humanity's ability to overcome challenges imposed by nature, allowing the development of civilizations across the globe. Today, the world's population has reached unprecedented levels, and mankind has imposed its presence in nearly every corner of the planet. We now face a new challenge. The very same technological advancements that have shaped our culture as we know it today are also threatening our existence by transforming the environment into an unknown landscape.

The consequences of keeping business as usual have already been highlighted as critical by the scientific community. In this context, new methods of providing the goods and services demanded by our societies are necessary. The construction and building industry stands out as one of the most influential sectors in terms of reshaping our environmental footprint. Firstly, construction materials are used in vast quantities worldwide. Secondly, their production requires significant amounts of natural resources and energy. It is estimated that approximately two-thirds of global energy consumption can be attributed to this sector.

This landscape presents new opportunities for developments in sustainable design for construction products. This thesis addresses this issue by proposing the development of technological solutions based on the utilisation of the Life Cycle Assessment (LCA) methodology. The latter serves as a scientifically proven famework for quantifying the potential environmental impacts of products and services. This endeavour is framed within the SUBLime project, a Marie Skodowska-Curie Action European Training NetworkInnovative Training Network (ETN ITN).

The core of this thesis lies in the computational formulation of LCA. This approach serves as a foundational contribution upon which new developments can be added or explored. Indeed, its structure comprises three primary scientific contributions in the form of peer-reviewed papers. These begin with the fundamental computational formulation of LCA and then venture into exploring new applications of LCA, specifically non-linear integration and stochastic analysis.

In recent decades, LCA has been repeatedly used as a reporting tool across a growing number of studies. While this reflects the status quo, the aim of this work is to redefine the use of LCA as a key supporting tool for the design of future materials. To achieve this goal, two critical aspects are examined. Firstly, the integration of material performance in terms of its structural and energy responses to a defined scenario is combined with its environmental performance. This approach enables to systematically analyse and compare different design solutions and material combinations. Results demonstrate that an optimal combination can be identified and future-oriented scenarios can be easily compared, providing a powerful tool at the early stages of design. Secondly, a comprehensive set of environmental benchmarks and an EPD database are developed. Facilitating easy and robust comparison is crucial during product development. Therefore, LCA-based key environmental performance indicators are disclosed in this work. The results not only showed that accuracy, measured in terms of standard deviation, can be improved up to seven times but also provides a reference baseline upon which new studies can be built.

In conclusion, this PhD thesis highlights the potential benefits of repositioning LCA as a design tool rather than merely a reporting one, making it possible to predict the environmental footprint of construction materials throughout their life cycle.

Zusammenfassung

Kalkbasierte Baustoffsysteme haben die Evolution der Menschheit im Laufe der letzten Jahrtausende begleitet. Einige dieser Strukturen sind noch heute auffindbar. Sie haben miterlebt, wie die Menschheit die Herausforderungen von Natur überwunden und somit die Entwicklung von Zivilisationen auf der ganzen Welt ermöglicht. Heutzutage hat die Weltbevölkerung beispiellose Höhen erreicht, und die Menschheit hat ihre Präsenz in nahezu jedem Winkel des Planeten durchgesetzt. Wir stehen nun vor einer neuen Herausforderung. Die gleichen technologischen Fortschritte, die unsere Kultur geformt haben, bedrohen auch unsere Existenz, indem sie die Umwelt in eine unbekannte Landschaft verwandeln.

Die wissenschaftliche Gemeinschaft hat bereits die Konsequenzen hervorgehoben, die mit dem Fortführen des bisherigen Geschäftsgangs einhergehen. In diesem Zusammenhang sind neue Methoden zur Bereitstellung der Waren und Dienstleistungen, die von unseren Gesellschaften gefordert werden, unerlässlich. Die Bau- und Baubranche ragt als einer der einflussreichsten Sektoren hervor, wenn es darum geht, unsere Umweltbilanz neu zu gestalten. Erstens werden Baumaterialien weltweit in enormen Mengen verwendet. Zweitens erfordert ihre Produktion erhebliche Mengen an natürlichen Ressourcen und Energie. Es wird geschätzt, dass etwa zwei Drittel des globalen Energieverbrauchs auf diesen Sektor entfallen.

Dieses Szenario bietet neue Möglichkeiten für Entwicklungen im Bereich nachhaltiges Design für Bauprodukte. Diese Dissertation adressiert diese Thematik, indem sie die Entwicklung von technologischen Lösungen vorschlägt, die auf der Nutzung der Life Cycle Assessment (LCA) Methodik basieren. LCA dient als wissenschaftlich bewährtes Rahmenwerk zur Quantifizierung der potenziellen Umweltauswirkungen von Produkten und Dienstleistungen. Dieses Bestreben ist im Rahmen des SUBLime-Projekts enthalten, einem Marie Skodowska-Curie Action European Training NetworkInnovative Training Network (ETN ITN).

Der Kern dieser Dissertation liegt in der Modellierung der LCA. Dieser Ansatz dient als grundlegender Beitrag, auf den neue Entwicklungen hinzugefügt werden können. Tatsächlich umfasst ihre Struktur drei wesentliche Veröffentlichungen in Form von peer-reviewed Papers. Diese

beginnen mit der grundlegenden Formulierung der LCA und gehen dann dazu über, neue Anwendungen der LCA zu erforschen, insbesondere nichtlineare Integration und stochastische Analyse. In den letzten Jahrzehnten wurde LCA als Berichtsinstrument in einer wachsenden Anzahl von Studien eingesetzt. Während dies den aktuellen Stand widerspiegelt, zielt diese Arbeit darauf ab, die Verwendung von LCA als ein wichtiges unterstützendes Werkzeug für die Gestaltung zukünftiger Materialien neu zu definieren. Um dieses Ziel zu erreichen, werden zwei wesentliche Aspekte untersucht.

Zum einen wird die Integration der Materialeigenschaften in Bezug auf ihre strukturellen und energetischen Leistungen mit ihrer Umweltleistung kombiniert. Dieser Ansatz ermöglicht die systematische Analyse und den Vergleich verschiedener Gestaltungslösungen und Materialkombinationen. Die Ergebnisse zeigen, dass eine optimale Kombination identifiziert werden kann und zukunftsorientierte Szenarien leicht verglichen werden können, was ein leistungsstarkes Werkzeug in den frühen Phasen der Gestaltung bietet.

Zum anderen werden ein umfassender Satz von Umweltvergleichsdaten und eine EPD-Datenbank entwickelt. Eine einfache und robuste Vergleichsmöglichkeit während der Produktentwicklung zu erleichtern, ist entscheidend. Daher werden in dieser Arbeit auf LCA basierende Schlüsselindikatoren für Umweltleistung offenbart. Die Ergebnisse zeigten nicht nur, dass die Genauigkeit, gemessen in Standardabweichungen, um das Siebenfache verbessert werden kann, sondern bieten auch eine Referenzbasis, auf der neue Studien aufgebaut werden können.

AbschlieSSend hebt diese Doktorarbeit das Potenzial hervor, LCA als ein Gestaltungswerkzeug neu zu positionieren, anstatt es nur als Berichtsinstrument zu betrachten. Dadurch wird es möglich, den ökologischen FuSSabdruck von Baustoffen über ihren gesamten Lebenszyklus hinweg vorherzusagen.

Contents

List of abbreviations

Abbreviation	Description
AP	Acidification Potential
CB	Clay Brick
CC	Climate Change
CF	Characterisation Factor
CSB	Calcium Silicate Brick
CV	Coefficient of Variation
DQI	Data Quality Indicator
EP	Eutrophication Potential
EPD	Environmental product declaration
EQ	Ecosystems Quality
ESPA	Enhanced Structural Path Analysis
ET	Ecotoxicity
FU	Functional Unit
GGBFD	Ground Granulated Blast Furnace Slag
GHG	Greenhouse gas
GNR	Getting the Numbers Right
HH	Human Health
HT-Cancer	Human Toxicity: Carcinogenic
HT-NonCancer	Human Toxicity: Non-Carcinogenic
HVAC	Heating Ventilation and Air Conditioning
IC	Impact Category
IR	Ionizing Radiation
KEPI	Key Environmental Performance Indicator

Abbreviation	Description
LCA	Life Cycle Assessment
LCC	Life Cycle Costing
LCI	Life Cycle Inventory
LCIA	Life Cycle Impact Assessment
LCSA	Life Cycle Social Assessment
LO	Land Occupation
ME	Mineral Extraction
MEF	Material Embodied Footprint
MIC	Mineral Component
MMD	Metals & Minerals Depletion
MRP	Mortar Renders & Plasters
NRE	Non Renewables Energy
ODP	Ozone Layer Depletion Potential
OE	Operational Energy
PCR	Product category rule
PDF	Probability Density Function
PM	Particular Matter
POCP	Photochemical Oxidation Potential
RA	Resource Availability
RI	Respiratory Inorganics
SCOP	Seasonal Coefficient of Performance
SLCA	Sustainability Life Cycle Assessment
SS	Single Score
TAP	Terrestrial Acidification Potential
TETP	Terrestrial Ecotoxicity Potential
UNFCCC	United Nations Framework Convention on Climate Change
WD	Water Deprivation
XML	Extensible Markup Language

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1 Introduction

1.1 Research background

Planet Earth is transgressing high-risk zones in most of the fundamental processes that are critical for maintaining stability and resilience on our planet due to human-related environmental forcing [1]. Despite the widespread attention given to climate change in recent years, other categories like biosphere loss, biogeochemical cycles, land system change, and freshwater change have been recognised as crucial [2]. Manufacturing, construction, and energy use in building sectors collectively represent around 30 % of global greenhouse gas (GHG) emissions [3]. Moreover, the industry and building sectors together made up 2/3 of global energy consumption in 2023, namely 320 EJ [4]. The latter being dominated by heating of buildings. Notably, the cement industry alone accounts for nearly 7 % of total GHG emissions worldwide [5]. However, it is also the world's second-most-used substance after water, which allows for cost-effective and energy-efficient infrastructure developments [6].

In the political context, Europe has recently introduced state-of-the art legislation aiming to shift the business as usual production philosophy to a sustainable one. The European Green Deal has set an ambitious target to reach climate neutrality as a continent by 2050 [7] and was written into law by the European Climate Law [8]. In addition, the circular economy action plan [9] and the environment action programme to 2030 [10] introduced the framework for sustainable production and consumption, focusing on resource use efficiency and protecting and restoring biodiversity, respectively, among other goals. Complementary to the legislation, EU has committed to mobilise at least 1 trillion of investments between 2020 and 2030 to support a just and green transition under the European Green Deal Investment Plan [11].

Despite the evident environmental crisis we are currently confronting, along with the legislation enacted to promote sustainable practices and developments, a significant barrier remains. While manufacturers are compelled to establish climate-related targets and adhere to carbon taxes under the European trading system, consumer adoption of these practices lags far behind implementation.

Environmental product declarations (EPDs) have emerged as an environmental passport for products and have gained significant traction, particularly within the construction sector. These reports are created using the Life Cycle Assessment (LCA) methodology and fall under the category of Type III eco-labels according to ISO 14025 [12]. They serve as a fundamental communication tool for both business-to-business and business-to-consumer interactions, providing comprehensive LCA-based environmental impact indicators that encompass a product's complete environmental footprint. Despite the increasing number of EPDs being published, there remains a gap concerning their practical utilisation.

First, comparing different EPDs proves challenging due to a lack of transparency in the disclosed information, often linked to confidentiality concerns. Results are presented deterministically, diminishing their reliability. Furthermore, although the product category rules (PCRs) set the conditions and rules for the calculation of a specific group of products, there is still room for interpretation, particularly when modelling downstream processes and activities. For instance, the relationship between insulation products and their later non-linear performance regarding operational energy consumption in buildings is usually disregarded. Secondly, the absence of a standardised and well-established framework for their application is a notable issue. While certain labels, such as BREEAM, incorporate scoring systems for products containing EPDs, there remains substantial room for improvement regarding the consumer-oriented utilisation of them. Designers and contractors, as key stakeholders, have yet to significantly engage with these types of reports. Finally, the current approach to EPD generation is often post-hoc, meaning that EPDs are a consequence of manufacturing practices rather than a deliberate target. The primary limitation lies in effectively integrating production practices and key operating parameters with LCA-based expected environmental performance scores.

In conclusion, there is a noticeable gap in the development of industry-specific tools that facilitate comprehensive calculation and communication of the associated environmental impacts of construction products. Addressing this gap requires the integration of such tools into current research and development practices, thereby shifting the traditional approach towards sustainable design and management.

1.2 Research objectives

This research aims to bridge the gap between LCA modelling and construction material production and design practices. This is achieved by developing a novel LCA-based tool that covers life cycle inventory (LCI) management, life cycle impact assessment (LCIA) calculation, integrated non-linear energy consumption modelling, and stochastic LCA modelling. Figure 1.1 shows the three main pillars followed in this research to accomplish the intended results.

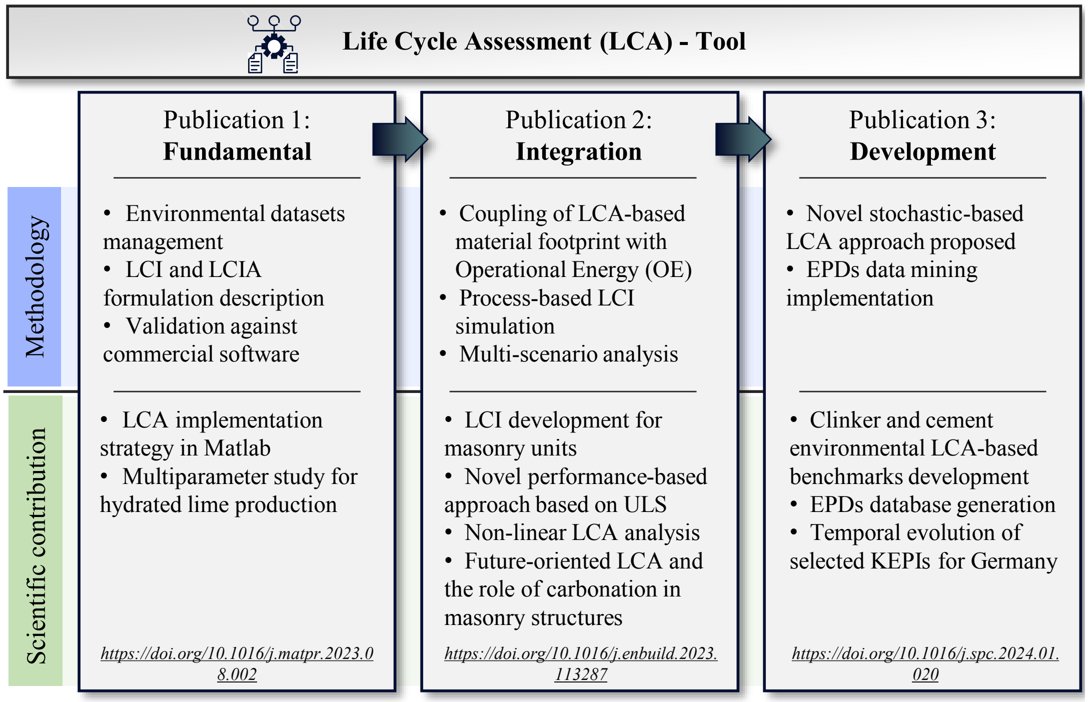

Figure 1.1: LCA-based tool development for the cement and lime industry.

The specific research objectives can be listed as follows:

1. To develop a novel LCA-based Tool for the environmental impact assessment of construction products.

2. To expand current LCA Framework in order to consider non-linear behaviour, stochastic analysis, time discretization and use phase simulation.

3. To apply the developed framework to produce a reference environmental benchmark for the cement and lime market.

4. To develop a process-based LCI for lime-based construction systems

1.3 Research scope

1.4 Outline

This dissertation is presented as a cumulative document comprising three publications. Figure 1.2 shows its structure along with the main contents of each chapter. The first one introduces the research background together with the specific research objectives and scope definitions. Then, the state of the art is presented in Chapter 2, providing fundamental knowledge about life cycle assessment modelling. Chapter 3 follows with the three peer-reviewed publications, namely:

Publication 1:

Title: Life cycle assessment modelling in Octave/Matlab: Hydrated lime manufacturing case study [13]

Journal: Materials Today: Proceedings

DOI: *https://doi.org/10.1016/j.matpr.2023.08.002*

Publication 2:

Title: A performance-based approach for coupling cradle-to-use LCA with operational energy simulation for Calcium Silicate and Clay Bricks in masonry buildings [5]

Journal: Energy & Buildings

DOI: *https://doi.org/10.1016/j.enbuild.2023.113287*

Publication 3:

Title: Environmental benchmarks for the European cement industry [14]

Journal: Sustainable Production and Consumption

DOI: *https://doi.org/10.1016/j.spc.2024.01.020*

Finally, Chapter 4 provides a comprehensive summary of the main findings and significant contributions of this research. Moreover, it delineates specific directions for future investigations, guiding subsequent research endeavours.

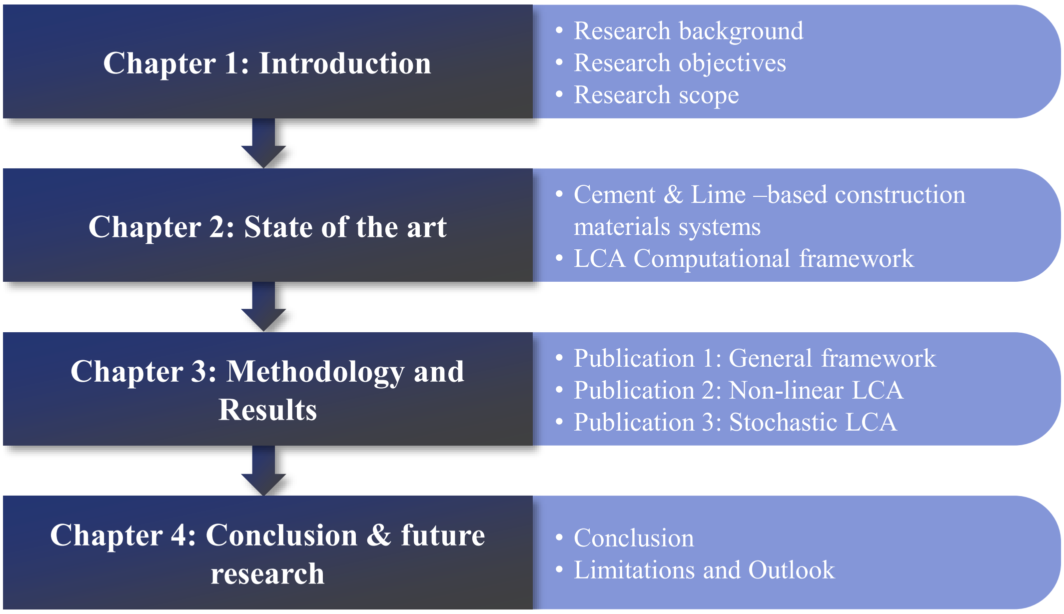

Figure 1.2: Dissertation outline

2 State of the art

2.1 Cement and Lime-based construction materials systems

2.1.1 Manufacturing and applications

Lime and cement stand as two of the most utilized construction materials worldwide. Their cost-effectiveness and versatility offer a wide range of possibilities in terms of applications and uses. Lime, with its historical significance, has been employed by various civilizations for thousands of years, dating back to its use 12,000 years ago [15]. Portland cement, as recognized in modern construction, was developed between 1824 and 1845 by Joseph Aspadin and Isaac Johnson, who obtained its precursor, the clinker [16].

Today, around 430 million tonnes and 4.6 billion tonnes of lime and cement are produced worldwide annually, respectively [6, 17, 18].

Lime

The manufacturing of lime involves six main steps, as outlined in Laveglia et al. [19], starting from the mineral extraction of limestone ($CaCO_3$) and proceeding through calcination, during which free lime (CaO) is obtained and CO_2 is released. Furthermore, lime can be slaked to produce hydrated lime ($Ca(OH)_2$). A representation of the system flow along with the mass balance is illustrated in the first publication in Fig. 3.1 [13]. Lime's versatility enables a wide range of applications, spanning from iron and steel production to soil neutralisation in agriculture. The construction sector represents 18% of the total European market share [20]. Its uses include the manufacturing of construction materials, bonding agents, fillers, and soil stabilisation agents.

Cement

Cement production follows a similar process to lime manufacturing, with the main differences lying in the addition of other types of raw materials alongside limestone, which introduce sources of silicon, aluminium, and iron [21]. The calcination of the raw meal, reaching temperatures up to 1450žC, facilitates the formation of clinker [22]. The resulting clinker can then be blended with various types of mineral additives to create a wide range of cement formulations.ăA representative system flow of cement manufacturing is illustrated in Fig. 2.1.

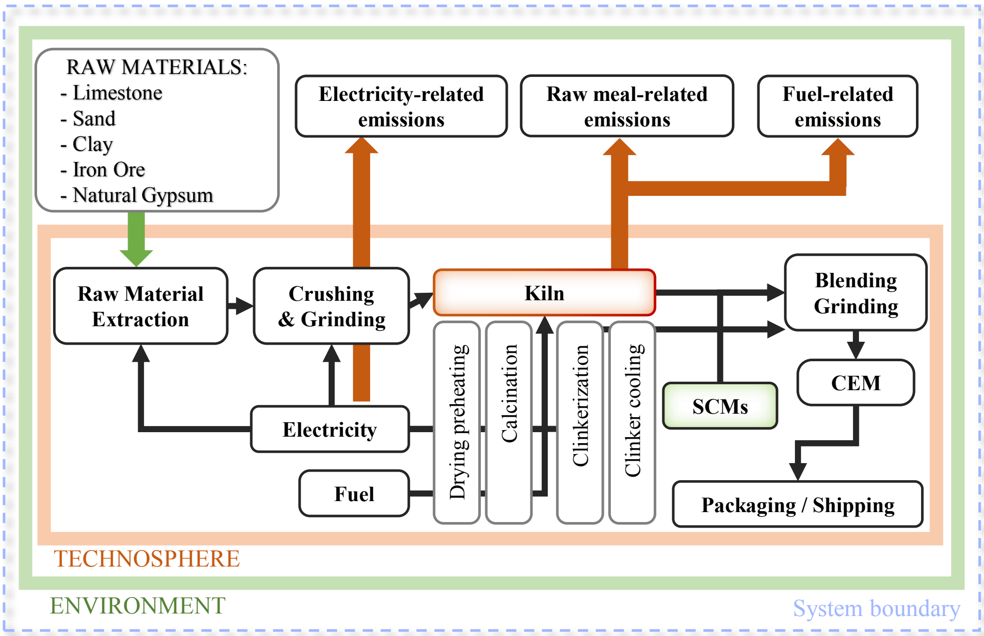

Figure 2.1: Cement manufacturing system flow, adapted from [21–23]

Cement is primarily used in the production of concrete, typically constituting 12% of the entire concrete mix [21]. However, its use extends to other construction materials such as mortars, renders, masonry units, among others.

Cement and lime-based construction materials systems

The current thesis is conducted within the framework of the SUBLime ITN-ETN project [1], which aims to investigate enhanced pathways of sustainable use of lime in the construction sector. To this end, the scope of this work extends to the following materials:

- Lime and hydrated lime
- Cement
- Clay masonry units
- Calcium-silicate masonry units
- Cement and lime-based mortars, renders and plasters

Typical compositions and manufacturing processes included during the analysis of the different publications in chapter 3 are addressed accordingly.

2.1.2 Environmental impact

As highlighted by numerous authors, the cement industry contributes to over 6% of GHG emissions [6, 24–26]. This can be attributed primarily to two factors: the substantial annual consumption of cement and the calcination process, as discussed before. However, these emissions may only be the tip of the iceberg, as the lime and cement industry is also associated with other environmental burdens. For instance, Li et al. [27] demonstrated that potential acidification in China, primarily driven by the use of hard coal as fuel, is as significant as global warming potential. Additionally, issues such as photochemical smog formation and eutrophication must also be considered. Interestingly, while GHG emissions contribute to global phenomena like climate change, other burdens tend to have a more localised or regional impact, predominantly affecting the surroundings of the emitting plant.

To comprehensively analyse a material's environmental footprint, the LCA methodology must be applied [28]. This allows for scientific quantification of all related environmental burdens associated with a product's process flow. A recent literature review conducted by Dahanni et al. [29] compared various LCA studies on cement manufacturing over the past decade. The authors highlighted the need to enhance the relationship between cement's performance and the LCA modelling. Indeed, this concept extends to any construction material, where design parameters

[1] https://sublime-etn.eu/

will impact not only in the environmental performance but also the product's mechanical and physico-chemical performance.

2.2 LCA: Fundamental

2.2.1 History and developments

Life Cycle Assessment (LCA) is a tool that assess the potential environmental impacts and resources used throughout a product's life cycle [30]. It's development can be tracked back to 1970, when the methodological foundation for environmentally extended input-output analysis was first introduced by Leontief [31]. Since them, numerous developments and milestones were achieved. The methodology shifted from a public-oriented concerns assessment tool, to become a harmonised science-based methodology, with the ability to model complex flows between processes [32]. Fig. 2.2 encompasses the main events that forged LCA to the methodology known today.

Methodological developments

From a methodological point of view, it can be seen that the frameworks regarding impact assessment methods were developed during the 1990s. The first introduced mid-point impact methodology was the CML92 method developed by the Institute of Environmental Sciences at Leiden University in the Netherlands [33]. Here, the authors introduced many of the environmental indicators being used today. The main goal was to shift from the traditional public-concern-oriented analysis towards independent environmental impact quantification, thus avoiding burden shifting [32]. In parallel, end-point impact methods like the Eco-indicator 99 [34] and the EPS method [35] were developed, focusing on the potential damage to ecosystems and human health rather than on the mid-point mechanistic impact.

During the first decade of the 2000s, the majority of LCA studies were attributional in nature. This means that the primary objective was to analyse the environmental performance of a specific product throughout its lifecycle without considering its impact on alternative markets. However, some researchers did focus on the latter issue, particularly concerning recycling and waste management [36, 37]. As emission modelling became more complex, two new branches emerged during the 2000s. On one hand, spatially differentiated inventories and impact methods were developed by Hauschild and Potting [38] and further investigated by Mutel and Hellweg [39]. On the other hand, time-dependent LCIA was developed, with significant contributions made by

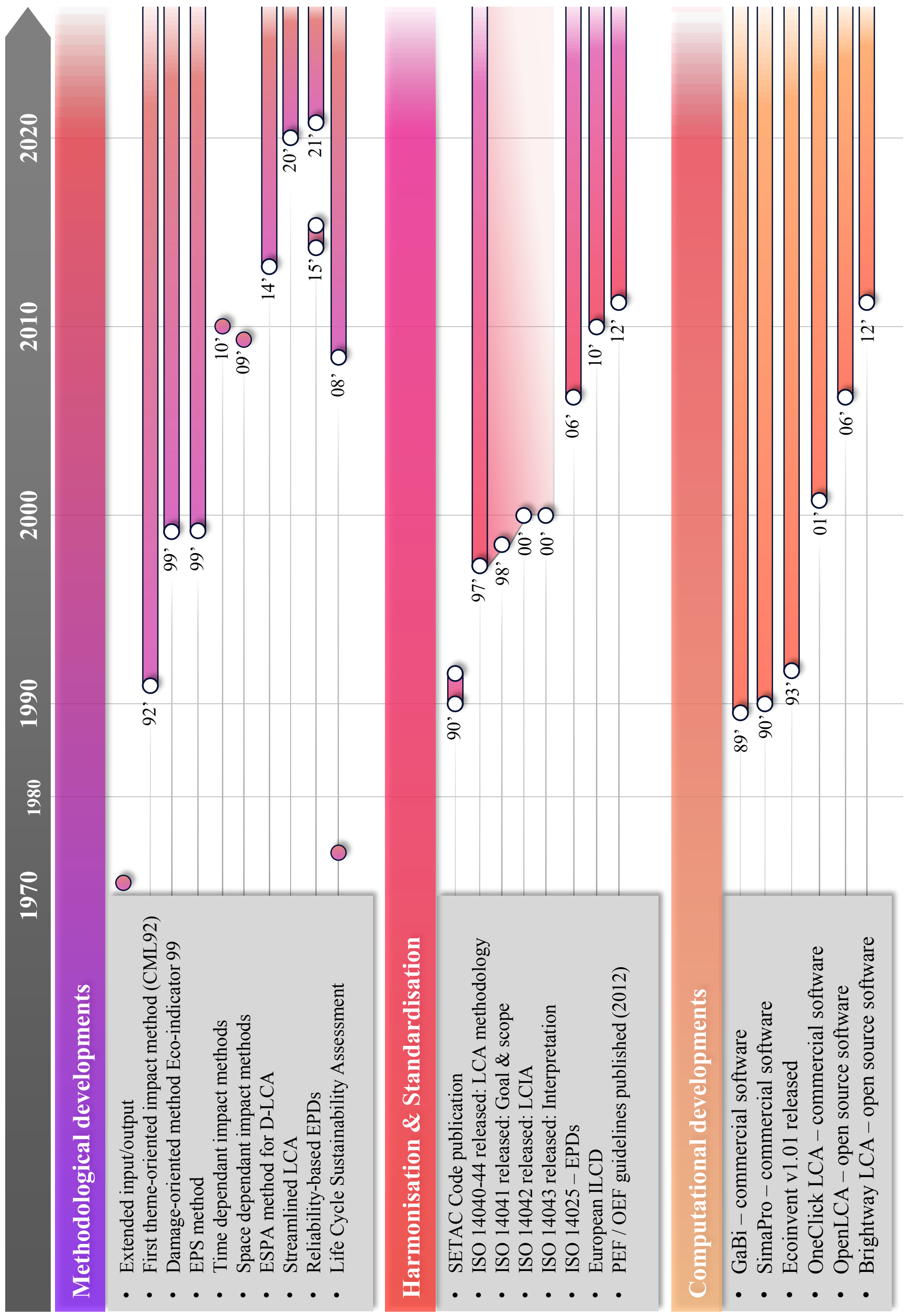

Figure 2.2: LCA milestones and developments. Adapted and expanded from [32]

Levasseur et al. [40]. These methods will continue to expand, as will be discussed later. Although stochastic-LCA analysis constitutes an entire branch that will be addressed in a later section of this chapter, its utilisation for disseminating results in the form of products' carbon footprints, or EPDs, as proposed by Henriksson et al. [41], Gregory et al. [42], and AzariJafari et al. [43], can be highlighted as a significant contribution.

In recent years, the term Sustainability Life Cycle Assessment (SLCA) has garnered attention. Its fundamental formulation, shown in Eq. 2.1, was introduced by Kloepffer [44]. The core concept is that sustainability can be assessed by integrating the economic and social dimensions alongside the traditional environmental aspects. Life Cycle Costing (LCC) and Life Cycle Social Assessment (LCSA) aim to encompass both the product's life cycle cost and its associated social impacts, respectively.

$$SLCA = LCA + LCC + LCSA \tag{2.1}$$

However, this notion of sustainability assessment can be tracked back to 1974, when Holdren and Ehrlich [45] introduced the famous IPAT equation:

$$I = P \cdot A \cdot T \tag{2.2}$$

Where **I** denotes the environmental impact, **P**, **A**, and **T** the number of people, their material affluence, and the technology intensity, respectively.

Standardisation

Looking into harmonisation and standardisation, the first official LCA code of practice was introduced in 1993 [46], following several technical events starting in 1990 [32]. This initial code of practice primarily focused on methodological guidelines for the inventory and impact assessment phases. Subsequently, the ISO standards family was introduced with the release of the 14040-44 series [28]. These standards provide a comprehensive framework that includes a dedicated volume for each of the four main phases in an LCA, namely:

i) Goal and scope definition

ii) Inventory

iii) Impact assessment

iv) Interpretation of results

Additionally, key terms such as functional unit (FU) and system boundary were defined. The complete ISO family concerning environmental management extends beyond LCA, covering eco-design (ISO 14062), greenhouse gas reporting (ISO 14064), and communication of environmental performance (ISO 14020, ISO 14025) [32]. The latter establishes the framework for the generation of EPDs. These reports have gained significant traction in the construction and building sector. Based on the international standard EN-15804 [47], LCA applied to construction materials is required to disclose their environmental impact according to the lifecycle phases shown in Figure 2.3. Due to the fact that a building's use phase typically spans over 50 years, the disclosure of impacts associated with stages B1 to B5 are usually based on steady-state projections, which represents one of the shortcomings of traditional LCA, as will be discussed in section 2.3.

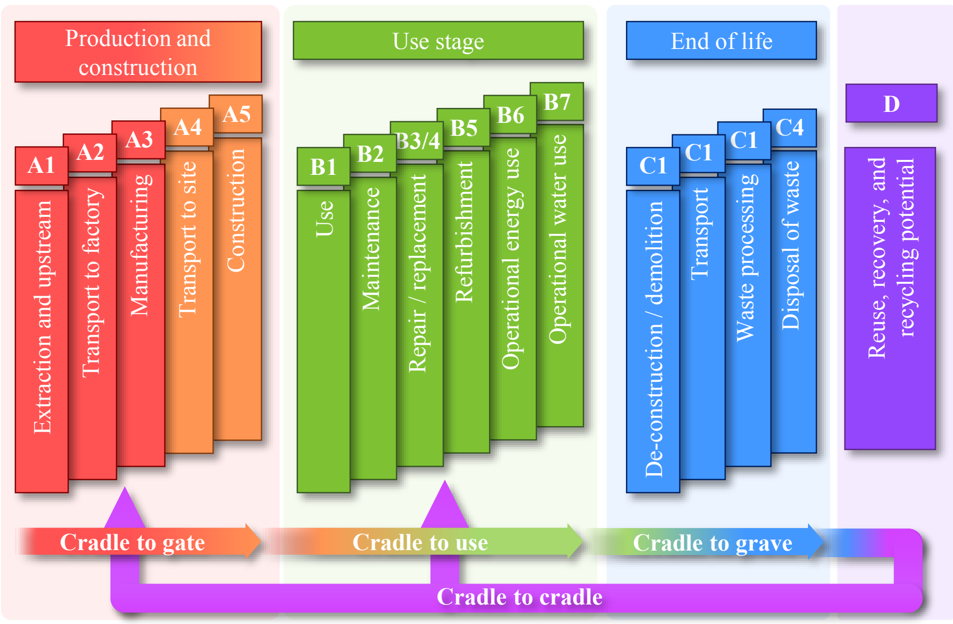

Figure 2.3: LCA stages definition according to EN-15804 Standard [47]

At the European level, a significant milestone was reached with the introduction of the European ILCD guideline [48] . This guideline aimed to address many of the methodological choices left open by the ISO standard, with the goal of achieving harmonisation and increased comparability among LCA studies. The ILCD guideline served as a foundation for the subsequent development of the Product Environmental Footprint (PEF) and Organisational Environmental Footprint (OEF) guidelines, launched by the EU Commission.

Computational developments

The LCA computational ecosystem began to take shape in the 1990s with the development and release of two commercial software programmes: GaBi and Simapro. These tools are now firmly established and widely used by companies and researchers. A few years later, the Ecoinvent v1.01 database was launched. Today, it stands as one of the largest LCA databases, with over 14,000 activities in its current version 3.10. In 2001, a new commercial LCA software specifically tailored for the construction industry was released. OneClick LCA has become widely recognised as the leading tool for producing EPDs in the construction products sector. In addition, two open-source software programmes were released in 2006 and 2012, namely OpenLCA and Brightway [49]. The first follows the traditional software structure, providing practitioners with a user interface (UI) for conducting comprehensive LCAs. On the other hand, Brightway, based on the Python programming language, is designed to offer a powerful tool for practitioners seeking flexibility in LCA analyses. This software is particularly appealing to researchers as it allows for the adaptation of LCA to new developments in a highly customisable manner.

2.2.2 Mathematical structure

The LCA mathematical structure was first introduced by Heijungs [50] in 1994 and later on formalized by Heijungs and Suh [51] in 2002. The matrix formulation is based on the concept that each process can be vectorized by describing its economic and environmental entities [50], as follows:

$$\begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} a_1 \\ \dots \\ a_r \\ b_1 \\ \dots \\ b_s \end{pmatrix} \tag{2.3}$$

Where a stands for any economic process such as raw materials, energy, and products, and b represents environmental flows like resources or emissions. They can be either inputs or outputs, with the general consensus being to display negatives for the former and positives for the latter [51]. When expanding this concept to the entire process tree, composed of n upstream activities, a production matrix can be written as:

$$\begin{pmatrix} A \\ B \end{pmatrix} = \begin{pmatrix} a_{11} & \dots & a_{1i} & \dots & a_{1n} \\ \vdots & \ddots & \vdots & \ddots & \vdots \\ a_{r1} & \dots & a_{ri} & \dots & a_{rn} \\ b_{11} & \dots & b_{1i} & \dots & b_{1n} \\ \vdots & \ddots & \vdots & \ddots & \vdots \\ b_{s1} & \dots & b_{si} & \dots & b_{sn} \end{pmatrix} \tag{2.4}$$

Where the new subscript denotes the ith upstream process and **A** and **B** are known as technology matrix and intervention or environmental matrix, respectively. Given a specific demand vector f, which depends on the functional unit (FU) analysed, the technology-related system can be linearly written as:

$$A \times s = f \implies s = A^{-1} \times f, \tag{2.5}$$

Where s represents the scaling vector needed to produce the demanded FU. Moreover, the associated environmental entities can be determined by:

$$g = B \times s, \tag{2.6}$$

Given space to the environmental vector g, which contains the LCI solution. The information contained in g can then be transformed into environmental impact-related scores by means of characterization factors. The latter are dependent on the impact method used. The final impact indicators can be obtained by:

$$h = C \times g, \tag{2.7}$$

Where **C** is the characterisation factors matrix and h the impact scores vector.

2.2.3 Information architecture

One of the primary challenges when modelling LCA is handling numerous interconnected processes, resulting in matrices containing thousands of rows by hundreds of columns, as illustrated in Eq. 2.4. To address this issue, ISO 14048 [52] outlines the requirements for data documentation, which serve as the foundation for the ILCD and ecoSpold formats. These formats are based on Extensible Markup Language (XML) and are widely adopted today by most LCA software providers and databases, such as Ecoinvent v3 [2], Brightway [3], and SimaPro [4].

The LCI structure can be arranged for each process activity related to the technosphere and environment, where intermediate exchanges and elementary flows are organised, respectively. Collectively, they constitute the fundamental modelling block known as the unit process (UPR). This UPR serves as a representation of any human activity, capturing the balance between exchanges with the environment and other activities. Fig. 2.4 illustrates the definition of the UPR, depicting the inputs and outputs expected from the environment and technosphere, respectively. For each activity, represented by a UPR, information is stored and structured in the fields shown in Fig. 2.5. From a modelling perspective, understanding this arrangement is crucial to accessing the necessary information and being able to shape it accordingly to one's research goal. Within each activity's subfield, various types of information can be accessed through node extraction. The basic syntax for achieving this is provided in the Section 5.1 of this thesis.

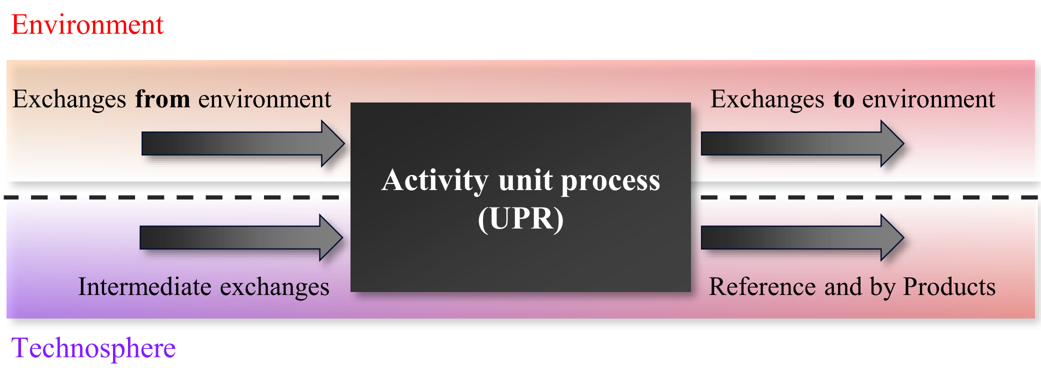

Figure 2.4: Unit process definition

[2]https://ecoinvent.org/
[3]https://docs.brightway.dev/en/latest/
[4]https://simapro.com/

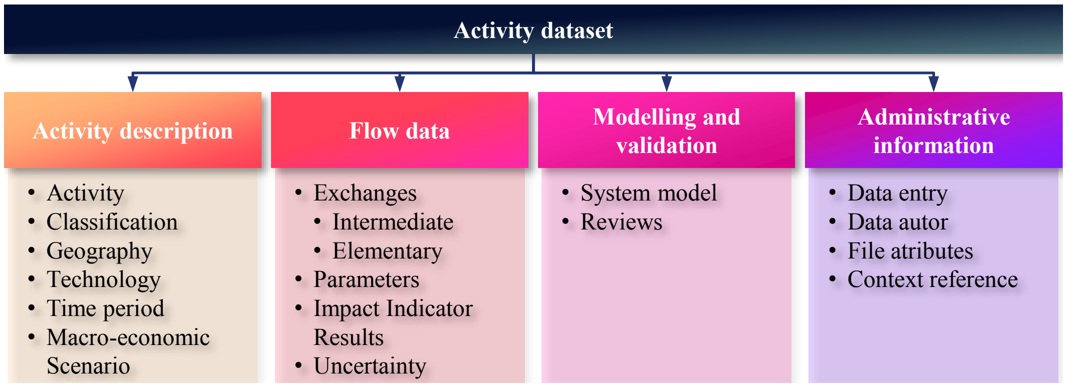

Figure 2.5: Data architecture at activity level: EcoSpold 2 format

Tecnoshpere

The term technosphere is used to describe any exchange related to human activities. These are defined as intermediate exchanges. While a specific activity will have a characterising name, represented by a <*@activityNameId*>, it is only after specifiyng the geography, time coverage, type of activity and system model used, that it becomes unique, obtaining an <*@activityIndexEntryId*>. This information corresponds to the first box in Fig. 2.5. Each of these distinct UPRs will in turn hold the information for all the upstream activities comprising the process tree mentioned in Eq. 2.4, by specifying intermediate exchanges under the flow data information.

Given a text file containing all the different activities in an environmental database (e.g., Ecoinvent v3.9), it is possible to search for a specific activity name and compile the results. Table 2.1 displays the different types of entries found for the activity *clinker production*. It can be observed that the same activity linked to different geographies represents a new type of entry. By accessing the combination of *"clinker production"* and *"Europe without Switzerland"* with the corresponding *Id*, it is possible to compile key dataset information, obtaining the details shown in Table 2.2. For sake of readability, both the *"intermediateExchangeId"* and the *"activityLingId"* are not displayed completely. Once the information is gathered, parameters can be easily adjusted to affect specific portions of the dataset, such as the raw materials used for clinker manufacturing. The code syntax needed to compile Table 2.2 is given in the Section 5.1.

Table 2.1: Activity structure example for clinker production

EntryId	Activity	ActivityId	Geography	GeoId
'3b83869a-...'	'clinker production'	"919cdfc8-..."	"CH"	"131278d6-..."
'b3714f88-...'	'clinker production'	"919cdfc8-..."	"CO"	"0cc6c45a-..."
'4a989885-...'	'clinker production'	"919cdfc8-..."	"US"	"13d387f6-..."
'054aa0c5-...'	'clinker production'	"919cdfc8-..."	"Europe without Switzerland"	"f9221622-..."
'0aa58e82-...'	'clinker production'	"919cdfc8-..."	"IN"	"0e6a7860-..."
'a79a3c73-...'	'clinker production'	"919cdfc8-..."	"ZA"	"12b21766-..."
'5fbc0ca8-...'	'clinker production'	"919cdfc8-..."	"PE"	"11387d6c-..."
'6fbf4404-...'	'clinker production'	"919cdfc8-..."	"CA-QC"	"868a66d1-..."
'd41dbe4d-...'	'clinker production'	"919cdfc8-..."	"BR"	"0a2c8c66-..."
'fce53f4e-...'	'clinker production'	"919cdfc8-..."	"RoW"	"7846b897-..."

Environment

Analogue to the technosphere information, the environmental intervention associated with a specific UPR is represented by *"elementary exchanges"*. These are classified in different ecosystems, defined as compartments and sub-compartments, as illustrated in Fig 2.6. According to Eq. 2.7, each specific elementary exchange will have an associated characterization factor. The latter will depend on the impact category under study and the sub-compartment classification of the elementary exchange. Applying the same concept as for the technology matrix, Table 2.3 presents key information regarding the elementary exchanges included in the clinker production dataset. It is worth stressing out that only the elementary exchanges consumed or emitted by the current UPR will be displayed. Exchanges related to the upstream activities are included in the parent activities. The syntax for generating Table 2.3 is presented in the Section 5.1.

Table 2.2: Key technosphere-related information compiled from clinker production activity in Europe

intermediateExchangeId	activityLinkId	name	amount	unitName	meanValue	mu	variance	Var_Pedigree
06b8d05b	2b2f21c9	ammonia, anhydrous, liquid	0.00090797	kg	0.000908	-7	0.01	0.0526
6e6b1247	3197dc09	bauxite	0.00012	kg	0.00012	-9.03	0.01	0.0526
0ae050ad	bb11eb0c	calcareous marl	0.46598393	kg	0.466	-0.76	0.01	0.0526
c08228bd	894541bb	cement factory	6.27E-12	unit	6.27E-12	-25.8	0.31	0.3526
e89b4064	c83bc239	clay	0.33098859	kg	0.331	-1.11	0.01	0.0526
b0f4c2fb	d43a967d	diesel, burned in building machine	0.01339954	MJ	0.0134	-4.31	0.01	0.0526
759b89bd	7a90d6ab	electricity, medium voltage	0.057998	kWh	0.058	-2.85	0.01	0.0526
0d3eda5a	6cb5d53a	hard coal	0.01565934	kg	0.0354	-3.34	0.01	0.0526
0d3eda5a	b067d1ad	hard coal	0.01973944	kg	0.0354	-3.34	0.01	0.0526
2966d161	e4681009	heavy fuel oil	0.02549912	kg	0.0255	-3.67	0.01	0.0526
4cc87eb6	fc2a2efb	industrial machine, heavy, unspecified	3.76E-05	kg	3.76E-05	-10.19	0.32	0.372
240c1a3c	fa5379a2	inert waste, for final disposal	-8.00E-05	kg	8.00E-05	-9.43	0.01	0.0126
b89dadb0	5675f213	light fuel oil	0.00037399	kg	0.000374	-7.89	0.01	0.0526
a00b7e35	1256ecaf	lime	0.840971	kg	0.841	-0.17	0.01	0.0526
e40cb987	e93948cf	lime, hydrated, loose weight	0.00391986	kg	0.00392	-5.54	0.01	0.0526
ea75b944	ba8ea029	lubricating oil	4.71E-05	kg	4.71E-05	-9.96	0.01	0.0526
9e36204d	94cd29a9	meat and bone meal	0.00960967	kg	0.00961	-4.645	0.01	0.062
27da8130	7924af82	municipal solid waste	-4.50E-05	kg	4.50E-05	-10.01	0.01	0.0126
a9007f10	c464302e	natural gas, high pressure	0.00017461	m3	0.00017462	-4.99	0.01	0.0526
eb6b5a9a	697b8cc6	petroleum coke	0.00390987	kg	0.00391	-5.54	0.01	0.0526
17c72eaf	bb505a72	refractory, basic, packed	0.00018999	kg	0.00019	-8.57	0.01	0.0526
d3e019ee	2cab1d74	refractory, fireclay, packed	8.21E-05	kg	8.21E-05	-9.41	0.01	0.0526
b230aa6e	a7b5b4a3	refractory, high aluminium oxide, packed	0.000137	kg	0.000137	-8.9	0.01	0.0526
f51d7ccf	cab96c7a	sand	0.00925968	kg	0.00926	-4.68	0.01	0.0526
c5246dbb	adeafd64	steel, chromium steel 18/8, hot rolled	5.86E-05	kg	5.86E-05	-9.74	0.01	0.0526
c5adb1fb	c3fda02d	tap water	0.33998828	kg	0.34	-1.08	0.01	0.0526

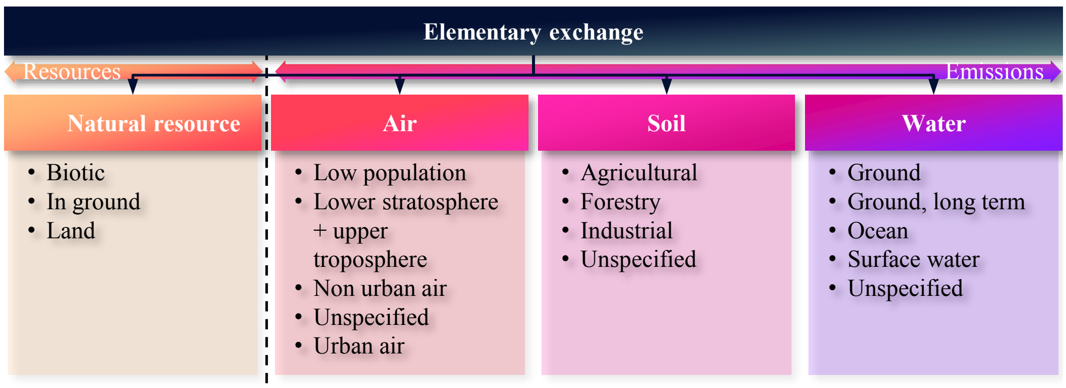

Figure 2.6: Elementary exchange data structure

2.3 LCA: Dynamic

The term Dynamic Life Cycle Assessment (DLCA) has been broadly used by different researchers to address the effect of time on traditional LCA studies. In general terms, the methodological

Table 2.3: Key environment-related information compiled from clinker production activity in Europe

intermediateExchangeId	name	compartment	subcompartment	amount	unitName	meanValue	mu	variance	VarPedigree
709dd019	Antimony ion	air	unspecified	2.00E-09	kg	2.00E-09	-20.03	0.66	0.7026
f03eada0	Arsenic ion	air	unspecified	1.20E-08	kg	1.20E-08	-18.24	0.05	0.0926
5db3ff71	Beryllium II	air	unspecified	3.00E-09	kg	3.00E-09	-19.62	0.05	0.0926
9aef1c4c	Cadmium II	air	unspecified	7.00E-09	kg	7.00E-09	-18.78	0.05	0.0926
4523bfdd	Carbon dioxide, fossil	air	unspecified	0.83897107	kg	0.839	-0.18	0.01	0.0526
5bf52322	Carbon dioxide, non-fossil	air	unspecified	0.01509948	kg	0.0151	-4.19	0.01	0.0526
4e3e6c7a	Carbon monoxide, fossil	air	unspecified	0.00047198	kg	0.000472	-7.66	0.13	0.1726
04677f10	Chromium III	air	unspecified	1.45E-09	kg	1.45E-09	-20.35	0.05	0.0926
32fe4d6d	Chromium VI	air	unspecified	5.50E-10	kg	5.50E-10	-21.32	0.05	0.0926
e14f6030	Cobalt II	air	unspecified	4.00E-09	kg	4.00E-09	-19.34	0.05	0.0926
c04f3788	Copper ion	air	unspecified	1.40E-08	kg	1.40E-08	-18.08	0.05	0.0926
0e7cbbd2	Dioxins,	air	unspecified	9.60E-13	kg	9.60E-13	-27.67	0.13	0.1726
62741a50	Hydrochloric acid	air	unspecified	6.31E-06	kg	6.31E-06	-11.97	0.05	0.0926
12eed8f8	Lead II	air	unspecified	8.50E-08	kg	8.50E-08	-16.28	0.66	0.7026
e81f954a	Mercury II	air	unspecified	3.30E-08	kg	3.30E-08	-17.23	0.05	0.0926
f72092ae	Methane, fossil	air	unspecified	8.88E-06	kg	8.88E-06	-11.63	0.13	0.1726
5cc8e1ac	NMVOC	air	unspecified	5.64E-05	kg	5.64E-05	-9.78	0.13	0.1726
e8a5fcb9	Nickel II	air	unspecified	5.00E-09	kg	5.00E-09	-19.11	0.05	0.0926
9559d1ca	Nitrogen oxides	air	unspecified	0.00107996	kg	0.00108	-6.83	0.05	0.0926
99e7c575	Particulate Matter, <2.5 um	air	non-urban...	2.41E-05	kg	2.41E-05	-10.63	0.31	0.3526
23798dba	Particulate Matter, >10 um	air	non-urban...	5.66E-06	kg	5.66E-06	-12.08	0.05	0.0926
6cf0a90a	Particulate Matter, >2.5 um and <10um	air	non-urban...	7.92E-06	kg	7.92E-06	-11.75	0.13	0.1726
bd4a4115	Selenium IV	air	unspecified	2.00E-09	kg	2.00E-09	-20.03	0.66	0.7026
50f9b0f6	Sulfur dioxide	air	unspecified	0.00035499	kg	0.000355	-7.94	0.05	0.0926
e79fd2ea	Thallium I	air	unspecified	1.30E-08	kg	1.30E-08	-18.16	0.05	0.0926
ecb0afdc	Tin ion	air	unspecified	9.00E-09	kg	9.00E-09	-18.53	0.66	0.7026
920e06e6	Vanadium V	air	unspecified	5.00E-09	kg	5.00E-09	-19.11	0.05	0.0926
efda1427	Water	air	unspecified	0.00029399	m3	0.000294	-8.32	0.04	0.0807
c4790ccb	Zinc II	air	unspecified	6.00E-08	kg	6.00E-08	-16.63	0.05	0.0926
c8a4915e	Water	water	unspecified	0.00166594	m3	0.001666	-6.59	0.04	0.0807
3b96bc04	Water, unspecified natural origin	natural resource	in water	0.00161994	m3	0.00162	-6.43	0.01	0.0526

Table 2.4: Dynamic LCA literature review

Scope	Sub-Scope	Ref
DLCI	Process-oriented	[56–58, 61–65]
	Future-oriented	[59, 60, 66]
DLCIA	CF and time horizon	[40, 67–71]
	Discrete timing of emissions	[40]
DLCI + DLCIA	Process-oriented + CF and time horizon	[53, 72–77]
	Future-oriented + CF and time horizon	[78, 79]
	Process-oriented + Discrete timing of emissions	[80, 81]

time dependency can be divided into inventory-related dynamics and impact assessment-related discounting rates, as proposed by Collinge et al. [53]. The former, commonly known as dynamic life cycle inventory (DLCI), can be subdivided into process-oriented and future-oriented analyses. The latter, corresponding to dynamic life cycle impact assessment (DLCIA), can be split into CF and time-horizon-related vs. discrete timing of emissions.

The lack of consideration of time in traditional LCA was already pointed out as a main limitation by Owens [54] in 1997. Since then, different approaches were developed in the literature to achieve its implementation in more complex systems covering both the LCI and LCIA. A recent review by Beloin-Saint-Pierre et al. [55] addresses the challenging task of setting the fundamental framework for future consideration of time in LCA, by introducing a common glossary, inventory definitions at database level and impact assessment implementation.

Table 2.4 summarises a literature review of DLCA regarding the aforementioned classification. The first steps in modelling time during the inventory phase can be attributed to Field, Kirchain, and Clark [56] and Björk and Rasmuson [57]. While the former focused on a fleet-based analysis showing that emissions follow a transient state in addition to the common steady state, the latter modelled time-dependent key parameters like moisture content in wood during drying, thus obtaining a set of time-dependent results. The fleet-based inventory approach was also applied by Stasinopoulos et al. [58], showing its benefits when comparing the dynamic changes of steel vs. aluminium body-in-whites energy consumption during their life-cycle. For this, linear mathematical relationships were used to describe the flow into and out of the fleet, together with the recycling of aluminium [58]. In parallel, Pehnt [59] and Zhai and Williams [60] analysed the effect of time by considering future scenarios. Although the authors did not consider time explicitly, they discussed the changing nature of LCA under different future-oriented conditions.

2.3.1 DLCI: process-relative temporal distributions

From the DLCI point of view, it can be seen that efforts were made to explicitly model the temporal relationship between processes. Today, two main tools are available for LCI modelling: DyPLCA and Temporalis [55]. These models are based on the depth-first and best-first graph search methods, respectively.

ESPA method

Beloin-Saint-Pierre, Heijungs, and Blanc [62] introduced the Enhanced Structural Path Analysis (ESPA) method, which propagated temporal information among the inventory by using product convolution. By combining Eq. 2.5 and 2.6, the system can be written as:

$$g = B \cdot (I - A)^{-1} \cdot f \tag{2.8}$$

Then, the authors use Taylor's expansion to solve the inverse, namely:

$$g = B \cdot (I + A + A^2 + A^3 + ... + A^j + ... + A^n) \cdot f \tag{2.9}$$

Finally, defining a product of convolution on the temporal dimension of the process-relative temporal distributions, Eq. 2.9 is written as:

$$g = B_{*temp} \cdot (I + A + A_{*temp}A + A_{*temp}A_{*temp}A + ...)_{*temp} \cdot f \tag{2.10}$$

The method was further developed step by step. From the inventory point of view, it was expanded to consider the spatial dispersion of emissions over time [64]. However, it was its combination with DLICA that boosted its development. Pinsonnault et al. [74] expanded it in the background system up to 13 tiers in combination with time-dependent characterization factors. Similarly, Cardellini et al. [76] applied it to the foreground system by using the best first search algorithm, based on the enhanced version developed by Beloin-Saint-Pierre et al. [75], who introduced the temporally differentiated LCI.

Depth-first method

In parallel, the use of graph search algorithms was already investigated by Tiruta-Barna et al. [63], who modelled the demand-supply relationships, therefore overcoming the until then limitations of the ESPA method. Here the authors expanded the matrix-based formulation to generate a graph with two main dynamic models: the process model and the supply model [63].

Implementing a productivity function $p(t)$ and an intervention function $e(t)$, the dynamic process can be written as:

$$\begin{aligned} P &= \int_{t_0}^{t_0+T} p(t)\, dt \\ E &= \int_{t_0}^{t_0+T} e(t)\, dt \end{aligned} \tag{2.11}$$

In order to calculate the parameters used in the matrix formulation in Eq. 2.4, a normalization step is required, thus giving:

$$\alpha_{i,i} = \frac{p_i(t)}{P_i} \tag{2.12}$$

The production function $\alpha_{i,i}$ can then be used to calculate $a_{i,i}$ as:

$$a_{i,i} = \int_{t_0}^{t_0+T} \alpha_{i,i}(t)\, dt \tag{2.13}$$

Similarly, the emission k related to a process i can be calculated as:

$$\begin{aligned} \beta_{k,i} &= \frac{E_{k,i}}{P_i} \\ b_{k,i} &= \int_{t_0}^{t_0+T} \beta_{k,i,i}(t)\, dt \end{aligned} \tag{2.14}$$

Tiruta-Barna et al. [63] also introduces a delivery function $\psi(t)$ that describes the exchange or acquisition of product j at plant i, dynamically as:

$$-a_{j,i} = \int_{t_0}^{t_0+T} \psi_{j,i}(t)\, dt \tag{2.15}$$

Finally, the authors present the analytical solution for a complete supply chain through all the processes defined in the system model.

2.3.2 DLCIA

Looking into DLCIA, it can be seen that a first attempt at considering time was made by Kendall, Chang, and Sharpe [68]. The authors focused on land use change (LUC) GHG emissions during the manufacturing of biofuels, using time correction factors to account for the amortisation of emissions over time. This early research already pointed out two important aspects: i) the timing of emissions and ii) the time value of emissions, especially when looking at LUC-project investments. This latter concept was further elucidated by Brandão et al. [66], who compared the time value of carbon sequestration and temporary storage. A main breakthrough in the DLCIA methodology is attributed to Levasseur et al. [40], for considering the temporal profile of emissions together with time-adjusted characterization factors for the GWP indicator.

The combination of DLCI with DLCIA was stressed as a main topic of development in LCA by Reap et al. [72] and Finnveden et al. [73]. Both authors believed that changes in the environment and dynamic variations between processes needed to be accounted for. However, it was Collinge et al. [53] who explicitly considered DLCA by transforming the mathematical matrix approach proposed by Heijungs and Suh [51] into a time-dependent matrix system, as follows:

$$h_t = \sum_{t=t_0}^{t_e} C_t \times B_t \times A_t^{-1} \times f_t \tag{2.16}$$

Where t denotes a specific point in time at which the values are known. As the author suggests, the notation in Equation 2.16 does not necessarily imply that the terms are functions of time, but rather indicates that they can change over time [53]. Specifically, the term C_t suggests that the underlying model used to compute the characterization factors may have temporal variability. This pivotal research divides an early DLCA period from a second era of rapid methodological improvements.

An interesting discovery was made by Shimako et al. [77], who performed a sensitivity analysis on temporal parameters, showing that temporal granularity during the LCI is not an influencing factor while the time horizon adopted in the dynamic LCIA heavily affects the results. More recently, Ferrari et al. [81] performed a DLCA by integrating the enterprise resource planning (ERP) system of a tile manufacturing company, giving birth to the *streamlined* DLCA. This promising approach captures live data from the production process and combines it with custom-made LCA software to compute real-time environmental impacts.

2.4 LCA: Stochastic

2.4.1 Uncertainty in LCA

LCA uncertainties have been highlighted as one, if not the biggest, drawback when analysing, comparing, or extrapolating results. They are classified into parameter, scenario and model uncertainties [82].

Fig 2.7 illustrates these three components for an example of cement manufacturing in Germany. Parameter uncertainty is related to the lack of information about the true value of an input element [83]. For instance, when modelling the CO_{2e} emissions during the clinker production, it is necessary to know the amount and type of raw materials and fuel used, for a certain kiln. It is possible to know the exact amounts at a plant scale. However, if the aim is to conduct a regional or even national analysis, there will inherently exist a range of applications with different frequencies. While the average value is commonly used, this approach introduces an unavoidable bias in the results, hindering the quality of the analysis. The same principle is applied to all the involved parameters in the LCI.

Model uncertainties commonly arise due to simplifications in both the inventory and impact assessment phases. These range from the modelling procedure, i.e., linear vs. non-linear modelling, spatial distribution and interaction of emissions with the receiving environment, and temporal distribution vs. steady state modelling. In the example illustrated in Fig. 2.7, the CO_{2e} emissions can be obtained from either a simplified carbon footprint factor or a more specific process-related mass balance.

Finally, scenario uncertainties are linked to normative decisions [82]. Here, the system boundary choice, i.e. plant, regional or national scale will have a direct impact, like the functional unit or allocation procedure adopted. In addition, the time boundaries are of particular importance, as was discussed before.

2.4.2 Uncertainty modelling

The handling of uncertainty in LCA is still a topic under development, although basic approaches were introduced more than two decades ago [84]. Table 2.5 encompasses a literature review with

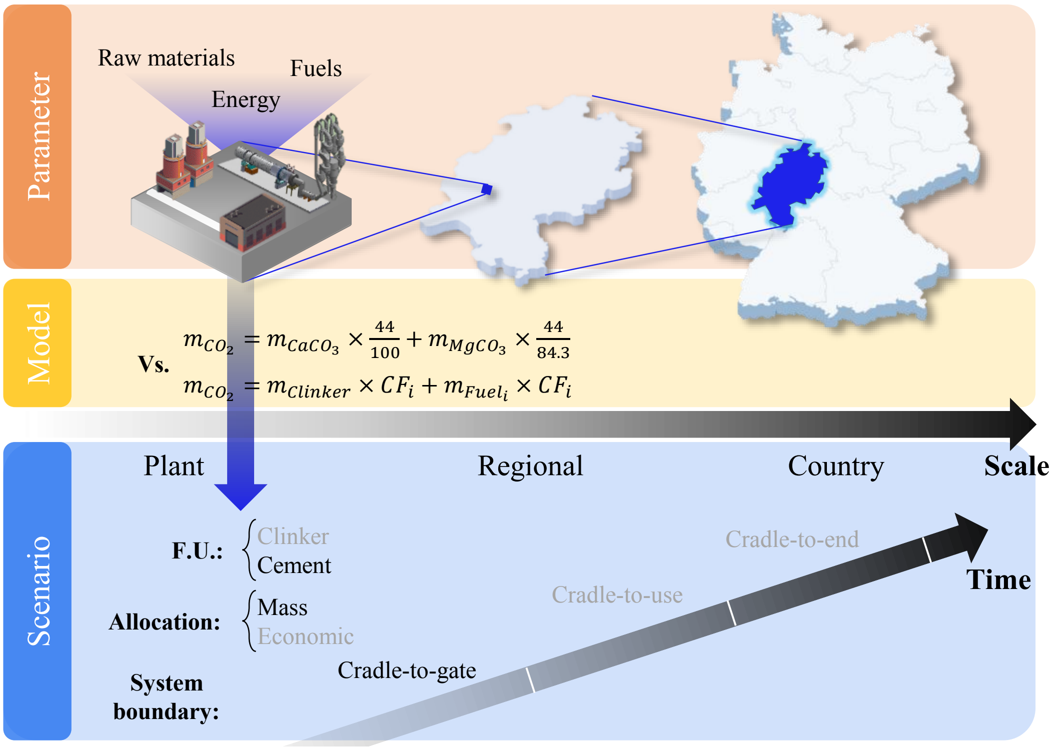

Figure 2.7: 3 levels of uncertainty in LCA

a classification into methodological, analysis, or datasets types of references. Moreover, the scope is also differentiated.

Table 2.5: Stochastic LCA literature review

Type	Scope	Ref
Methodology	LCA	[82, 84–89]
	Reports and communication	[41–43, 96, 97]
Analysis	LCA	[90, 91]
	CO2 footprint	[92–95]
Dataset	LCA	[98, 99]
	CO2 footprint	[100, 101]

From a methodological point of view, a first attempt to quantify LCA uncertainty was made by Weidema and Wesnaes [84] under the data quality indicators (DQI) framework. Here, a basic parameter uncertainty is combined with five additional variances in the form of a pedigree matrix to judge the quality of data. The latter aims to quantify deficiencies in the data linked to its reliability, completeness, temporal, geographical, and technological correlation. Table 2.6 shows the criteria used for the assignment of quality level. However, as pointed out by Coulon et al. [85], uncertainty and data quality are two distinct attributes. While the first represents the inherent variability of the data itself, the second should speak for its adequacy. Therefore, the authors introduced a stochastic approach to handle the first source of uncertainty. These were the foundations upon which the stochastic LCA was developed until today. For instance, Canter et al. [86] employed a combination of DQIs with stochastic analysis to enhance LCA-based decision-making accounting variances. The framework was further developed to consider a sensitivity analysis, its application in Ecoinvent v3 database and the development of empirical uncertainty factors to replace the expert-derived ones normally include in databases [87–89].

The omission of uncertainty analysis in LCA has a direct impact on the results. Huijbregts et al. [82] analysed the three types of uncertainties discussed previously, showing that all of them have a significant impact on the outcome. Furthermore, Henriksson et al. [41] performed an extensive review of LCA studies, that considered uncertainty, and its effect on eco-labelling frameworks. The authors concluded that disclosing point-estimate results is misleading in terms of environmental comparisons of products and suggested that product carbon footprints should be supported by quantitative uncertainty estimates.

Table 2.5 lists other studies that analysed the variability of both CO_{2eq} footprint and LCA results when considering variable input data [90–95]. However, it is not common practice among LCA practitioners to perform stochastic analysis. There are two critical aspects that need to be overcome: i) data availability remains a challenge ; and ii) comprehensive frameworks that rely on stochastic-based LCA studies to fairly compare products' environmental performance.

2.5 Challenges and gaps

In light of the literature review discussed above, it is certain that the construction industry requires the development of industry-specific LCA-based tools that offer flexibility and customisation opportunities to analyse the environmental footprint of new material designs. Furthermore, directing innovation to surpass stochastically determined environmental indicators will enable the industry to advance its environmental agenda, thereby enhancing sustainable developments. Additionally, LCA practitioners are urged to transition from traditional steady-state analysis towards a more comprehensive time-dependent LCA modelling approach.

In this context, this research pursues three main objectives. Firstly, it will delve into the computational structure and implementation strategy required for a tool to ensure its effectiveness and functionality.ă Secondly, the dynamic and non-linear interaction between energy performance, and material footprints will be studied, providing insights into optimising both aspects simultaneously. Lastly, this research aims to develop robust environmental benchmarks specifically tailored for comparing current and future cement-based materials, facilitating informed decision-making towards more sustainable construction practices.

Table 2.6: LCA pedigree matrix [84, 89]

Indicator	Score				
	1	2	3	4	5
Reliability	Verified data based on measurement	Verified data partly based on assumptions or non-verified data based on measurements	Non-verified data partly based on assumptions	Qualified estimate (e.g. by industrial expert)	Non-qualified estimate
Complete-ness	Representative data from a sufficient sample of sites over an adequate period to even out normal fluctuations	Representative data from a smaller number of sites but for adequate periods	Representative data from an adequate number of sites but from shorter periods	Representative data but from a smaller number of sites and shorter periods or incomplete data from an adequate number of sites and periods	Representative-ness unknown or incomplete data from a smaller number of sites and/or from shorter periods
Temporal correlation	Less than 3 years of difference to year of study	Less than 6 years difference	Less than 10 years difference	Less than 15 years difference	Age of data unknown or more than 15 years of difference
Geo-graphical correlation	Data from area under study	Average data from larger area in which the area under study is included	Data from area with similar production conditions	Data from area with slightly similar production conditions	Data from unknown area or area with very different production conditions
Further techno-logical correlation	Data from enterprises, processes and materials under study	Data from processes and materials under study but from different technology	Data from processes and materials under study but from different technology	Data on related processes or materials but same technology	Data on related processes or materials but different technology

3 Results

3.1 Publication 1: Life cycle assessment modelling in Octave/Matlab: Hydrated lime manufacturing case study

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3.1.1 Abstract

Life Cycle Assessment (LCA) modelling of several scenarios are time consuming if performed manually and the results are typically calculated as a single time point estimate. Furthermore, uncertainty in the input variables is high, making comparisons between different solutions challenging. This work introduces an LCA-algorithm tool that improves upon existing commercial software by offering flexibility in considering various factors, such as probability density functions, parameter study, regression and optimisation requiring multiple scenarios. It enables the resolution of inventory problems and impact assessment calculations, following ISO 14040/44 standards, while allowing for easy simulation of different scenarios and boundary conditions. In this paper, LCA implementation strategy in Octave (freeware) and Matlab (proprietary) programming language is presented, following the Mathematical structure of the LCA algorithm. Special focus is on the implementation of the Inventory data manipulation and LCA impact analysis. In order to demonstrate the benefits and potentiality of this methodology, a theoretical case study for

hydrated lime manufacturing industry in Europe is presented, developed under the European SUBLime network.

A comparison with open source software OpenLCA is carried out to validate the presented Octave/Matlab development. Both methods delivered results with negligible relative errors in all evaluated impact categories. After the validation, a parametrized study on the fuel and electricity composition and consumption of the theoretical plant and influence of transport distances was carried out. Results demonstrate benefits of the Octave/Matlab implementation approach, especially when looking for strategies to improve sustainability indicators.

3.1.2 Introduction

The manufacturing and construction sector was responsible for the production of 6.30 billion tonnes of CO_2e in 2019, making it the third more contributing category worldwide [3]. After the Paris Agreement [102], the race for climate neutrality has begun and companies are setting ambitious goals towards this target. Today, a revolution in the design principles and the adoption of construction materials is taking place, where the environmental performance of an entire building or a part of it is as important as the mechanical or aesthetic one. Almost every new development of a construction material incorporates an evaluation of the environmental performance by means of LCA. There are still some limitations. While the goal of many LCA studies is the comparison of different solutions for a certain problem, the reproducibility of this studies and the extrapolation of the results is arduous, since they are often very case specific. Furthermore, when considering the life cycle inventory (LCI), poor discretization in terms of the processes involved is often to be found, relying on generic background datasets that already contain upstream information. For this reason, sensitivity analysis and simulations are often not possible. Besides, the use of available software such as Simapro (proprietary) or OpenLCA (open source) limits the freedom in terms of the different analysis that can be implemented, such as non-linear relationships, parametric studies or different boundary conditions definitions.

The computational structure of LCA has been extensively addressed by Heijungs and Suh [51], by dedicating a complete book to the explanation of the matrix representation of the mathematical treatment of LCA. Since them, different authors have made important contribution towards the improvement of this methodology. For instance, Peters [103] explored different iterative techniques in order to solve the inventory problem more efficient. Later on, Heijungs, Settanni, and Guinée [104] published an expression that allowed to incorporate the LCC calculation within the matrix formulation that was further developed by Moreau and Weidema [105]. On a different approach, authors like Collinge et al. [53], Beloin-Saint-Pierre, Heijungs, and Blanc [62], and Tiruta-Barna et al. [63] have explored the dynamic aspect in LCA with different approaches.

Despite recent developments, research in the field of LCA still heavily relies on manual case-specific analyses, which may hinder transparency and limit broader applicability and integration with available computational libraries, such as probabilistic, non-linear regression and optimisation tools. Researchers would greatly benefit from a flexible LCA calculation tool, enabling them to simulate and analyse multiple scenarios freely in automatized fashion. Different commercial software are currently available with interesting features, such as parametric process definition or sensitivity analysis by means of Monte Carlo simulation. However, they usually lack simulation flexibility, e.g. when considering different types of probability density functions and reliability methods, non-linear behaviour between parameters, multiple scenario analysis or time dependent variables. The current work presents an LCA-algorithm tool that allows solving the inventory problem and the impact assessment calculation of the system under study, following ISO 14040/44 standard. Accessing the computational level of LCA enhances the understanding of how environmental impacts are determined in relation with every elementary flow of each process, but also allows to easily simulate different scenarios and boundary conditions.

The aim of this paper is to bridge the gap between traditional case-specific and manual LCA approaches and computational implementation strategies. This is accomplished through three main steps:

i) Describing a complete implementation of an LCA calculation tool within the Octave and Matlab computational environment,

ii) Applying the methodology outlined in (i) to a specific case study focusing on hydrated lime manufacturing. This practical application of the LCA calculation tool demonstrates its effectiveness in assessing the environmental impact of a real-world scenario.

iii) Conducting a parametric analysis that explores various factors, including kiln fuel consumption, plant electricity usage and the impact of transport distance. By examining these parameters, researchers can gain valuable insights into the sensitivity of the environmental assessment and identify potential areas for optimisation.

By combining a comprehensive and automatized implementation of the LCA calculation tool, a practical case study, and parametric analysis, this paper aims to provide a robust framework for more accessible LCA research, fostering greater transparency and facilitating informed decision-making in sustainable design and manufacturing practices.

3.1.3 Methodology

The methodology followed in this paper is aligned with the different stages included in ISO 14040/44 [106]. For this reason, the implementation strategy is presented in three main categories, namely the data acquisition, the inventory definition with its solution and the environmental impact calculation. Special attention is given to the data format Ecospold2, upon which the datasets are build. Additionally, the life cycle impact method Impact 2002+ is implemented as a reference, but a generalisation towards any impact method is also presented. During each stage comprising the LCA analysis, an example is described regarding the hydrated lime manufacturing process in Germany, following a previous publication from the authors [19].

Fig. 3.1 shows a simplified version of the cradle-to-gate system boundary used. Note that not all the inputs needed for the inventory are displayed, for more information the reader is invited to follow the beforementioned publication [19].

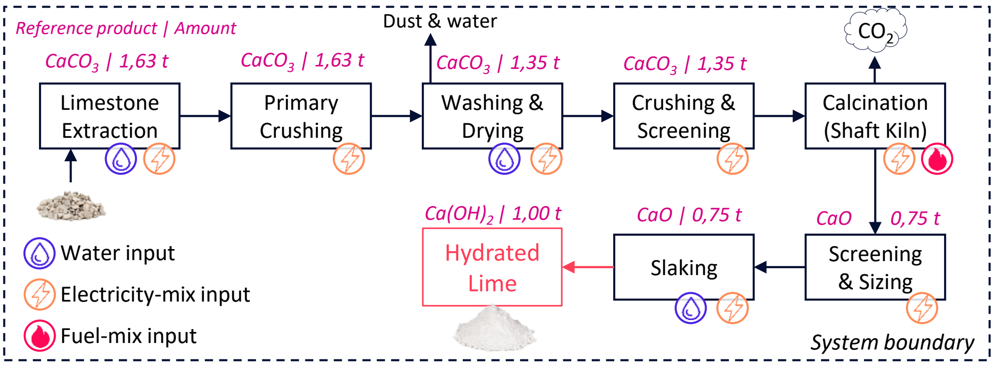


Figure 3.1: System boundary and unit processes modelled

Data import and organization

As already highlighted by many authors, the quality of the results in an LCA analysis highly depends on the inputs considered [32]. As a consequence, the best practice in terms of building a reliable inventory is to develop a process-based LCI, where each step in the manufacturing process is modelled. At a certain point, background data will be needed in order to reproduce upstream activities. In this paper, Ecoinvent database is considered for this purpose. Figure 2, shows the information structure related to the Ecospold2 format [1]. Typically, the inventory information in any database is stored in xml format, because of the compatibility with the nested organization. The use of structures in the programming language is recommended. It can be seen, that for any datapoint, e.g. a process, a dataset number identifies it unequivocally. Furthermore, two types of information groups are defined. On one hand, the meta-information highlights the dataset name, reference amount and unit. On the other, the flow-data shows all the different flow exchanges related to it. A flow exchange can be defined as the acquisition of a resource or the emission of a chemical from or into a defined environment, namely inputs and outputs respectively. For any process in the database, a total of 258 inputs and 1287 outputs are defined and specified into different categories of environments as shown in Fig. 3.2. The information contained in this part of the structure is the one related to the environmental intervention matrix defined by Heijungs and Suh [51].

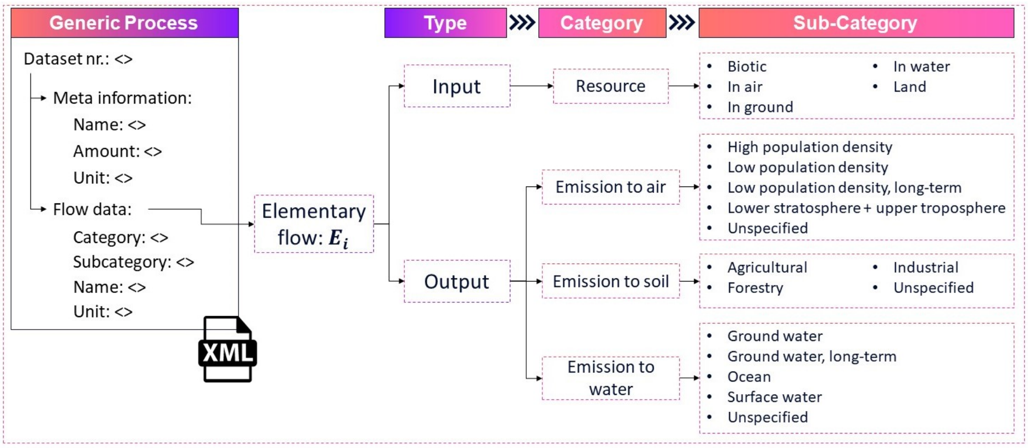


Figure 3.2: Information structure for a generic process and its classification of inputs and outputs according to the Ecospold2 format

Inventory

There is no single way to build and solve the inventory problem. While the complete production chain can be directly modelled as one big connection of processes, the presented approach here is to split it into smaller unit processes as shown in Figure 1, because it allows a better interpretation

[1] https://support.ecoinvent.org/ecospold2

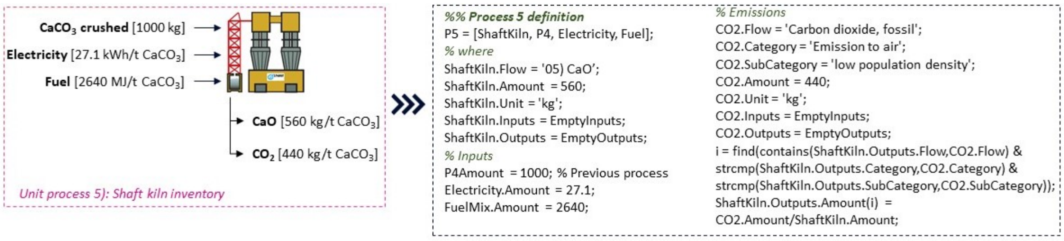


Figure 3.3: Shaft kiln unit process and the corresponding Octave/Matlab structure

Table 3.1: Pseudocode for the balancing, normalization and allocation procedure

Octave / Matlab pseudocode	Reference
a = ones(size(c));	% Definition of allocation vector
a(2:end) = value;	% Setting the allocation value (1 meaning no allocation)
cNorm = 1/c(1).Amount;	% Normalization value
for i = 1 : length(c)	
c(i).Amount = c(i).Amount *cNorm*a(i);	% Scaling the unit process amount to the normalized one times the corresponding allocation value
c(i).Inputs.Amount = c(i).Inputs.Amount*c(i).Amount;	% Scaling and allocating the input elementary flows
c(i).Outputs.Amount = c(i).Outputs.Amount*c(i).Amount;	% Scaling and allocating the output elementary flows
end	

of the results in a later stage. Following the type of structure presented before, a new unit process can be created by defining this information. For this purpose, a dummy file containing hollow inputs and outputs elementary flows is used and filled in order to define the flow exchanges of the corresponding processes that affect that activity. A template is given in the supplementary material. Next, the inventory needs to be formulated, i.e. the relationship between economic activities should be established. For this, a new process is created for each unit and all the relative inputs and outputs are modelled following the basic structure showed in Figure 2. An example of the Shaft Kiln unit process is shown in Fig. 3.3.

It should be stressed out at this point, that correlation between processes can be easily treated by simply writing the linking equations that relate the amount needed for each exchange of processes.

Once the process unit is defined, normalization and allocation take place. Since the unit process will be requested by other units, all the different inputs and outputs should be normalized to a basic reference unit. Furthermore, allocation may be needed for the cases where multifunctional process exists. An example can be seen for the case of the fines released during the secondary crushing in the reference scenario [19]. A generalized pseudocode is given Table 3.1. Assuming that c is the corresponding structure for a certain unit process, a normalization array c_{norm} multiplies the corresponding allocation vector as follows:

Table 3.2: Pseudocode for the Technology Matrix

Octave / Matlab pseudocode	Reference
A = eye(length(flows));	% Definition of identity matrix
for i = 1:length(flows) & for j = 1:length(LMTotal)	% Setting the length of iteration to the system boundary
u = find(strcmp(flows(i), string({LMTotal{1,j}.Flow})'));	
if isempty(u) == 1	% Meaning no relation was found
A(i,j) = 0;	
else	% Meaning a relation was found
A(i,j) = -LMTotal{1,j}(u).Amount;	% Negative values for inputs, positive for outputs
end; end; end; end	
A = A - diag(diag(A)) + diag(abs(diag(A)));	% Replacement of diagonal values for positive ones

Technology matrix and inventory solution

The technology matrix introduced by Heijungs and Suh [51], aims to link the economic related flows between each other. As already stated by the author, the cut-off problem needs to be solved. In the approach presented here, the method of hollow processes is followed. For more information the reader should refer to the beforementioned literature. Since an economic flow can be linked to more than one processes, an algorithm is developed in order to find the relation between all the processes contained in the system boundary and displayed them into the technology matrix **A**. Lets consider ***flows*** as a vector containing the name of all the different economic flows in the system boundary and **LMTotal**, a cell structure containing all the different unit processes, with the categories defined according to Fig. 3.2. The technology matrix can be filled following the pseudocode shown in Table 3.2.

Once the technology matrix is built, the inventory solution in terms of the environmental intervention can be calculated. For this, the scaling vector needs to be computed following Eq. 2.5 where **A** denotes the technology matrix, **f** the demand vector and **s** the scaling vector. Noted that when using Octave and Matlab, the use of backslash operator is preferred, shown in Eq. 3.1, as it allows a faster and more accurate calculation than inverting the matrix and then multiplying by the demand vector. This operator uses Gaussian elimination without explicitly building the inverse matrix.

$$
\begin{aligned}
s = f \Leftrightarrow s &= A^{-1} f \\
s &= A \backslash f
\end{aligned}
\tag{3.1}
$$

Life Cycle Impact Assessment

During the LCIA, all the different elementary flows, already scaled up during the inventory solution, need to be translated into impact categories. Midpoint, endpoint and single score (SS) can be defined. Depending on the selected impact methodology, different selection of flows or coefficient factors (CF) could arise. Nevertheless, the general approach follows Eq. 3.2, for the case of mid-point impact categories.

$$IS_c = \sum_i (CF_i \cdot E_i) \tag{3.2}$$

Where IS_c stands for the midpoint impact score under a certain category c; and CF_i is the characterization factor for a given elementary flow E_i, classified according to Fig. 3.2. The basic idea is to link a predefined set of elementary flows from a corresponding category and subcategory, as defined in the data import section, with a set of coefficients that relate the undergoing environmental problem with a reference unit. The derivation of the different characterization factors and the explanation of the undergoing environmental mechanism is well described by Hauschild, Rosenbaum, and Olsen [32]. From the algorithm point of view, given that once the impact method is selected and thus the types of flows and the CFs are defined, it is more efficient to predefined a vector containing the relative location of each flow inside the intervention matrix, instead of searching them upon each iteration. It should be stressed out, that the order in the elementary flows should be maintained. For the damage-related endpoint scores, the following expression can be used:

$$DS_c = \sum_i (EF_i \cdot IS_c i) \tag{3.3}$$

Where DS_c references the damage score (e.g. damage to human health) and EF_i are the endpoint characterization factors for a specific mid-point impact score IS_{c_i}. Table 3 shows the midpoint impact categories considered and the corresponding endpoint characterization factor. The abbreviation used for each impact category can be also found under $RefName$ column.

Regarding the algorithm structure, the implementation for the case of the impact method Impact2002+, can be easily integrated. HH, EQ, RES and CC stands for Human Health, Ecosystems, Resources and Climate Change damage categories respectively.

Defining $Impact_m id$ as the vector containing the mid-point impact scores results for each impact category, namely the second column shown in Table 3.3, and $END_C F$ as the matrix containing

Table 3.3: Midpoint impact categories and the relationship with endpoint areas of damage

Impact Category	RefUnit	RefName	HH	EQ	RES	CC
'Acidification potential'	'kg SO2 eq'	'AP'	-	-	-	-
'Aquatic ecotoxicity'	'kg TEG water'	'ET'	-	8.86E-05	-	-
'Aquatic eutrophication'	'kg PO4 P-lim'	'EP'	-	-	-	-
'Carcinogens'	'kg C2H3Cl eq'	'HT-Cancer'	2.80E-05	-	-	-
'Global warming'	'kg CO2 eq'	'GWP'	-	-	-	1.00E+00
'Ionizing radiation'	'Bq C-14 eq'	'IR'	2.10E-10	-	-	-
'Land occupation'	'm2org.arable'	'LO'	-	1.09E+00	-	-
'Mineral extraction'	'MJ surplus'	'ME'	-	-	1.00E+00	-
'Non-carcinogens'	'kg C2H3Cl eq'	'HT-NonCancer'	2.80E-04	-	-	-
'Non-renewable energy'	'MJ primary'	'NRE'	-	-	1.00E+00	-
'Ozone layer depletion'	'kg CFC-11 eq'	'ODP'	1.05E-03	-	-	-
'Respiratory inorganics'	'kg PM2.5 eq'	'RI'	7.00E-04	-	-	-
'Photochemical oxidation'	'kg C2H4 eq'	'POCP'	2.13E-06	-	-	-
'Terrestrial acidification'	'kg SO2 eq'	'TAP'	-	1.04E+00	-	-
'Terrestrial ecotoxicity'	'kg TEG soil'	'TETP'	-	8.86E-05	-	-

```
Impact_End = pagemtimes(Impact_mid,END_CF);    Octave / Matlab syntax
```

all the end-point characterization factors (columns 5 to 8), the final end-point impact vector $Impact_End$ can be then calculated by using the pagemtimes command as follows:

Finally, a Single Score SS can be calculated as:

$$SS = \sum_i (WF_c \cdot DS_c) \tag{3.4}$$

Where WF_c represents the weighting factor for a specific end-point area of damage and DS_c the corresponding score. It should be noted, that while considering a single score enables a straightforward and easy compare between results, there is still no agreement among researchers on the selection of the weighting factors and results should be analysed carefully. As far as the author concern, all the three type of scores should be communicated together, since they are complementary rather than contrasting.

Table 3.4: Baseline scenario results and validation

Impact Category	Unit	OpenLCA	LCA - Algorithm	Rel. Difference
'Aquatic acidification'	'kg SO2 eq'	4.71E-01	4.71E-01	8.83E-06
'Aquatic ecotoxicity'	'kg TEG water'	2.62E+04	2.62E+04	4.41E-07
'Aquatic eutrophication'	'kg PO4 P-lim'	9.21E-02	9.21E-02	2.03E-05
'Carcinogens'	'kg C2H3Cl eq'	9.96E-01	9.96E-01	3.52E-06
'Global warming'	'kg CO2 eq'	8.23E+02	8.23E+02	6.06E-09
'Ionizing radiation'	'Bq C-14 eq'	6.91E+02	6.91E+02	1.45E-09
'Land occupation'	'm2org.arable'	4.77E+00	4.77E+00	6.77E-07
'Mineral extraction'	'MJ surplus'	2.29E+00	2.29E+00	1.12E-06
'Non-carcinogens'	'kg C2H3Cl eq'	1.02E+00	1.02E+00	4.66E-06
'Non-renewable energy'	'MJ primary'	3.29E+03	3.29E+03	3.48E-10
'Ozone layer depletion'	'kg CFC-11 eq'	1.82E-05	1.82E-05	2.08E-07
'Respiratory inorganics'	'kg PM2.5 eq'	8.26E-02	8.25E-02	2.33E-05
'Photochemical oxidation'	'kg C2H4 eq'	3.43E-02	3.43E-02	9.41E-05
'Terrestrial acidification'	'kg SO2 eq'	2.33E+00	2.33E+00	9.56E-08
'Terrestrial ecotoxicity'	'kg TEG soil'	6.76E+03	6.76E+03	5.68E-10

3.1.4 Results

Validation

In order to validate the developed algorithm, a direct comparison between the results of the baseline scenario and OpenLCA is carried out. All the modelled background processes are equal in both cases. The complete inventory used can be found in an authors previous publication [19]. Results regarding all the mid-point impact categories are shown in Table 3.4. It can be seen, that both methods are comparable.

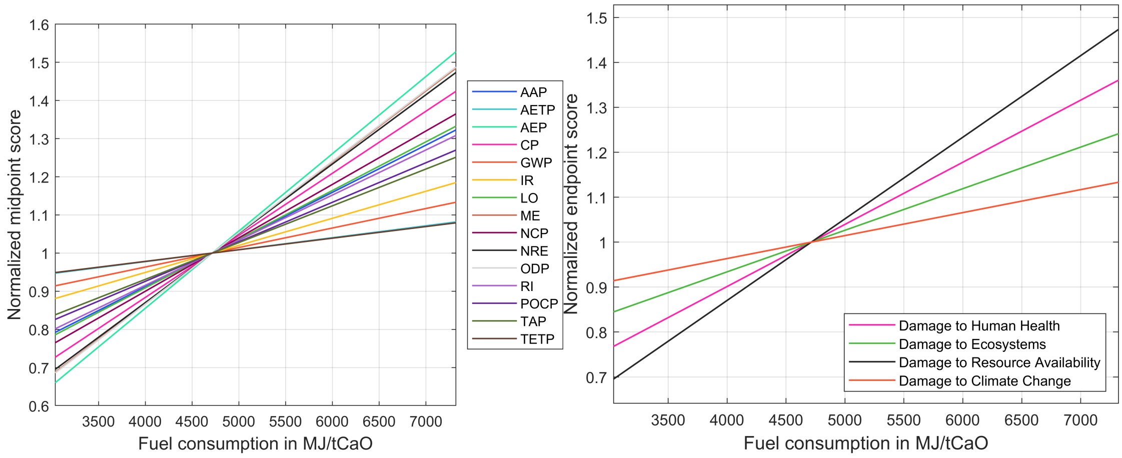
Parametric analysis

In order to show the benefits of the proposed methodology, the influence of three parameters among the midpoint and endpoint impact scores is presented. First, the effect of the fuel consumption in the kiln is studied, since this is one of the most contributing parameters to the lime environmental footprint. Then, the consequence of the transition towards renewable-based electricity sources is analysed, following the procedure presented in Sambataro et al. [5]. Finally, the response of the environmental impact to the transport distance of the dispatched material is evaluate.

Fig. 3.4 shows the normalized midpoint and endpoint impact scores regarding the fuel consumption in the kiln. As it is expected, the less fuel is consumed, the less environmental impacts can be expected for all the different categories. It is nevertheless interesting from an operation point of view, to analyse the sensitivity of each impact category against this parameter. For instance, while the GWP increases around 13% with a 55% increase in the fuel consumed, the EP increases more than 50%. This is mainly because of the release of high amounts of phosphate when lignite is burned. Similarly, when looking at endpoint indicators, the damage to resource availability is much more sensitive to the amount of fuel consumed than the damage to climate change, which can be explained through the consumption of non-renewables resources such as hard coal, lignite, oil and natural gas.

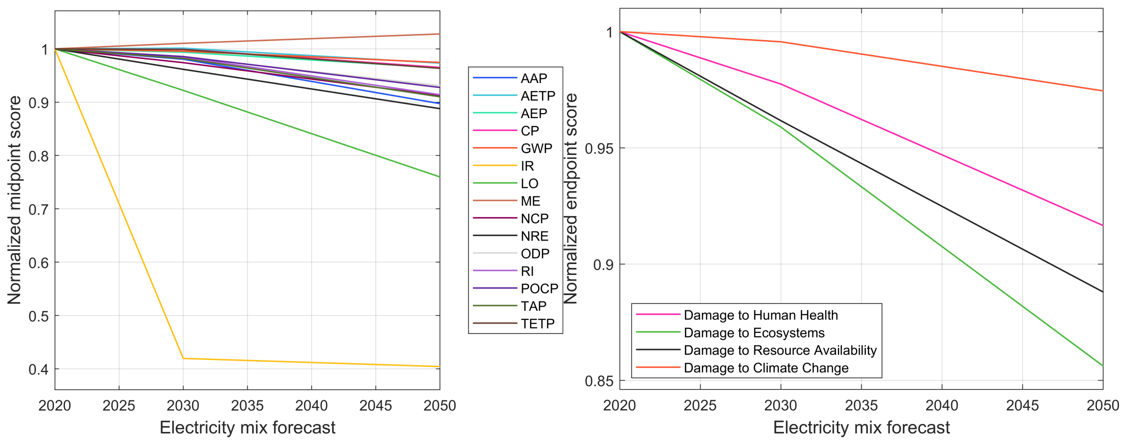
The electricity mix was forecasted for 2030 and 2050 by considering the increase share of renewables as stated in a recent report published by the German Ministry for Economic Affairs and Energy [107, 108]. The exact mixes considered can be seen in the supplementary material. Fig. 3.5 shows the expected evolution of the midpoint and endpoint indicators when a more renewable-based electricity mix is used. It is worth highlighting, that while 14 out of 15 indicators improve their performance, the mineral extraction impact increase. This is mainly because the consumption of precious metals needed for the wind electricity generation. The most affected midpoint score is Ionizing Radiation, due to the expected phase-out of nuclear energy. In terms of areas of damage, the abatement in the consumption of fossil fuels leads to a major benefit in the ecosystems quality.

Regarding the transport distance, the process *transport freight lorry 16-32 metric ton, EURO6, transport freight lorry 16-32 metric ton, APOS-S, RoW*, from Ecoinvent was used in order to evaluate the relative impact of transporting the hydrated lime beyond the gate of the factory. Different transport distances were simulated, ranging from 0 km (i.e. baseline scenario from cradle-to-gate) till 350 km. As it can be seen in Fig. 3.6, the midpoint non-carcinogens is highly affected by this parameter, which is also reflected in the Human Health area of damage category. As was shown in Table 3, there is a big contribution of the HT-NonCancer indicator in the HH endpoint score. Climate Change on the other hand, is the less affected indicator by this parameter, meaning that actions towards the electrification of the transport fleet should be placed in second order of priority.



(a) Midpoint (b) Endpoint

Figure 3.4: Normalized scores against fuel consumption in the Kiln

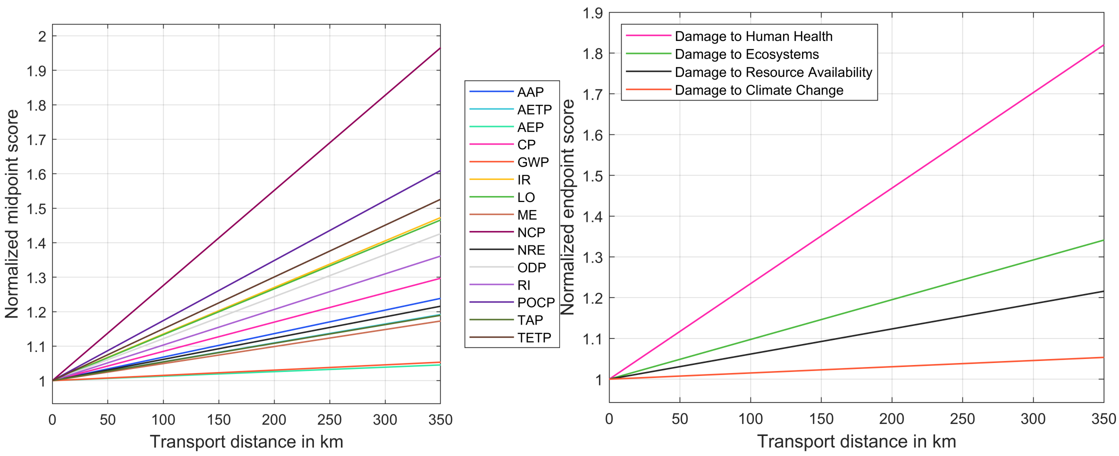


(a) Midpoint (b) Endpoint

Figure 3.5: Normalized scores against electricity mix forecast

3.1.5 Conclusions

This paper describes an implementation strategy of the LCA analysis in the Octave and Matlab programming language. Moreover, an application is developed for the hydrated lime manufacturing process, where different production parameters are studied from an environmental perspective.



(a) Midpoint (b) Endpoint

Figure 3.6: Normalized scores against transport distance

The following conclusions can be drawn:

- A new Octave/Matlab algorithm was developed that can perform a complete Life Cycle Assessment, including the main stages specified in ISO14040/44 standard, by following the matrix formulation. In addition, given the programming flexibility, thousands of different analyses can be calculated in less than a minute with a regular notebook. This results especially beneficial for scenario analysis.

- A case study regarding the hydrated lime manufacturing process in Germany was implemented and validated. Furthermore, the explicit formulation was used in order to analyse the influence of three operation parameters in the final environmental footprint. The effect of the fuel consumption in the kiln, the expected electricity forecast and the transport distance in regards to the midpoint and endpoint impact scores were studied. This is an example on how beneficial this approach could be for manufacturers and designers as a decision-making tool towards more sustainable production.

- The presented work shows a good prospect to continue exploring the limits of the LCA implementation in a computational code that can be applied by any practitioner. The next research lines will explore the effect of time discretization in the analysis.

CRediT authorship contribution statement

Luciano Sambataro: Conceptualization, Methodology, code development, and processing, LCI, LCIA, discussion, Writing original draft, paper preparation, Writing review and editing, results and discussion. Agustin Laveglia: Review and editing. Neven Ukrainczyk: Resources, Writing review and editing, results and discussion and Supervision. Eddie Koenders: Resources, Writing review and editing, results and discussion, Supervision.

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

Data will be made available on request.

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Supplementary data

Supplementary data to this article can be found online at

https://doi.org/10.1016/j.matpr.2023.08.002.

3.2 Publication 2: A performance-based approach for coupling cradle-to-use LCA with operational energy simulation for Calcium Silicate and Clay Bricks in masonry buildings

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3.2.1 Abstract

A performance-based approach for assessing the environmental impact of masonry buildings is proposed. This new method combines Life Cycle Assessment and operational energy (OE) simulations to compare the cradle-to-use environmental performance of a reference building composed of single core masonry walls made of Calcium Silicate Bricks (CSB) and Clay Bricks in Germany over a period of 50 years. To achieve this, a detailed process-based life cycle inventory and a methodology that combines material embodied footprints with operational energy simulations is developed, while also considering the vertical limit state for loading the walls. The study also considers the impact of future electricity mixes, the efficiency of heating, ventilation and air conditioning systems and the effect of lime-based construction materials carbonation on the optimal insulation thickness for a reference building. Results show that the OE consumption is the dominant phase in the overall environmental performance of current masonry buildings. Moreover, the balance between the material embodied footprint (MEF) and the OE at use phase, strongly depends on the impact category under study. If fully renewable-based electricity supply and highly efficient heat pumps are implemented, the role of MEF plays a decisive role, particularly in terms of climate change and resource availability damage areas. Moreover, the role of carbonation in CSB may contribute to up to 20% of carbon footprint reduction at a building scale.

3.2.2 Introduction

The global Green-House-Gas (GHG) emissions grew 0.9% in 2022 [109], and with this heavily jeopardizing the Paris Agreement's target on keeping the global temperature increase below 1.5 řC [102]. The manufacturing, construction, and energy use in buildings contributed for nearly 30% of these emissions [3]. While the cement industry is often cited for its large share of the global anthropogenic GHG emissions, lime-based construction materials also produce significant amounts of CO_2 emissions due to a similar kind of calcination process [19]. Moreover, the European Lime Association (EuLA) disclosed a growing trend in CaO production in the past years, especially emphasizing the construction materials sector, which represents 11.6% of the European lime market share [110]. Along with this, Life cycle assessment (LCA), as defined by ISO 14040/44 [106], is commonly used as a methodology to evaluate a buildings environmental footprint from a holistic point of view, while considering the various life cycle stages as stated in the European Standard EN-15804 [111]. A recent study by Bahramian and Yetilmezsoy [112] showed that on average, the operational energy (OE) requirement of a building is the predominant phase that represents typically over 60% of the total life cycle energy, while the embodied energy of materials is around 40%. However, the variability of the OE ratio relative to the total life cycle energy ranges from 25% to 95%, depending on the buildings lifetime. As about 60% of the building sector's energy use is delivered by fossil fuels [113], further investigation is needed to understand its environmental consequences.

Many studies focus on the LCA of masonry systems at a material level while lacking a clear coupling with a model that provides the analyses of the energy performance during use phase. While some studies compare materials as such, they often disregard a consideration of the building-scale performance [114–117]. Conversely, studies that consider operational energy (OE) simulation often lack sufficient detail in life cycle inventory (LCI) developments [118], when using generic environmental datasets. Some studies use optimization methods related to energy retrofitting and LCA, LCC (Life Cycle Costing), and LCSA (Life Cycle Social Assessment) [119], but lack a detailed inclusion of a process-based LCI connected to the environmental performance analysis [120].

Masonry buildings LCA

Specific research related to clay bricks (CBs) LCA was published by many authors. For instance, De Souza et al. [114] conducted a comparative LCA of exterior walls made from ceramic bricks, concrete bricks and cast-in-place reinforced concrete in Brazil. In this study, the environmental impact of manufacturing and assembling the different solutions, as well as the end of life

(EoL) phase were analysed. Muñoz et al. [115] performed an LCA to analyse the environmental benefits of the inclusion of Waelz slag into fired bricks, with particular attention given to raw material extraction, manufacturing process and EoL treatment. Similarly, Muneron et al. [116] compared the environmental performance of ceramic bricks and concrete blocks in vertical systems using a cradle-to-grave LCA approach. Results highlighted the contribution of fossil fuels during firing of ceramic bricks, without showing a connection with the share of various energy sources needed during operation of the building. In fact, none of the before mentioned studies considered the thermal or mechanical performance of these materials and its relation with the OE requirement. Moreover, Albuquerque Landi et al. [117] recently published an LCA of a smart clay brick monitoring system for masonry buildings, including a comprehensive literature review on environmental information related to clay bricks manufacturing and detailed information on the cradle-to-gate LCI. However, no performance in terms of OE requirement was published, and conclusions were drawn with emphasis on comparing different solutions at a material level.

Many studies that focus on design optimization, tend to rely on generic environmental datasets such as Ecoinvent and Gabi, lacking of the necessary level of detail in their LCI. For instance, Antipova et al. [119] developed a mathematical approach for optimizing an LCA of building retrofitting, including the economic performance of the solution through total cost calculation. However, in this study the LCI information needed for evaluating the environmental performance was disregarded. Instead, the environmental impact of different energy sources (natural gas and electricity) was employed directly. Toosi et al. [120] proposed a methodology for life cycle sustainability assessment (LCSA) of building retrofitting, which included LCC and SLCA. Although the study conducted a comprehensive literature review on optimization methods, energy retrofit, LCA, LCC and SLCA, a detailed process-based LCI in the environmental performance analysis was disregarded. Rather, generic information on direct mid-point impact categories was calculated based on the Ecoinvent database. Finally, the study highlighted the fact that reducing energy consumption in the operational phase may result in an environmental load-shift towards other life cycle phases.

Coupled LCA and OE

To couple the material embodied footprint (MEF) with the OE demand of a building, it is necessary to define basic design parameters such as building geometry, location, construction system, heating ventilation and air conditioning (HVAC) system, among others. Since a buildings energy saving potential is heavily influenced by its envelope components and therefore by MEF, a non-linear, iterative procedure of analysing the final environmental impact using LCA methodology is required. In a study by Landuyt et al. [118], a balance between the material-related environmental impact and OE requirement was found for a specific case study in Belgium. The study also examined the optimal insulation thickness of a prefabricated house called TheMobble, as well as its relationship with design parameters such as HVAC system efficiency and user comfort, using a single score indicator. However, like the aforementioned studies, a clear link between the material manufacturing process and the end-point and mid-point impact indicators was ignored. Combining a detailed process-based LCI with the OE requirements during the use phase offers numerous benefits for various stakeholders. For manufacturers, it provides a comprehensive understanding of the impact of their products at final use stage, enabling them to identify areas for improvement and optimization opportunities. For designers, it offers the ability to incorporate holistic environmental indicators into the early stages of design. Additionally, for policy makers, it provides an in-depth understanding through simulations of the interplay of all the parameters involved in the production and use of construction materials, such as the use of different energy sources. This can support the development of more sustainable construction policies. The aim of this paper is to bridge the gap between the current knowledge of LCA at materials manufacturing level and their lifecycle performance, according to i) proposing a methodology to calculate the LCA at a building level, which incorporates both the material manufacturing and the OE requirements in an integrated manner from the cradle-to-use phases, ii) providing a detailed and transparent process-based LCI for the production of two building materials, namely calcium silicate brick (CSB) and CB, to determine their environmental performance, and finally, iii) determining the optimal combination of materials to produce the lowest environmental impact and conduct a parametric study of the HVAC system efficiency, as well as the electricity mix used, with respect to the optimal insulation thickness while considering future trends in energy use and technological advancements.

3.2.3 Methodology

A coupled process-based LCA and OE simulation model was developed for assessing the environmental performance of masonry buildings. The main novelty of this approach is the combination of a detailed LCI along with the performance of the building materials to analyse the cradle-to-use environmental performance of multiple solutions in different impact categories. The case of CSB and CB, along with lime-based Mortar, Render and Plaster (MRP) was investigated for Frankfurt, in Germany. Furthermore, a detailed process-based LCI was developed and disclosed for the two types of bricks. For this case study, the MOD 910 building from ASHRAE (American Society of Heating Refrigerating and Air-Conditioning Engineers) Standard was employed, while analysing the OE requirement for 50 years of use. The effect of the current and forecasted electricity mix, the HVAC efficiency and carbonation potential of the materials was studied as well.

Goal of the study

A methodology is developed that enables an easy comparison of the environmental impact of multiple masonry construction unit combinations. The methodology couples the various manufacturing phases and related impacts of each construction material with the expected building-scale energy performance. The mechanical performance of materials is taken into account by adjusting the quantity of material required to meet the vertical loading limit state. This approach, previously introduced by Dobbelaere, De Brito, and Evangelista [121] for concrete structures, aims to ensure a fair comparison among different materials. As demonstrate by Simone Souza et al. [122], the choice of FU can introduce bias in building-LCA results. In fact, Bahramian and Yetilmezsoy [112] analysed the FU used in different studies regarding the LCA of buildings, showing that they may vary considerably. In this study, the FU is set to the unit of gross floor area. This means, that the total amount of material needed for each scenario and the total OE requirement is divided by the buildings gross floor area. Since the goal of the analysis is to compare different wall solutions, neither the roof nor the floor is accounted for in the LCA, although they are considered in the OE requirement simulation.

In the end, this methodology, along with the LCI, is applied to determine the most environmentally friendly solution for the construction of masonry walls made with CSB and CB for the particular case study in Frankfurt. The analysis considers 12 wall combinations, composed with a render, an insulation, a brick and a plaster layer for a standard 1- story building over 50 years. Moreover, for each combination, an iterative procedure for calculating the environmental performance is conducted by means of an LCA, along with the energy simulation, while the thickness of the insulation material changed from 0 cm to 40 cm. The optimal insulation thickness is calculated by finding the minimum environmental impact in each category. The study also provides the backgrounds of the Matlab modelling following the ISO14040/44 [106] LCA methodology.

Coupling methodology

As shown in Figu. 3.7, four main steps are followed in the approach for the coupling methodology. First, all background environmental data needed for the LCI definition and calculation is imported from Ecoinvent v3.8 [123] into Matlab. All different manufacturing processes related to production of construction materials are modelled and parametrized as functions. This allows each product to be used either directly in the functional unit calculation or to be requested by other processes during manufacturing of a new material. To account for regional representativeness, a country-specific electricity mix and an industry-specific fuel mix is modelled and presented in Table A-1 of the supplementary material. Once all processes are defined based on their reference amount (e.g. 1 kg of CSB), links are established between upstream and downstream related processes. For example, the lime manufacturing function is linked to the CSB production, since it is one of the input materials. Secondly, the inventory definition at both, building and material scale has to be conducted. For this, basic material input data is taken from an own made construction material database (CM-DB) build from different sources like Environmental Product Declarations (EPDs), research papers and manufacturer catalogues. Based on the buildings main properties, different wall compositions are defined and compared through the differences in mechanical properties of the materials. In this study, the vertical loading limit state of the wall is calculated following the European Standard EN1996-1-1 [20] and an equivalent depth capable of withstanding a similar vertical load is determined for each wall. A Matlab algorithm is developed to solve the LCI by following the matrix structure defined by Heijungs and Suh [51]. The production of each material works as an individual function, where the technology matrix A is parametrized and solved. Thirdly, all possible combinations are normalized to the system FU of 1 m2 of the buildings gross area. The OE requirement of the reference building is obtained from the open source EnergyPlus software [2] and an OE profile is established for each wall combination. Finally, the Life Cycle Impact Assessment (LCIA), following IMPACT 2002+ methodology, is implemented in Matlab in order to automatically calculate all different scenario results. Midpoint, endpoint and single score indicators are calculated and compared by focussing on the relative contribution of the different processes on the overall score.

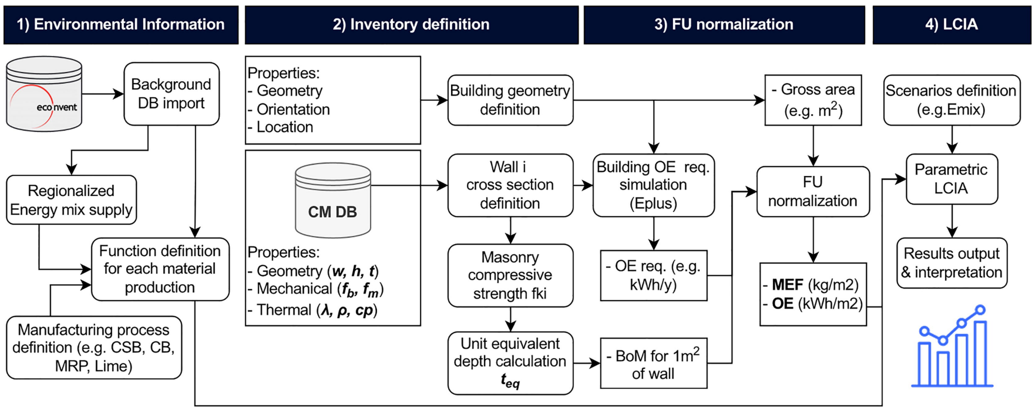


Figure 3.7: Four step coupling methodology scheme

Non-Linear Life Cycle Assessment calculation

It is common to build up an LCI normalized to the systems functional unit, allowing to easily

[2]https://energyplus.net/

scale it while considering a new vector of demand. Nevertheless, this requires that all the flows in the system are linearly correlated. However, this is uncommonly the rule in engineering practice. In reality, non-linearities arise at almost every step of the LCA analysis. For instance, for the manufacturing phase, Eden et al. showed that while the mean primary energy requirement for the manufacturing of 1 ton of Calcium Silicate Brick in Germany in 2010 was 120 kWh, this value could vary non-linearly between 80 kWh and 140 kWh depending on the raw materials temperature before entering the autoclave [124]. Similarly, the OE requirement of a building exhibits a non-linear dependency on materials properties such as thickness, thermal conductivity, heat capacity, and other relevant parameters. As discussed by Hollberg [125], decisions made in the early stages of the design process have the greatest influence on the operational and embodied environmental impacts, but the information available is rather scarce and uncertain. For this reason, it is of great importance to develop LCA-models that can overcome this limitation and be flexible enough to simulate non-linearities in the assessment. In this research, non-linear behaviour linked to the operational energy requirement are considered, while the ones arising from the manufacturing phase are disregarded.

General Matlab structure for solving LCA

The mathematical approach followed in this paper for solving LCA systems is based on a set of linear equations that were inverted following the matrix inversion method which was firstly implemented by Heijungs and Suh in 2002 [51]. They introduced the concept of technology matrix **A**, intervention matrix **B**, demand vector **f** and scaling vector **s**. The inventory system can be written as provided in equation 3.5. Inverting the matrix A leads immediately to the solution of the inventory problem. Once the scaling vector is found, it is possible to calculate the inventory vector **g**, by scaling the environmental flows in **B**, and then to calculate the related impacts according to equation 3.6, where **h** is the impact category vector and **C** represents the matrix of characterization factors (CFs), that depend on the selected impact method.

$$s = f \Leftrightarrow s = A^{-1} f \tag{3.5}$$

$$\begin{aligned} g &= Bs \\ h &= Cg \end{aligned} \tag{3.6}$$

Life cycle inventory solution

Regarding the LCI solution, three main steps were followed, schematized in Fig. 3.8. First, a technology matrix A_i comprising all relevant processes listed in the inventory table for manufacturing each individual material i is defined. It should be noted that hollow processes were created whenever necessary to achieve a square matrix for a unique solution when inverting this matrix. Secondly, the corresponding demand vector f_i for each material is calculated to fulfil the systems FU. During this step, a list of commercially available bricks is used to analyse multiple solutions that adapt to the market reality. The bricks compressive strength f_b is taken from each products technical sheet. The amount of bricks and mortar needed is calculated based on the listed geometry and the joint width and height. Once the total surface of bricks and mortar is known for 1 m2 of wall, an equivalent depth is determined based on structural performance, as described before. Eq. 3.7 is used to calculate the equivalent thickness w_{eq}, where f_k is the characteristic compressive strength of the masonry, calculated following the European Standard EN1996-1-1 [126] considering the corresponding expression related to the brick and mortar type. In Eq. 3.7, w_{max} denotes the thickness of the wall with the highest compressive strength value f_{kmax}.

$$w_{eq} = w_{max} \times \frac{f_{kmax}}{f_k} \tag{3.7}$$

This generalized method allows to automatically compute multiple combinations based on a material database. Furthermore, different compositions like binder proportions can be studied for a reference mortar.

Thirdly, the operational energy requirement is simulated for the different wall profiles, by introducing the building design parameters and the materials thermal properties into EnergyPlus software. It should be noted that the energy requirement input, here as electricity due to the use of a heat pump, should be selected by considering the type of fuel and efficiency of the system used to deliver the energy. A technology and intervention matrix A_{ope} and B_{ope} are defined for this process.

For each combination under study, once the reference amount f_i has been calculated, the contribution of each process, i.e. the scaling vector s_i, has to be determined. This includes the corresponding environmental flows g_i. A final inventory vector **g** can be calculated for each wall combination $Wall_j$.

Life Cycle Impact Assessment

The environmental impact analysis was conducted across fifteen mid-point categories, four end-point categories and a single score indicator, following the IMPACT 2002+ method [127]. It should be emphasised, that the proposed methodology is applicable to any impact method.

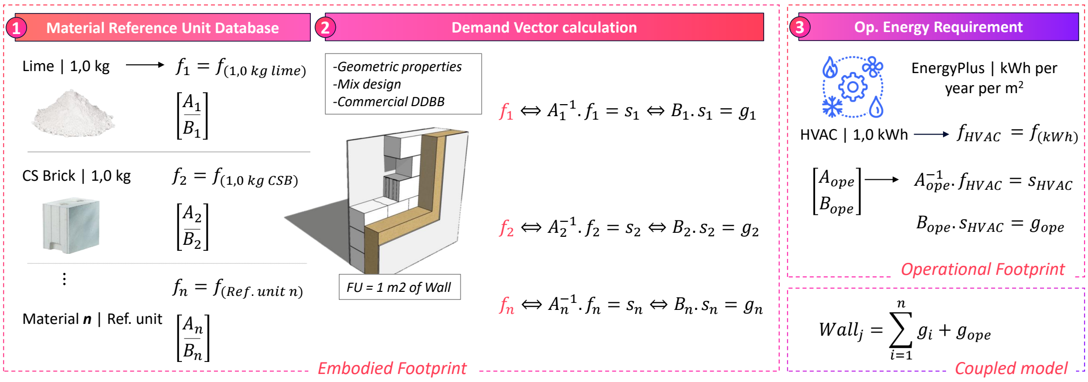


Figure 3.8: Information flow of the LCI

Table 3.5 shows the different mid-point impact categories considered, along with the used conversion factors to calculate the end-point indicators. These are then multiplied by the normalization factors shown below and summed to express the single score point. The environmental impact is calculated for each wall combination and the information about the contribution of each process is stored. Results are then plotted as a function of the variable insulation and the different impact categories. By calculating the minimum environmental impact value, it is possible to find most environmentally friendly combination along with the relative contribution of each process to the overall score.

Life Cycle Inventory development

The LCI phase as part of an LCA links all unit processes needed for manufacturing the product under study [32]. This is often the most time-consuming and critical aspect of an LCA, as the results heavily rely on the feasibility of the input variables. Although the ISO 14040/44 standard recommends using primary data, this is not always available from research reports due to confidentiality constrains. The present study, however, was conducted as part of the European SUBLime project [3], where 11 industries and 6 academic institutions collaborate on examining sustainable lime-based applications. The study also benefited from close collaboration with the German Calcium-Silicate Brick Association [4], which allowed for the gathering and validation of inventory data used in the analysis. The system boundary considered in this study is illustrated in Fig. 3.9.

[3]https://sublime-etn.eu
[4]https://www.ks-original.de

Table 3.5: Mid-point and End-point impact categories and conversion and normalization factors

Impact Category	Reference Unit	Reference Name	Conversion Factors			
Mid-point			HH	EQ	RA	CC
Acidification potential	kg SO2 eq	AP	-	-	-	-
Aquatic ecotoxicity	kg TEG water	ET	-	8.86E-05	-	-
Aquatic eutrophication	kg PO4 P-lim	EP	-	-	-	-
Carcinogens	kg C2H3Cl eq	HT-Cancer	2.80E-05	-	-	-
Global warming	kg CO2 eq	GWP	-	-	-	1.00E+00
Ionizing radiation	Bq C-14 eq	IR	2.10E-10	-	-	-
Land occupation	m2org.arable	LO	-	1.09E+00	-	-
Mineral extraction	MJ surplus	ME	-	-	1.00E+00	-
Non-carcinogens	kg C2H3Cl eq	HT-NonCancer	2.80E-04	-	-	-
Non-renewable energy	MJ primary	NRE	-	-	1.00E+00	-
Ozone layer depletion	kg CFC-11 eq	ODP	1.05E-03	-	-	-
Respiratory inorganics	kg PM2.5 eq	RI	7.00E-04	-	-	-
Photochemical oxidation	kg C2H4 eq	POCP	2.13E-06	-	-	-
Terrestrial acidification	kg SO2 eq	TAP	-	1.04E+00	-	-
Terrestrial ecotoxicity	kg TEG soil	TETP	-	8.86E-05	-	-
End-point						
Human Health	DALY	HH				
Ecosystems Quality	PDF m2 year	EQ				
Resources Availability	MJ	RA				
Climate Change	kg CO2 eq	CC	**Normalization Factors**			
Single Score	persons year	SS	7.10E-03	1.38E+04	1.16E+04	1.52E+05

In this paper, three types of CSB and CB and two types of mortar, i.e. normal joint mortar and thin joint mortar, are considered, giving a total of 12 wall combinations. Furthermore, the insulation layer composed by mineral wool, is modelled as variable ranging from 0 cm to 40 cm every 1 cm. Table 3.6 shows all the material properties considered, including the thermal conductivity and the density . Regarding the mortar mixes, it is assumed that for both the thin layer mortar and the joint normal mortar, the mean compressive strength fm is 12 N/mm2. Both mix designs were taken from published EPDs. For the first one, 1% and 0.1% of plasticizer and air entrainer was employed relative to the binder content, respectively. For the latter, these amounts were set to 0.5% and 0.0% respectively. No additives were included for the plaster and the render mix design. Each production process of each material was treated as an individual function and the electricity and fuel mixes were defined as separate functions to enable flexible regional and industry-specific simulations.

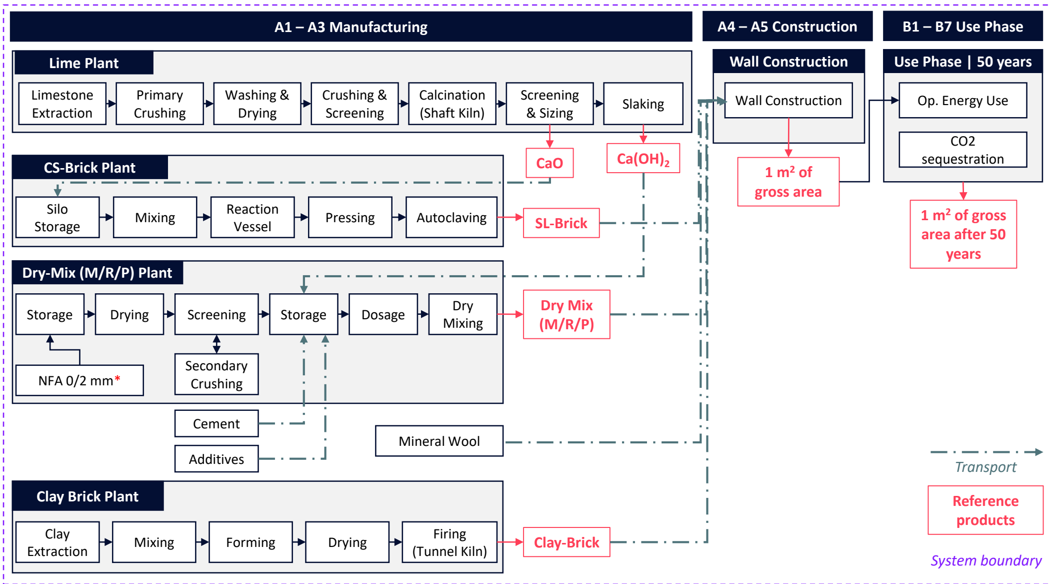


Figure 3.9: System boundary

Table 3.7 shows the total number of wall combinations with regards to the quantity of materials. Both the amounts of brick and mortar are calculated with the equivalent thickness method described before in Eq. 3.7. The render and plaster thickness are set constant to 20 mm for all wall designs. The amount of insulation is not specified, as it changes with the variation of its

Table 3.6: Material properties

Bricks properties							
Name	Type	Length (mm)	Thickness (mm)	Height (mm)	fb (N/mm2)	(W/m.K)	(kg/m3)
CSB-1400	CSB	248	175	248	12	0.7	1400
CSB-1800	CSB	248	175	248	12	0.99	1800
CSB-2000	CSB	248	175	248	20	1.1	2000
CB-600	CB	248	175	244	6	0.09	650
CB-600b	CB	248	365	244	6	0.09	650
CB-1200	CB	248	365	244	12	0.12	900
Mortar Render & Plasters mix and properties							
Type	H. Lime (kg)	CEM I (kg)	Sand (kg)	Plasticizer (kg)	Air entrainer (kg)	fm (N/mm2)	(W/m.K)
Joint Thin	0	350	611.5	35	3.5	12	-
Joint Normal	30	310	642	18	0	12	-
Render	225	150	625	0	0	-	0.51
Plaster	300	0	700	0	0	-	0.51
Insulation properties							
Type	Thickness (mm)	(W/m.K)	(kg/m3)	LCI dataset			
Mineral Wool	Variable [0:10:400]	0.035	70	Ecoinvent V3.8 | stone wool production packed, APOS S-RoW			

thickness.

The manufacturing of each construction material was considered by simulating the process flows of the production plants shown in Fig. 3.9. Additionally, direct processes for the cement, additives and mineral wool were used from the Ecoinvent v3.8 database. For cement, a CEM type I was modelled by the process *cement production Portland, APOS-S, Europe without Switzerland*. Regarding the additives shown in Table 3.6, the processes *carboxymethyl cellulose production, powder | APOS, S RoW* and *alkylbenzene sulfonate, linear, petrochemical | APOS, S RoW* were selected as plasticizer and air entraining agent respectively. This was done, since no direct dataset was found and, according to the authors, these two alternatives can be considered as a most feasible representative option, which is based on literature [128]. The mineral wool production was simulated by the process *stone wool production packed, APOS-S RoW*.

Lime Manufacturing

Lime has been used as a construction material for many centuries [129]. Some authors date back its use to 10,000 BCE [15]. In recent years, interest in this material has gained renewed attention because of its carbonation potential during its service life, and with this, its possible use in carbon sequestration applications, which will be discussed later. The approach introduced by the authors in [130] will also be followed in this work. Based on the conservation of mass principle and the stoichiometry of reactions, each unit process comprising a theoretical lime production plant is balanced. Detailed information of the considered inventory can be found in the corresponding article [130].

Table 3.7: Wall combinations and amount of materials used per FU

Wall	Brick				Mortar		Render I Plaster
Name	Type	fk (N/mm2)	teq (mm)	Amount (kg/m2)	Type	Amount (kg/m2)	Amount (kg/m2)
CSB-1.4T	CSB-1400	6.61	270.2	497.2	Joint Thin	4.4	40.6 I 40.6
CSB-1.4N	CSB-1400	6.60	270.7	443.7	Joint Normal	65.9	40.6 I 40.6
CSB-1.8T	CSB-1800	6.61	270.2	639.2	Joint Thin	4.4	40.6 I 40.6
CSB-1.8N	CSB-1800	6.60	270.7	570.4	Joint Normal	65.9	40.6 I 40.6
CSB-2.0T	CSB-2000	10.21	175.0	460.0	Joint Thin	2.8	40.6 I 40.6
CSB-2.0N	CSB-2000	9.44	189.3	443.3	Joint Normal	46.1	40.6 I 40.6
CB-0.6T	CB-600	3.44	519.4	443.8	Joint Thin	8.4	40.6 I 40.6
CB-0.6N	CB-600	4.06	439.7	334.6	Joint Normal	107	40.6 I 40.6
CB-0.6bT	CB-600b	3.44	519.4	443.8	Joint Thin	8.4	40.6 I 40.6
CB-0.6bN	CB-600b	4.06	439.7	334.6	Joint Normal	107	40.6 I 40.6
CB-1.2T	CB-1200	6.20	288.2	340.9	Joint Thin	4.7	40.6 I 40.6
CB1.2N	CB-1200	6.60	270.7	285.2	Joint Normal	65.9	40.6 I 40.6

Calcium silicate brick manufacturing

Since its patenting in 1886 in UK, CSB became a major building material in Europe, especially in Germany, The Netherlands, UK and Russia [131]. Today, CSB are the second most used type of bricks in Germany, making up almost one third (30%) of Germanys brick industry market. They represented a 406.5 Mio EUR industry in 2020. The rest of the market is divided between ceramic bricks (47% share, 636.7 m EUR), autoclaved aerated concrete blocks (20% share, 267.7 m EUR) and lightweight concrete blocks (4% share, 51.1 m EUR) [132]. The manufacturing process of CSB is composed by four main stages, as shown in Fig. 3.9. First, the raw materials, namely lime (CaO) and sand, are transported and stored into silos. It was assumed that the sand is extracted directly near the plant and therefore only transportation by conveyor belt is considered. The lime transport distance was assumed to be 95 km, since it can range between 10 km and 200 km [133]. Next, each material is weighted and placed in the mixer. The amount of required water depends on the sand humidity (usually in the range of 4% to 6%). A typical composition is made of 0.07 tonne CaO per ton of CSB and around 0.93 tonne sand per ton CSB [134], although fillers may also be included. After an intensive mixing process, the sand-lime-water mix is stored in a reaction vessel for about 1 hour where the complete hydration reaction of the lime takes place. An incomplete reaction could lead into undesired expansions during the autoclaving process and the associated risk of cracking [135]. Different size configurations are defined in DIN 20000-402, although an increasing number of manufacturers are producing customizable blocks, meaning they sized them to perfectly fit within the buildings design and therefore minimize the waste during construction. Most energy intensive process in the manufacturing of calcium silicate bricks is the autoclaving process. A recent report performed by the German Calcium Silicate Brick Association showing different strategies to achieve climate neutrality by 2050, exhibits that around 87% of the total energy for CSB manufacturing is required for the water vapour production. During autoclaving, the relative weak physical bond between the component elements (CaO, SiO2 and H2O) is transformed, under pressurized steam, at around 180 200 žC and 12 18 bar for 4 to 12 hours, into strong chemically bond calcium silicate hydrates (CSH) phases [136–138].

Clay brick manufacturing

Although CBs have been present as a traditional construction material since the Mesopotamian, Egyptian and Roman periods, its manufacturing process remained almost identical [139]. As for other ceramic products, its process may be divided into three main stages: i) powder processing, ii) shaping and iii) firing [140]. The latter represents the most energy-intensive stage during its manufacturing, because of the heat requirement in the kiln [141]. Despite the transition towards less CO_2 intensive fuels, such as natural gas or hydrogen [142], this step still remains critical, as shown by Almeida et al. [143]. A literature review carried out by Huarachi et al. [144] showed that regardless of the country of production, the main stages still remain.

First, the raw materials, which are most commonly different types of clays, are excavated from open pits. For this, the use of hydraulic excavators and transportation trucks were considered in this study. In general, excavation sites are located close to the manufacturing plant and, therefore, the transport distance can be minimised [145]. Once the clay is extracted, it is sized down in different steps until the desired granulometry is achieved. The use of a rotary crusher with rated power of 112 kW and an 80-tonnes production rate was simulated to break down the large lumps of clay. Then, through the secondary crushing process the clay grain size is further reduced to below 15 mm. For this, a regular pan mill was selected. The clay is then mixed with water to obtain a homogenized mass with a predefined plasticity. The amount of water used is related to the forming method, ranging from hand-made moulding, semi-dry pressing, to soft mud extrusion, etc. In this study, the latter was considered for the LCI. For this, a total content of 11% of water is added to the mix. The extruder delivers a clay column that is then subjected to the cutting process to form the bricks. Following, the drying process takes place at a temperature that usually range between 75-90 žC, where the excess heat from the kiln is used [145]. After drying, the bricks usually contain less than 3% of water and are subjected to the firing process at a temperature between 800-1000 žC [143, 145–147]. A tunnel kiln was adopted as the most representative technology for Europe [148].For the processes described in Fig. 3.9 (Clay Brick), different sources of LCI were used in order to quantify the mean input values and the standard deviation used in every stage as shown in Table 3.8.

Dry-Mix Mortar, Plasters and Renders Manufacturing

Table 3.8: Literature review on the Life Cycle Inventory for the production of 1 kg of finished Clay Brick

Clay Bricks	Loc.	Inputs for the production of 1 kg of finished Brick				Share of Primary Energy		
Author (year)	Code	Clay [kg]	Water [kg]	Sand [kg]	Energy [kWh]	Electricity	Diesel	Fuel
German National Association of Brick Industries (1998) [146]	DE	1.17	0.19	0.20*1	0.62	9.0%	5.0%	86.0%
Ecoinvent 3.8 - "clay brick production, GLO" (2002) [149]	GLO	1.35	0.03	0.01	0.52	8.0%	2.0%	90.0%
Koroneos (2007) [141]	GR	1.21	0.16	0.00	0.58	2.5%	11.5%	86.0%
Almeida (2010) [143]	PT	1.22	0.10	0.00	0.35	10.0%	2.0%	88.0%
Gomes (2012) [145]	BR	1.30	0.003	0.00	1.39*2	0.2%	0.1%	100%
Kua Wei H. & Kamath S. (2014) [87]	SG	1.11	0.13	0.00	0.91	17.0%	0.0%	83.0%
Giama & Papadopoulus (2015) [150]	GR	0.96	0.08	0.00	0.41	No information		
Souza et al. (2016)[114]	BR	1.59	0.13	0.00	0.91	4.0%	5.0%	91.0%
Muñoz (2018)[115]	ES	1.25	0.19	0.00	1.07	No information		
	Avg.	**1.24**	**0.11**	**0.00**	**0.67**	**8.4%**	**4.3%**	**87.3%**
	Std.	**0.16**	**0.06**	**0.00**	**0.26**	**0.05**	**0.04**	**0.03**

In this study 4 different types of mixes were used for the analysis. A pure hydrated lime mortar mix was considered for the plaster layer, while a cement-based mortar mix was used for the render layer as well as for the normal and thin laying mortar composition. Mix proportions, thermal and mechanical properties for each layer are presented in Table 3.6. The inventory information for MRP manufacturing was based on the detailed process-based inventory of Cuenca-Moyano et al. [151]. An additional step comprising the drying process of natural sand was included, by considering the amount of heat necessary for drying the sand from 5% to 1% water content, equal to 0.06 kWh per kg of dry sand, while using natural gas as fuel. To account for geographical correlation, the electricity mix in the processes was substitute to the corresponding local mix in Germany displayed in Table A1.

Construction and Use Phase

Construction related activities are not covered in the present work, since there are no significant differences between the analysed wall compositions. The transport distances from the manufacturing plants to the construction site were taken as 100 km for both CSB and CB, while 80 km were taken for the MRP and insulation material, based on average distances published in EPDs [152, 153]. The use phase of a building, analogue to the time when living beings age [154], is strictly related to the materials service life and their performance. In fact, a proper definition of the system boundary, representing the goal, scope and definition of the timespan employed in the analysis, will have a direct influence on the final environmental impact [155]. In the present work, it is considered that all included construction materials withstand the studied service life of 50 years, and thus, no activities regarding maintenance is assessed. Regarding the scenarios for simulating each different insulation thicknesses, Eq. 3.8 provides the emissions for each calculation step. E_i

Table 3.9: Roof and floor properties considered in the MOD-910 simulation

Element	[W/m/K]	Thickness [m]	U [W/m2/K]	R [m2.K/W]	Density [kg/m3]	Cp [J/kg/K]
Roof						
Internal Plaster	0.51	0.01	51.00	0.020	1700	960
Plasterboard	0.16	0.01	16.00	0.063	950	840
Fiberglass Quilt	0.04	0.3	0.358	2.794	12	840
Roof Deck	0.14	0.019	7.386	0.136	530	900
Floor						
Insulation	0.04	1.007	0.040	25.175		
Concrete slab	1.13	0.08	14.125	0.071	1400	1000

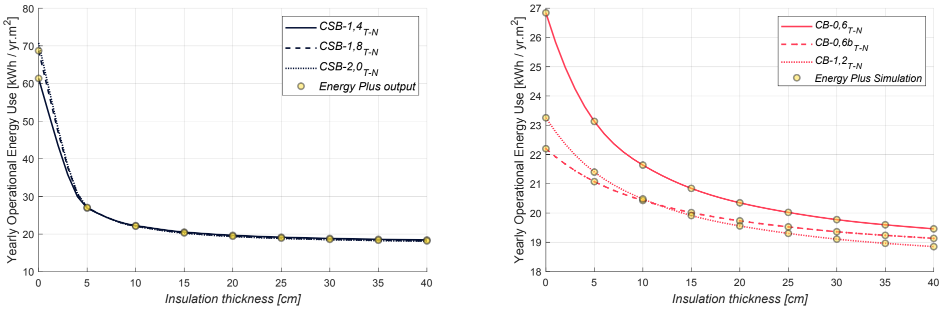
represents each emission or input flow. For each new calculation step, the additional embodied footprint related to the transport (E_T) and manufacturing (E_W) of the insulation material as well as the reduction of OE (E_{HVAC}) is considered in the analysis.

$$E_i = E_{i-1} + E_t \times \Delta M_{wi} + E_{HVAC} \times \Delta OE_i \tag{3.8}$$

Operational energy use in reference building

The open-source software Energy-Plus[5] was used to quantify the energy requirement profile of each wall combination. The building model selected for the simulation is the MOD-910, based on ASHRAE Standard [156]. This choice was made due to its well-documented theoretical design, which allows for a robust validation. The simulation utilized a typical meteorological year (TMY) from the Climate-OneBuilding database, representing the climatic conditions of Frankfurt [6]. Specific properties for the roof and floor construction systems are outlined in Table 3.9, while supplementary material provides additional details on windows glazing and the building characteristics. It should be noted that no distinction was made between thin joint mortar and normal mortar configurations, and the thermal coefficient of the brick was considered representative. Furthermore, this study did not explicitly model user behaviour, but set heating and cooling limit temperatures at 20 řC and 28 řC, respectively. Different insulation thicknesses were modelled as discrete scenarios and then interpolated via cubic spline in Matlab. The simulation results are shown in Fig. 3.10, where the yearly OE requirement for each wall profile in relation with the insulation thickness is displayed, while normalized to the buildings surface and HVAC efficiency. In this study, the seasonal coefficient of performance (SCOP) is set to 3, based on the technology average efficiency values reported by the STRATEGO project [157].

[5] https://energyplus.net
[6] https://climate.onebuilding.org



(a) Calcium silicate bricks (b) Clay bricks

Figure 3.10: Yearly Operational Energy requirement as a function of the insulation thickness

Sensitivity analysis and scenario descriptions

Sensitivity of indicators

One of the main benefits of the proposed methodology are the various possibilities to interpret the results and parametric studies that can be conducted. The fact that an LCA methodology is inherent deterministic where uncertainties are included in the input parameters and assumptions made, it is vital to understand up to what extent the results are reliable, and up to which degree they are modify with changes in the input parameters. For this, two approaches are followed. Firstly, the sensitivity of each mid-point and end-point indicator as a function of the insulation thickness was studied. All different indicators were normalized to their minimal value in order to be able to compare them in a single matrix. This type of analysis delivers valuable insights in the buildings environmental behaviour and should be included in any design process. Secondly, the influence of the main parameters dominating the results were studied. These were the electricity mix used for the buildings OE requirement, the SCOP considered for the HVAC system and the potential carbon sequestration of the lime-based materials.

Forecasted electricity mix and SCOP

As considered in the FU, the analysis represents the operation of a reference building for 50 years. This means that the energy provided to satisfy the OE requirement will be in accordance with Germanys electricity mix development. Looking at the countrys decarbonization pathway and recent energy polices [158], GHG neutrality will be achieved by 2045. In this study, this milestone was selected for the simulation. The corresponding distribution of the electricity mix and background data used is provided in Table A1. The SCOP of HVACs has a direct influence in the buildings OE requirement. As stated by the IRENA agency [113], one of the main strategies of Europe is to achieve climate neutrality with emphasis on the energy efficiency of buildings. For this reason, in this case study also the effect of an increasing SCOP is considered.

Lime carbonation

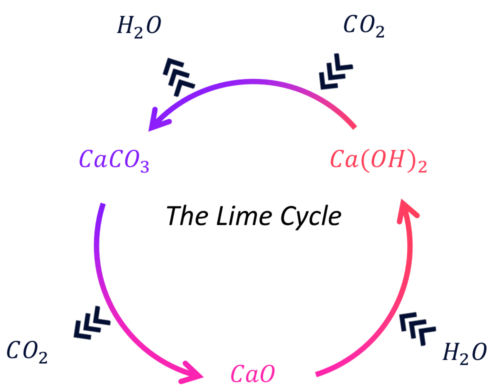
The lime cycle, represented in Fig. 3.11, theoretically allows for an infinite loop of limestone usage, resulting in net zero CO_2 emissions after a full cycle. In practice, the production of 1 tonne of lime generates approximately 1.2 tonnes of CO_2e emissions, which is nearly 1.53 times the process related emissions (786 kg CO_2e per ton CaO) and is due to the use of fossil fuels during the kiln operation and electricity generation [19]. A recent report published by EuLA [7], address different projects that examine the quantification of the carbonation potential of lime in different fields of applications. Furthermore, an extensive literature review on natural and enhanced carbonation of lime has been carried out by Grosso et al. [159] and Campo et al. [160] upon request of EuLA. According to this research, a carbonation rate between 80-92% and even 20-23% after 100 years, with affected material depths less than 191 mm can be expected for pure air lime mortars and mixed air lime mortars respectively. Moreover, while the carbonation potential of these materials is well studied, the one regarding calcium silicate bricks is less conclusive. In the latest roadmap published by the German CSB Association, based on 20 observations of CSB from 1903 onwards, a carbonation rate of 90% can still be expected after 50 years of service life [161]. Therefore, these values are also applied in the present simulation for evaluating the impact of the maximum disclosed carbonation potential of lime on the building's carbon footprint. For the case of MRP, Eq. 3.9 introduced by Grosso et al. [159], this was employed to estimate the carbonation potential after 50 years (CR50). The max CO_2 uptake modelled in this study are shown in Table 3.10. Based on the carbonation reaction of Fig. 3.11, around 0.59 kg of CO_2 will be absorbed for each kg of portlandite to form calcium carbonate. Here, *MCR* represents the maximum natural carbonation rate, *K* is the carbonation constant and *t* the time in days.

$$CR(\%) = \frac{MCR \times K \times \sqrt{t}}{depth} \tag{3.9}$$

[7] https://eula.eu/

Table 3.10: Maximal carbonation of lime-based construction materials

Material	MCR	K [mm/day]	CR50	Ca(OH)2 content [kg/FU]	Max CO2 - uptake [kg/FU]
Render	0.92	0.25	0.15	9.12	0.84
Plaster	0.92	1.00	0.62	12.16	4.49
CSB	-	-	0.90	42.55	22.77



$CaCO_3(s) \rightarrow CaO(s) + CO_2(g)$
$\Delta H^{o} = 177.8\ kJ/mol$ **Reaction 1**

$CaO(s) + H_2O(l) \rightarrow Ca(OH)_2\ (s)$
$\Delta H^{o} = -65.2\ kJ/mol$ **Reaction 2**

$Ca(OH)_2\ (s) + CO_2(g) \rightarrow CaCO_3(s) + H_2O(l)$
$\Delta H^{o} = -113.4\ kJ/mol$ **Reaction 3**

Figure 3.11: The Lime Cycle composed of three main reactions

3.2.4 Results and Discussion

Life Cycle Inventory

This section provides a detailed and transparent overview of the LCI developed for the present study. It summarizes each step during manufacturing of CSB and CB, following the procedure described above. Regarding the electricity mix, table A.1 (supplementary material) shows the relative amount of each energy source along with the background processes used to model its production. From this, Table 3.11 shows the LCI for the production of CSBs and Table 3.12 for CBs manufacturing.

Table 3.11: LCI - Calcium Silicate Brick manufacturing

CSB Manufacturing Process		Processed Amount Amount	Unit	Inventory Amount Amount	Unit	Source & Notes
Storage and mixing						
Input	Sand	9.10E-01	kg	9.10E+02	kg / t CSB	Resource, in ground
	Sand quarrying	1.13E-02	MJ	1.15E+01	MJ / t CSB	Ecoinvent - "diesel burned in building machine, APOS S, GLO"
	Sand | Transport by conveyor belt	3.64E-06	kWh	4.00E-03	kWh / t sand	Electricity Mix - SUBLime designed
	Lime	7.00E-02	kg	7.00E+01	kg / t CSB	Lime manufacturing - SUBLime
	Lime | Transport	6.65E-03	t.km	9.50E+01	km	Ecoinvent - "transport freight lorry 16-32 metric ton, EURO6, APOS S, RoW"
	Mixer operation	3.92E-03	kWh	4.00E+00	kWh / t CSB	Electricity Mix - SUBLime designed
Output	CSB - Dry Mix	9.80E-01	kg			
Reaction Vessel						
Input	CSB - Dry Mix	9.80E-01	kg			
	Water	2.25E-02	kg	3.22E-01	kg/kg lime	Ecoinvent - "tap water production, conventional treatment, APOS S, Europe without Switzerland"
Output	CSB - Wet Mix	1.00E+00	kg			
Pressing						
Input	CSB - Wet Mix	1.00E+00	kg			
	Press operation	7.12E-03	kWh	7.10E+00	kWh / t CSB	Electricity Mix - SUBLime designed
Output	CSB - Raw	1.00E+00	kg			
Autoclaving						
Input	CSB - Raw	1.00E+00	kg			
	Fresh water in steam	2.03E-01	kg	2.02E+02	kg / t CSB	Ecoinvent - "tap water production, conventional treatment, APOS S, Europe without Switzerland"
	Fuel | Steam generation	3.24E-01	MJ	3.24E+02	MJ / t CSB	Natural Gas: 95% Ecoinvent Heat and power co generation, natural gas 1MW electrical lean burn, APOS S, Europe without Switzerland
	Fuel | Steam generation	1.71E-02	MJ	1.70E+01	MJ / t CSB	Light Fuel Oil: 5% Ecoinvent heat production heavy fuel oil at industrial furnace, 1MW, APOS S, Europe without Switzerland
Output	CSB	1.00E+00	kg			

Table 3.12: LCI - Clay Brick manufacturing

CB Manufacturing		Processed Amount		Inventory Amount		Source & Notes
Process		Amount	Unit	Amount	Unit	
Clay Quarry						
Input						
	Clay	1.24E+00	kg	1.24E+00	t / t brick	Resource, in ground
	Clay quarrying | hydraulic excavators and dump trucks considered	1.04E-01	MJ	8.36E+01	MJ / t clay	Ecoinvent - "diesel burned in building machine, APOS S, GLO"
Output	Clay extracted	1.24E+00	kg			
Milling						
Input	Clay extracted	1.24E+00	kg			
	Prim. Crushing | Rotary Crusher	1.74E-03	kWh	1.40E+00	kWh / t clay	Electricity Mix - SUBLime designed
	Water	1.24E-02	kg	1.00E+01	kg / t clay	Ecoinvent - "tap water production, conventional treatment, APOS S"
	Sec. Crushing | Pan Mill	4.46E-03	kWh	3.60E+00	kWh / t clay	Electricity Mix - SUBLime designed
Output	Clay sized	1.25E+00	kg	1.23E+01		
Forming						
Input	Clay sized	1.25E+00	kg			
	Water	1.36E-01	kg	1.10E+02	kg / t clay	Ecoinvent - "tap water production, conventional treatment, APOS S"
	Forming | Extruder with mixer	3.01E-02	kWh	2.40E+01	kWh / t clay mix	Electricity Mix - SUBLime designed
	Cutting	1.63E-03	kWh	1.30E+00	kWh / t clay mix	Electricity Mix - SUBLime designed
Output	Green brick	1.39E+00	kg			
Drying & Firing						
Input	Green brick	1.39E+00	kg			
	Tunnel Kiln | Heat	2.11E+00	MJ	2.11E+03	MJ / t brick	Ecoinvent - Heat production natural gas at industrial furnace 100kW, APOS_S, Europe without Switzerland
	Tunnel Kiln | Operation	2.01E-02	kWh	2.01E+01	kWh / t brick	Electricity Mix - SUBLime designed
Output	Clay Brick	1.00E+00	kg			
	Water	1.49E-01	kg	1.20E+02	kg / t clay	Emission to air

Life Cycle Impact assessment

This section presents the life cycle impact assessment findings of the analysed wall compositions. For each wall type, the results are displayed as a function of the insulation thickness. The abbreviations used for each impact category are referenced in 3.5. The wall compositions with the best performance, using CSB and CB, were selected for the sensitivity analysis regarding the electricity mix composition, the SCOP efficiency, and the effective CO_2 sequestration by carbonation as discussed in previous sections.

Fig. 3.12 and 3.13 display all the mid-point and end-point impact scores of each analysed combination, while compared with the insulation thickness, respectively. Although the interpretation may seem challenging, some general information can be easily extracted. For instance, it can be seen that those impact categories that show considerable differences in the impact score for small insulation thicknesses are rather controlled by the OE requirement, because the insulation property of the CSB and the CB differ considerably. In fact, CSB-wall compositions require 3 times more energy when using insulation thicknesses between 0 and 5 cm. On the contrary, impact categories that show similar values for low amounts of insulation are rather MEF-controlled and are very sensitive to the addition of mineral wool. It is also possible to see that there is a dependency between the MEF and the OE requirement of the building for each analysed environmental impact. Moreover, the optimal thickness insulation is lower for clay bricks than for calcium-silicate bricks because of their lower thermal conductivity. The wall combinations that employ thin layer mortar (represented by dashed lines) consistently produce environmentally friendlier results compared to the same wall systems with normal joint mortar. Despite having a higher cement content in the thin layer mortar mix, the lower material requirements in the functional unit (see Table 3.7) leads to better environmental outcomes. Furthermore, the structural performance of thin layer mortars is higher when considering the characteristic compressive strength of masonry, which makes the equivalent thickness lower and is thus lowering the amount of material needed to satisfy the same FU.

It is observed that in some impact categories such as TAP, ODP, NRE and IR, a better environmental performance can be reached with CSB even with a higher amount of insulation placed. However, on the contrary, when considering HT-Cancer, LO, ME and POCP, clay bricks perform better when employed in their optimum combination. When looking at AP, ET, EP, GWP, HT-NonCancer, RI and TETP, similar behaviour can be reached for both type of bricks when selecting the appropriate insulation thickness. To explain this behaviour, a connection between mid-point and end-point scores is reported.

Human health (HH) related impacts

The HH end-point score is a linear combination of HT-Cancer, IR, HT-NonCancer, ODP, RI and POCP and is represented in terms of DALY (Disability-Adjusted Life Years), which is calculated by the mortality and morbidity that characterizes the disease severity [127]. From the aforementioned mid-point indicators, HH is heavily controlled by the human toxicity indicators, namely HT-NonCancer and HT-Cancer (around 80% and 6% of the impact score, respectively) and the particle matter formation, RI (around 10%). It can be seen that the dominant process governing HT-NonCancer and thus the HH indicator is the OE requirement, followed by the mineral wool manufacturing process. Therefore, the interaction between OE consumption and insulation happens at low values of the insulation thickness, while the absolute value of the indicator reaches a better performance for the CB wall composition. When looking at the HT-NonCancer of the CSB and CB, similar values can be found, namely 0,09 and 0,10 kg C2H3Cleq. Interestingly, the main chemical substance controlling this indicator is the arsenic ion emitted to the surface water during electricity production, especially in the case of biofuel and hard coal usage. On the contrary, when looking at the HT-Cancer, the main affecting process is the combustion of natural gas emitting aromatic hydrocarbons in the air. For this reason, the partial contribution of CB is around 1.7 times as much as those related to CSB (0.19 kg C2H3Cleq vs 0.11 kg C2H3Cleq). Again, the contribution of lime production inside CSB manufacturing is considerable. Regarding the particulate matter formation, represented by the IR indicator, the electricity production which uses 25% of hard coal as fuel is predominantly responsible of the generation of fine particulates. Moreover, the quarrying operation for sand obtention in both the CSB and CB manufacturing process releases high amounts of nitrogen oxides which also contributes to this indicator.

Ecosystems quality (EQ) related impacts

With the EQ indicator, the LCA analysis aims to understand the potential damage to biodiversity loss. By looking at the results along with the conversion factors from Table 3.5, it can be seen that the governing mid-point category is LO, which is responsible for 90% of this impact. This indicator is heavily controlled by the electricity production, in particular the biofuel process. For this reason, the LO impact score shows a decreasing tendency with increasing insulation thickness. This behaviour is further extrapolated to the end-point indicator.

Resource availability (RA) related impacts

The RA or requirement is an unweighted combination of the NRE and ME requirement. When looking at the mid-point values in Fig. 3.12 it becomes clear that the end-point impact category is controlled by the NRE. This impact category accounts for the extracted total non-renewable primary energy. As can be seen, this indicator is heavily depending on the OE requirement, since around 43% of the electricity used in the building comes from non-renewable sources such as hard coal and/or natural gas. Nevertheless, there is a substantial contribution related to the material production, which can be observed when looking at the minimum score of each combination. In fact, the NRE requirement for CSB production to fulfil the systems FU is around 294 MJ, while the corresponding for CB is almost 500 MJ. This difference can be explained by comparing the two manufacturing processes. As it is shown in the LCI, the amount of energy requirement during autoclaving CSB is around 6,18 times less than the amount needed for firing CB. Moreover, the biggest contribution to the CSB NRE-footprint is related to the lime production rather than to the bricks themselves, which requires almost half of the energy (140 MJ) for operating the lime kiln. The natural gas alone needed for the CB firing process makes up 317 MJ, while the rest comes from the electricity production (129 MJ) and diesel combustion during the quarrying of clays (47 MJ).

Climate Change (CC)

The CC endpoint category displays the same result as the mid-point indicator GWP. As a reference, 1000 kWh of OE electricity consumption, which corresponds to 20 kWh per m2 per year times 50 years of service life, produces around 407 kg of CO_2e emissions. More than 90% of these emissions are generated by the hard coal (259 kg CO_2e) and natural gas (113 kg CO_2e) combustion. This highlights the significance of the OE requirement as a driver to reduce the buildings stock carbon footprint. When looking at the CSB and CB manufacturing process, it can be observed that the energy requirement of CB production is much higher than the one of CSB. This is because of the higher temperature needed during the firing process, where roughly 17.8 kg CO_2e are emitted to produce 340.9 kg of CB, represented by the CB-1.2T wall combinations (Fig. 3.13). Moreover, the production of 460 kg of CSB in the case of the CSB-2.0T, releases almost 42.5 kg of CO_2e emissions, from which the manufacturing of lime is responsible for almost 35.0 kg, which is more than 80% of the GHG emissions of the CSB manufacturing process. From this, each cm of mineral wool added to the wall cross section adds around 1.2 kg CO_2e. For this reason, the threshold between OE and MEF tends to higher insulation thickness, especially for the CSB wall combinations.

Single score point

The single score point, displayed in Figure 8, facilitates the comparison across different impact categories. In fact, it represents the tendency previously mentioned, without providing specific details on the different impact indicators. It summarizes the results of the assessment into one single numerical value, related to the total impact of a certain category divided by the European population [127]. Both the CSB-2.0T and CB-1.2T wall compositions present the best environmental performance, here represented by the lowest number of points, and will, therefore, be considered for a detailed analysis.

Sensitivity analysis and scenarios results

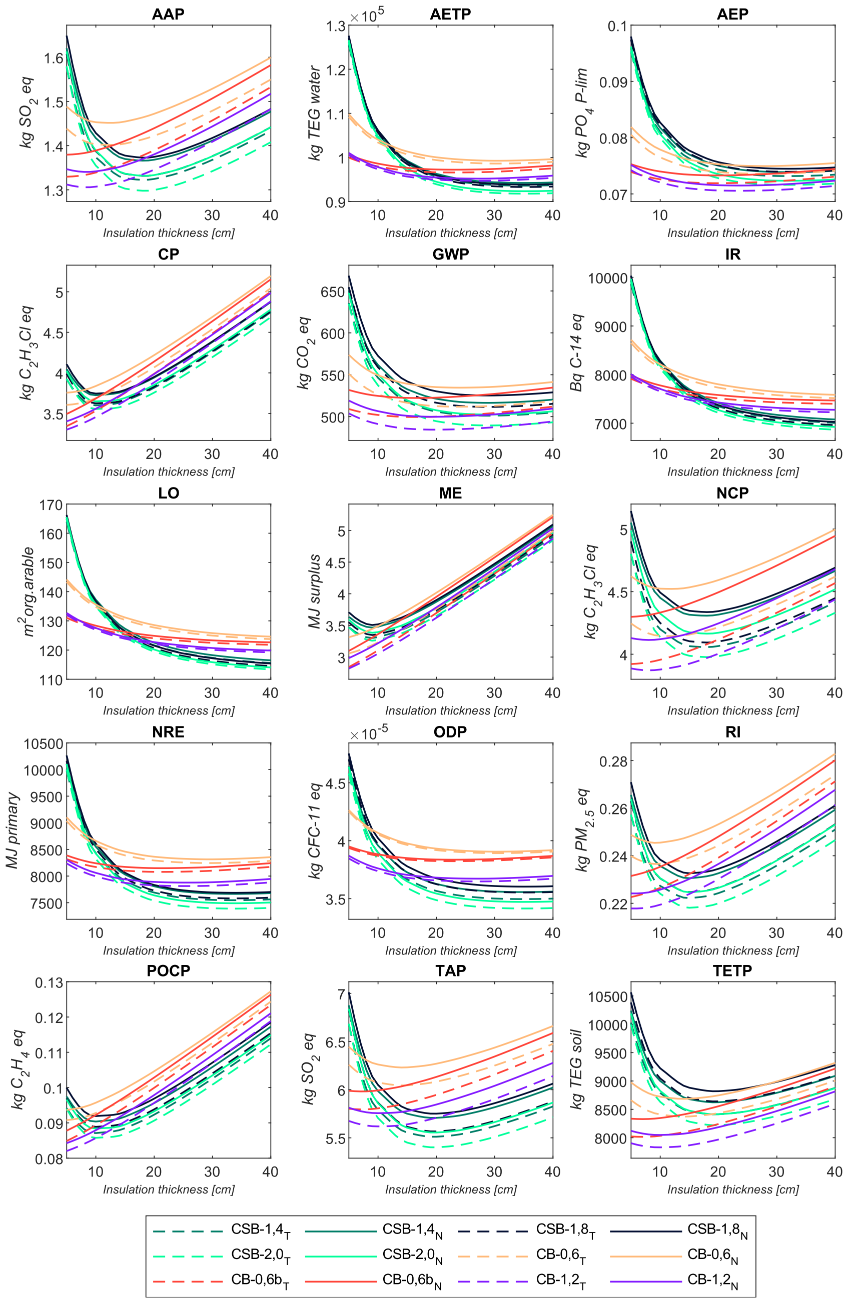


Figure 3.12: Mid-point impact scores for the reference wall combinations per FU

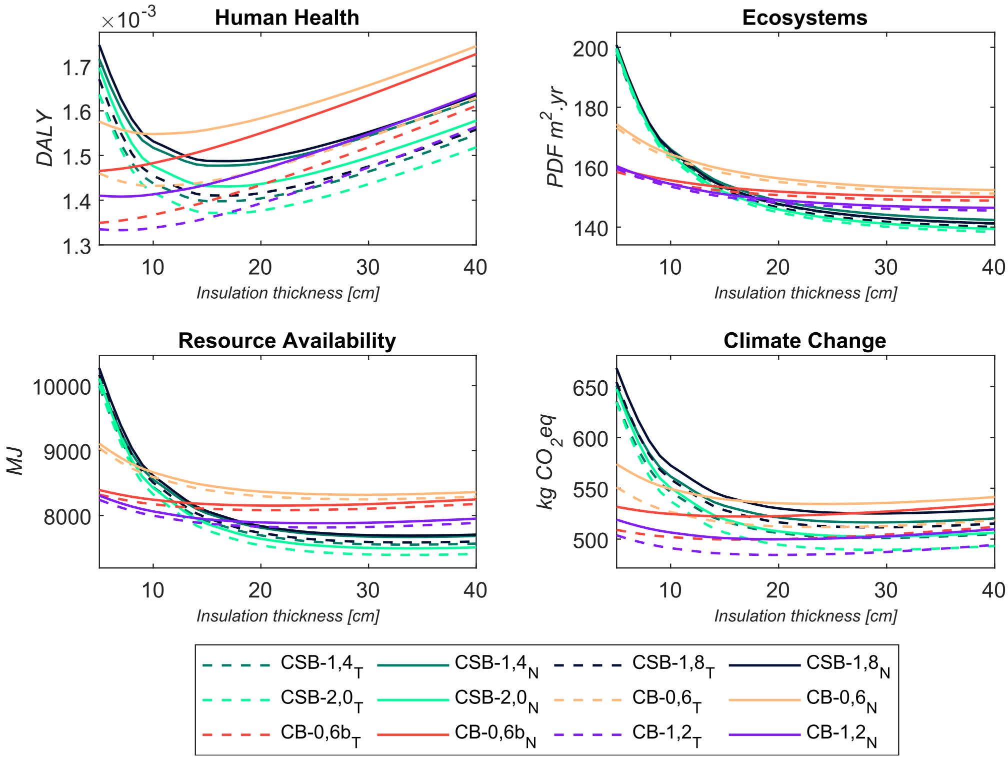


Figure 3.13: End-point areas of damage for the reference wall combinations per FU

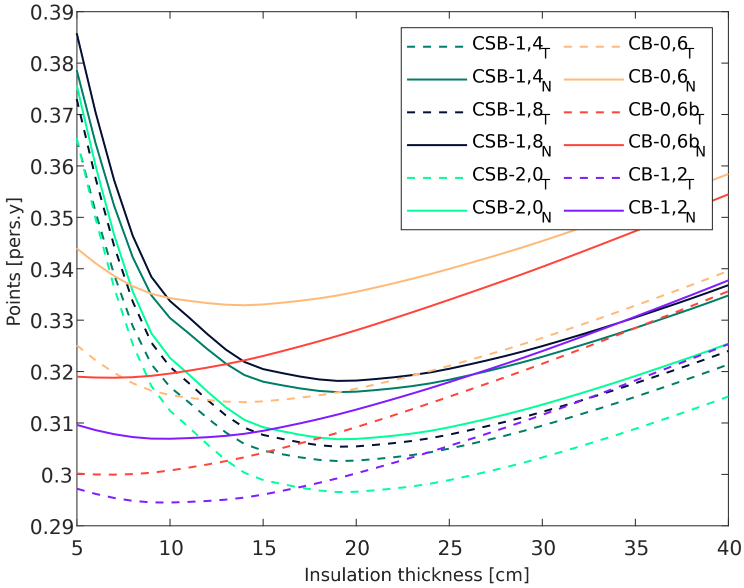
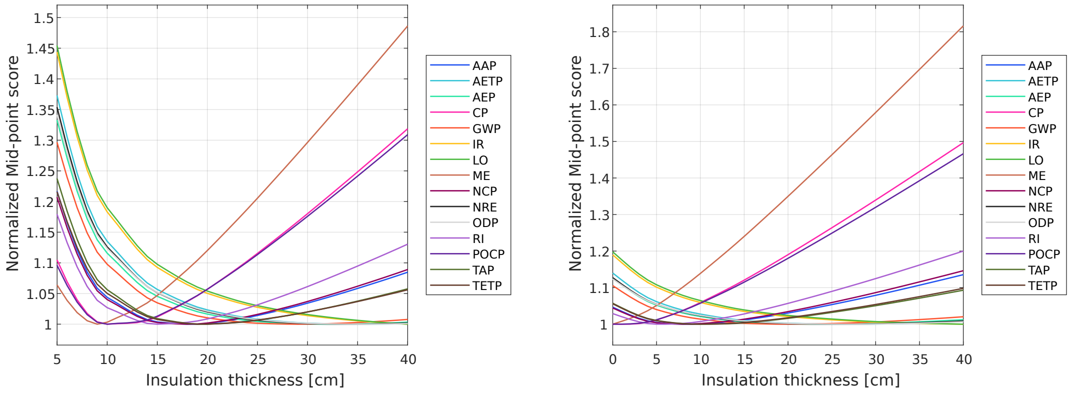


Figure 3.14: Single score for the reference wall combinations per FU

Fig. 3.15 shows the variation of each mid-point indicator for the two selected walls as function of the insulation thickness (CSB-2.0T and CB-1.2T). For both cases it can be observed that a first group of impact categories such as LO, IR, ET, EP, GWP, ODP and NRE are OE-controlled, meaning that they benefit from an increase in the insulation thickness and a consequential lower OE requirement. In fact, even if the insulation thickness reduces beyond the optimal solution, the expected increase in the impact score is below 1.03 times the optimum one. As discussed before, these indicators are heavily related to the non-renewable electricity consumption and therefore represent such behaviour. A second group of impact categories like AP, HT-NonCancer, RI, TAP, TETP, are in a balanced position, where they benefit from the reduction of the OE requirement up to a certain threshold where the MEF begins to dominate it. Along with this, in both directions these indicators can increase between 1.05 to 1.20 times the value of the optimum solution. A third group are the impact categories ME, HT-Cancer and POCP that can be highlighted as MEF-controlled, particularly because of the use of mineral wool as insulation material. These indicators have optimum solutions values at the lower range of insulation thickness and can increase their absolute value up to 1.5 to 1.8 times for CSB and CB respectively. The HT-Cancer is heavily affected by high amounts of aromatic hydrocarbons, especially benzo(a)pyrene, emitted to the air during the stone wool manufacturing. Similarly, the emissions of non-methane volatile organic compounds (NMVOC) are strongly responsible for the rapid increase of the POCP impact score. Regarding the ME category, although aluminium is the most occurring metal in the manufacturing of mineral wool (0.015 kg per kg of insulation), the use of copper is as critical because of its over 15 times higher impact conversion factor to the MJ surplus. Fig. 3.16 shows the analogue analysis at end-point categories. It can be observed that the EQ, RA and CC indicators are OE-controlled and therefore any measure taken to reduce the energy requirement of the building will positively affect these indicators. On the contrary, when looking at HH, the selection of materials plays a determining role and over-dimensioning the mineral wool thickness can lead to an increase of the damage to human health of up to a factor 1.18.

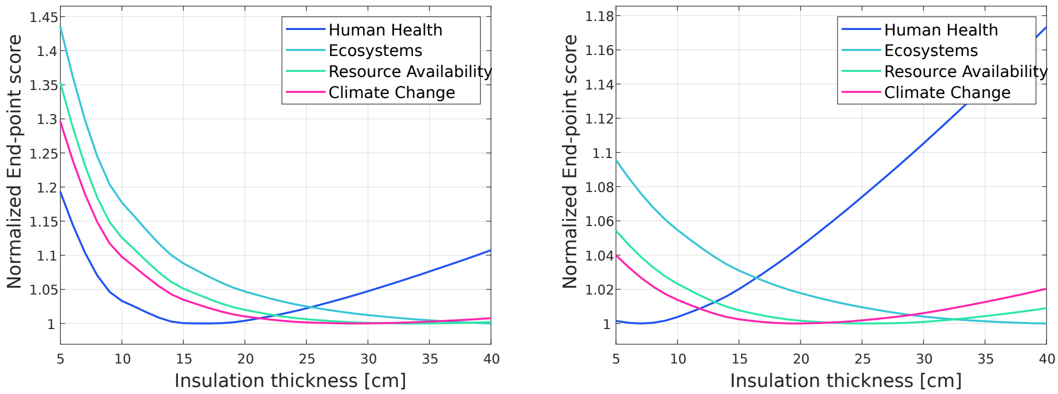
Contribution analysis

In terms of interpretation of LCA results, the contribution analysis is a key aspect. It allows to further understand and explain the relationships between mid-point, end-point and processes considered within the system boundary. The following sections analyse the contribution analysis related to the different sensitivity scenarios described before. Results regarding end-point categories are given in Table 3.13. Additionally, Figures A1 to A4 show the contribution of the mid-point and end-point environmental impacts on the different components of the walls. It can be seen, that the optimum insulation thickness for walls made with CSB ranges from 9 to 40 cm, while for CB this ranges from 0 to 29 cm, which is consistent with the previous results. Choosing any extreme of this range may result in an increase of more than 125% of the impact in the OE-controlled categories. Secondly, OE usage has a significant contribution to nearly



(a) $CSB-2.0_T$ (b) $CB-1.2_T$

Figure 3.15: Normalized Mid-point impact score for



(a) $CSB-2.0_T$ (b) $CB-1.2_T$

Figure 3.16: Normalized End-point impact score for

every impact category, with the production of mineral wool being the second largest contributor, particularly for mid-point categories of HT-Cancer, ME and POCP. Lastly, the MEF accounted for 4 to 13% of the total end-point impact, highlighting the importance of considering both MEF and OPE in a comprehensive evaluation of the environmental impact of buildings.

Electricity mix forecasting and SCOP efficiency

Table 3.13: End-point scores for the reference and forecasted scenarios

End-point per FU		CSB-2.0T					CB-1.2T				
HH [DALY]		Total	MEF	OE	M. wool	topt [cm]	Total	MEF	OE	M. wool	topt [cm]
Reference	Emix ǀ 2020	1.37E-03	1.29E-04	1.06E-03	1.78E-04	17	1.33E-03	1.33E-04	1.13E-03	7.34E-05	7
Scenario 1	Emix ǀ 2050	9.22E-04	1.29E-04	6.46E-04	1.47E-04	14	8.59E-04	1.34E-04	6.84E-04	4.19E-05	4
	Reduction	33%	0%	39%	18%	18%	36%	0%	39%	43%	43%
Scenario 2	SCOP 10	5.87E-04	1.29E-04	3.63E-04	9.44E-05	9	5.08E-04	1.34E-04	3.75E-04	0.00E+00	0
	Reduction	57%	0%	66%	47%	47%	62%	0%	67%	100%	100%
EQ [PDF m2 yr]											
Reference	Emix ǀ 2020	1.38E+02	3.75E+00	1.30E+02	4.99E+00	40	1.46E+02	5.40E+00	1.35E+02	4.99E+00	40
Scenario 1	Emix ǀ 2050	4.85E+01	3.76E+00	4.10E+01	3.75E+00	30	5.12E+01	5.41E+00	4.33E+01	2.49E+00	20
	Reduction	65%	0%	68%	25%	25%	65%	0%	68%	50%	50%
Scenario 2	SCOP 10	4.73E+01	3.76E+00	3.99E+01	3.62E+00	29	5.00E+01	5.41E+00	4.21E+01	2.49E+00	20
	Reduction	66%	0%	69%	27%	28%	66%	0%	69%	50%	50%
RA [MJ]											
Reference	Emix ǀ 2020	7.39E+03	5.24E+02	6.35E+03	5.18E+02	34	7.82E+03	7.37E+02	6.70E+03	3.80E+02	25
Scenario 1	Emix ǀ 2050	1.20E+03	5.26E+02	5.34E+02	1.37E+02	9	1.29E+03	7.38E+02	5.50E+02	0.00E+00	0
	Reduction	84%	0%	92%	74%	74%	84%	0%	92%	100%	100%
Scenario 2	SCOP 10	2.84E+03	5.26E+02	2.03E+03	2.89E+02	19	3.02E+03	7.38E+02	2.15E+03	1.37E+02	9
	Reduction	62%	0%	68%	44%	44%	61%	0%	68%	64%	64%
CC [kg CO2e]											
Reference	Emix ǀ 2020	4.89E+02	7.58E+01	3.78E+02	3.53E+01	29	4.84E+02	6.13E+01	3.99E+02	2.43E+01	20
Scenario 1	Emix ǀ 2050	1.26E+02	7.60E+01	3.91E+01	1.10E+01	9	1.02E+02	6.14E+01	4.03E+01	0.00E+00	0
	Reduction	74%	0%	90%	69%	69%	79%	0%	90%	100%	100%
Scenario 2	SCOP 10	2.18E+02	7.5 9E+01	1.22E+02	1.95E+01	16	1.98E+02	6.14E+01	1.28E+02	8.52E+00	7
	Reduction	55%	0%	68%	45%	45%	59%	0%	68%	65%	65%
Scenario 3	S1 + S2 + carbonation	6.80E+01	4.79E+01	1.41E+01	6.09E+00	5	6.57E+01	5.61E+01	1.21E+01	0.00E+00	0
	Reduction	86%	37%	96%	83%	83%	86%	9%	97%	100%	100%

Figures 3.17 and 3.18 show the relative contribution of the OE use, embodied material, and insulation manufacturing to the four endpoint categories in the forecasted electricity mix scenario. As can be observed, there is a general trend in all categories for less insulation thicknesses as the optimum solution. Moreover, Table 3.13 shows the absolute amount of each indicator along with the reduction percentage of the different scenarios, when compared with the reference case. It can be observed that increasing the SCOP (scenario 2) leads to better results in terms of HH and EQ while decarbonising the electricity mix (scenario 1) affects RA and CC in both types of walls. This is explained by a reduction of the optimum insulation thickness for each scenario.

Regarding scenario 1, the direct impact of OE decreases between 39% to 92% depending on the analysed damage area. This has two different effects: Firstly, it helps to reduce the final environmental performance directly between 33% (HH) and 84% (EQ). Secondly, it promotes the reduction of the threshold between MEF and OE, inducing a decrease in the amount of insulation required and therefore further reducing its environmental impact. Particularly for the RA and CC impact categories, the role of the MEF in scenario 1 represents the largest contribution. This can be explained by the fact that by decreasing the amount of fossil fuels used to deliver the OE requirement, both the CO_2e footprint and the NRE use decreases more than 90%. It should be mentioned that although the considered mix relies only on renewable energy sources, neither the GWP nor the NRE is zero. For instance, the production of electricity by solar energy requires natural gas to operate the plant, which will directly affect both indicators.

Moreover, it turned out that the MEF environmental performance without the insulation remain the same in absolute terms although its relative share of the final environmental impact increased for all cases. This highlights the role that construction material manufacturing will play in the coming decades. In fact, when looking at Fig. 3.18 the optimum insulation thickness for RA and CC is zero. This means, that the mineral wool production plays a decisive role in the building design. Such findings can justify the need to consider bio-based or mineral insulation materials.

Regarding scenario 2, the increase in HVAC efficiency has positive effects on all end-point impact categories, especially in the ones that are more affected by mineral wool production. The reduction potentials range between 57% and 66% for HH and EQ respectively. The latter corresponds to a reduction in the insulation thickness from 40 cm to 29 cm and 20 cm for CSB and CB respectively, with an added drop of the OE relative contribution. It can be seen that, although the main driver behind the use of renewable energy sources for the electricity production is the decarbonization of the German industry, this also leads to other benefits which include the reduction of potential damage to human health and ecosystems.

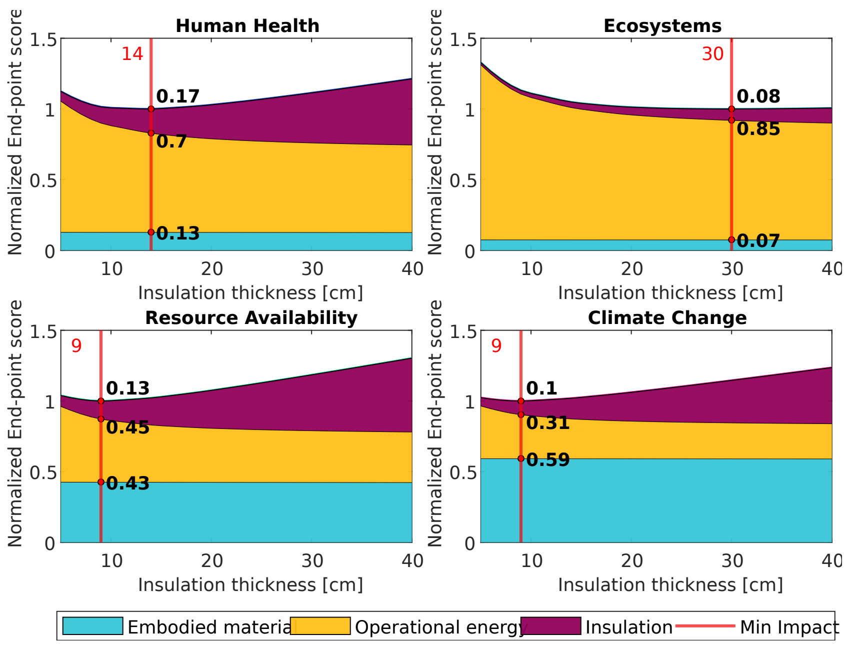


Figure 3.17: Normalized end-point impact scores and contribution analysis per FU for CSB-2.0T and 2050 forecasted electricity mix

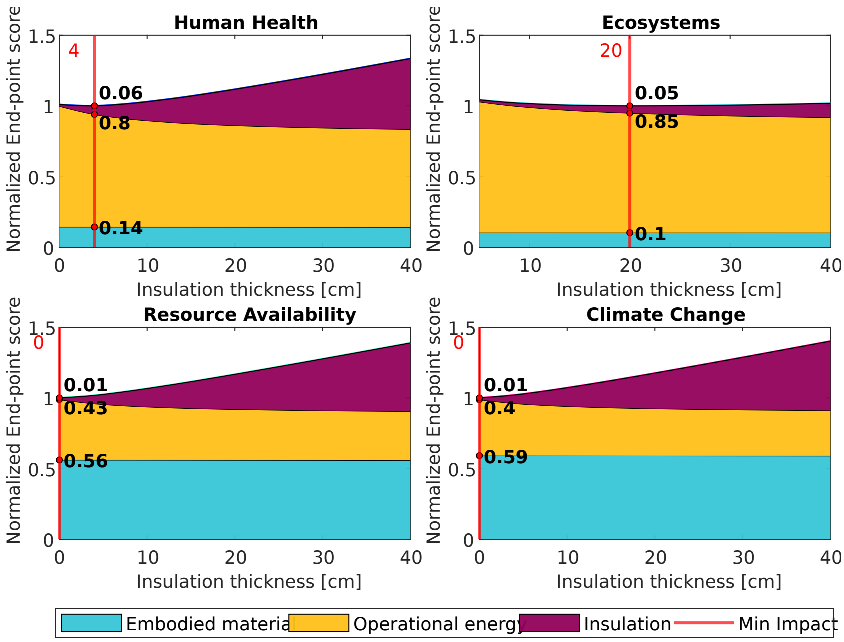


Figure 3.18: Normalized end-point impact scores and contribution analysis per FU for CB-1.2T and 2050 forecasted electricity mix

Carbonation

The contribution of the carbonation potential is analysed for the GWP mid-point indicator, since CO_2 emissions to the air are not considered in other impact categories. Two scenarios are shown in Fig. 3.19 and 3.20. First, the reference scenario with the current electricity mix and a SCOP of 3 is analysed. Then, the addition of scenario 1 and 2 are modelled and introduce scenario 3, which is shown in Table 9. It can be appreciated, that the carbonation of the render and plaster layers contribute to 1% of the FU carbon footprint. For the case of CSB-2.0T wall, this value increases up to 5% with the additional carbonation of CSB. If a fully renewable electricity mix is considered and the HVAC systems efficiency is increased to 10 (scenario 3), the relative contribution of the carbonation potential increases. It can be seen, that the absolute GWP impact decreases from 489 to 68 kg CO_2e per m2. In this context, the relative contribution of CSB carbonation plays a major role, namely more than 20% of the total impact. Additionally, the CO_2e uptake of the render and plaster is approximately 7% of the total emissions. These results suggest, that even if the maximum potential carbonation of lime-based materials is considered, the CO_2 uptake suffers from an attenuation effect when analysed at a building scale in the current scenario. Firstly, because the amount of material used is much lower than the structural and insulation ones and secondly because the role of the MEF in general is dominated by the OE requirement footprint. Furthermore, since a large share of the GHG emissions linked to lime manufacturing is produced by the combustion of fossil fuels in the kiln, there is a remaining amount of CO_2 that will not be re-captured. This finding highlights the importance of developing low-carbon content fuels and carbon capture strategies in the lime manufacturing industry. Finally, results also highlight the significance of the potential role that carbonation of CSB can play in the future. For this reason, more research is needed to comprehend and quantify the carbonation potential of these materials.

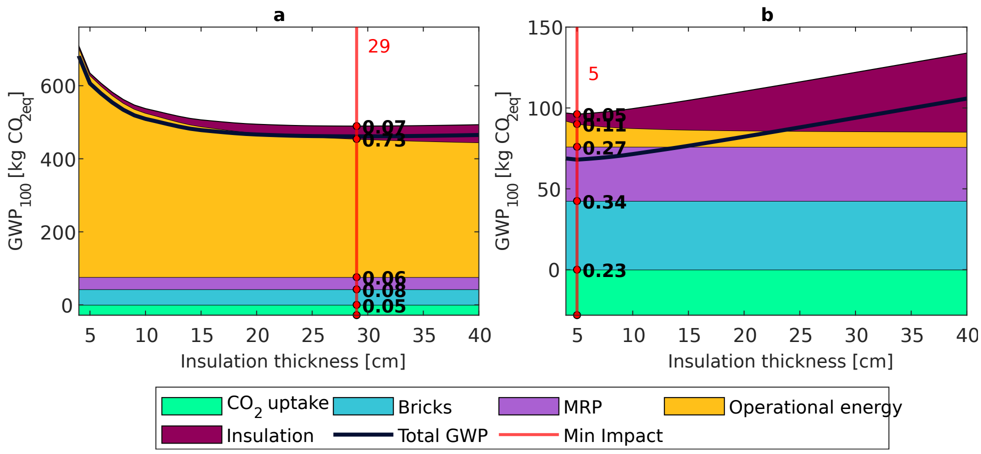


Figure 3.19: GWP per FU for $CSB-2.0_T$ with CO_2 uptake: a) Emix-2020, SCOP=3.0 b) Emix-2050, SCOP=10

3.2.5 Limitations

It should be noted that the presented results have certain modelling limitations. Firstly, some buildings elements were excluded from the LCA analysis as specified in the system boundary definition (Fig. 3.9). Secondly, the carbonation potential of CSBs was based on the maximum reported values found in literature and did not explicitly consider the presence of render layer on top of the bricks, potentially leading to lower carbonation values. Lastly, this paper deliberately omitted end-of-life scenarios, as its main focus was to model the interaction between process-based manufacturing and use-stage performance of building materials. However, exploring end-of-life scenarios remains a potential avenue for future research.

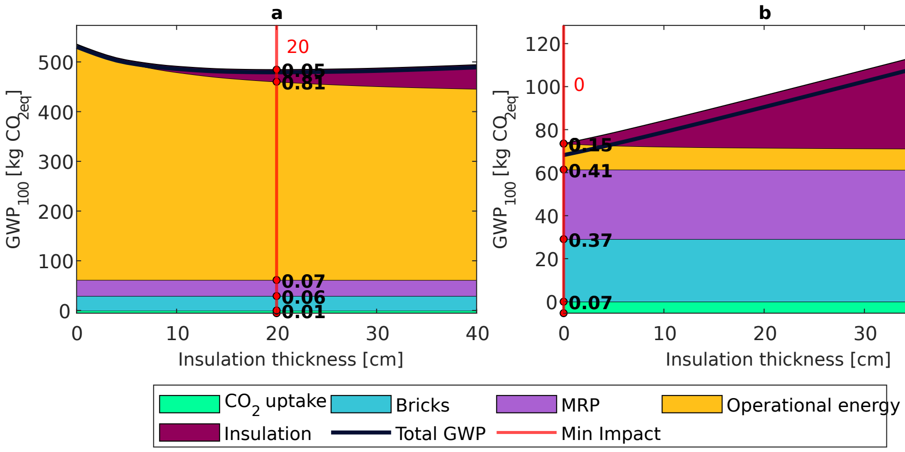


Figure 3.20: GWP per FU for $CB-1.2_T$ with CO_2 uptake: a) Emix-2020, SCOP=3.0 b) Emix-2050, SCOP=10

3.2.6 Conclusions

From the results of this study, the following conclusions can be drawn:

Coupling methodology

- By defining the manufacturing process of any construction material and linking it with OE requirement simulation at the building scale, comprehensive insights on the environmental performance can be achieved at an early stage of design.
- A link between MEF and OE exists, which, in this study, is represented by the insulation thickness, but its definition will depend on the environmental impact category considered. Mid-point impact categories like LO, IR, ET, EP, GWP, ODP and NRE are rather controlled by the OE requirement, while ME, carcinogenics and POCP by the MEF. Moreover, at end-point and mid-point levels, this study provides valuable insights that cannot be obtained when looking at a SS only.

Life Cycle Inventory and impact assessment

- A process-based LCI was successfully develop for the manufacturing of CSB and CB, providing valuable data that can be employed by different stakeholders to analyse the environmental performance of such materials.

- Thin-layer mortars outperformed normal joint mortars in every impact category. From the 12 different wall compositions, CSB-2.0T and CB-1.2T consistently delivered the best results in their respective groups after considering the masonry vertical load capacity with the equivalent thickness method.

- Looking at end-point areas of damage, CSB-2.0T performed better in terms of EQ and RA, while CB-1.2T did so for HH and CC. This is due to energy requirement during the firing of CB which heavily depends on fossil fuels. In addition, the lime manufacturing process is responsible for more than 80% of the GHG emissions of the CSB.

Scenario analysis

- A transition towards renewable-based energy sources for electricity production may significantly contribute to reductions of damage to HH, EQ, RA and CC of 33%, 65%, 84% and 74% respectively. This also leads to a reduction of the amount of insulation material required to achieve the best environmental performance of a building.

- The use of more efficient HVAC systems leads to a major relative effect of the MEF in the total environmental impact outcome of the masonry unit, resulting in a drop in optimum insulation thickness.

- Lime-based plasters and renders have a limited capacity to reduce CO_2 emissions by carbonation, with only around 1% reduction at the building scale in the reference scenario. However, if the carbonation potential of CSB would be fully realized, it can have a significant impact on the GWP indicator, leading to a 5% reduction in GHG emissions in the reference scenario. This effect can be further enhanced by combining it with a high HVAC efficiency (with a SCOP of 10) and 100% renewable-based sources for the buildings OE, resulting in a total reduction of 86

CRediT authorship contribution statement

Luciano Sambataro: Conceptualization, Methodology, code development, and processing, LCI, LCIA, discussion, Writing original draft, paper preparation, Writing review and editing, results and discussion. Agustin Laveglia: Review and editing, results and discussion. Neven Ukrainczyk: Resources, Writing review and editing, results and discussion and Supervision. Eddie Koenders: Resources, Writing review and editing, results and discussion, Supervision.

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

Data will be made available on request.

Acknowledgements

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Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.enbuild.2023.113287.

3.3 Publication 3: Environmental benchmarks for the European cement industry

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3.3.1 Abstract

The urgent need to address climate change has pushed Europe to the forefront of environmental legislation initiatives, such as the Environment Action Program (EAP) within the European Green Deal and the disclosure of Environmental Product Declarations (EPDs) in the construction sector. The cement industry plays a vital role in this transition because it is one of the biggest contributors to greenhouse gas emissions worldwide. EPDs have managed to articulate the environmental information flow across different stakeholders, allowing them to incorporate sustainability design practices at the manufacturing, construction, and design levels. However, current EPDs are deterministically disclosed and lack benchmarks, hindering effective comparison and impeding sustainable material development. To address this challenge, the present research introduces a novel Life Cycle Assessment (LCA)-based probabilistic analysis to develop clinker and cement benchmarks. The proposed method incorporates data from industry reports, environmental databases, and EPDs, to generate the stochastic benchmarks. Moreover, a wide range of environmental performance indicators at a national level in Europe are covered, offering a holistic perspective beyond climate change. The results highlight the benefits of using country-specific environmental benchmarks, reducing the standard deviation of results by 2 to 7 times compared to background datasets. The reduction of clinker content proved to reduce 7 to 9 kg CO_{2eq}/t for every 1% reduction in all countries. However, it also increased other indicators depending on the mineral component used as a replacement, underscoring the need for holistic analysis. The research also exposes discrepancies between EPDs and industry-related data, accentuating the need for stochastic information disclosure to enhance reliability and facilitate decision-making by stakeholders. Another significant contribution of this research is the development of an extensive open-access database, providing a reference for future developments regarding sustainable cement and concrete.

3.3.2 Introduction

The consequences of climate change are visible today. The International Panel on Climate Change (IPCC) reported a surge in global adverse impacts on health and wellbeing on cities, settlements, and infrastructure linked to climate change in their latest report [162]. Moreover, the recent update on the planetary boundaries framework [1], first introduced by Rockström et al. [2], reveals that Earth is already surpassing high-risk zones concerning biosphere integrity, novel entities, biogeochemical cycles, land system change, and freshwater change, besides climate change. In this context, Europe is taking a lead role by introducing cutting-edge legislation to accelerate the transition toward a balanced relationship with the environment. Key initiatives include the Environment Action Programme (EAP), built on the European Green Deal, the Circular Economy Action Plan, the EU Industrial Policy, and the European Climate Law.

The cement industry plays a decisive role in this transition. On the one hand, it contributes nearly 7% of global anthropogenic greenhouse gas emissions [5]. On the other hand, cement stands as the worlds second most used substance, after water, enabling cost-effective and energy-efficient infrastructure development [6]. Despite these advancements, challenges persist in integrating environmental data into the early stages of building design. Environmental Product Declarations (EPDs) have emerged as pivotal tools, employing the Life Cycle Assessment (LCA) methodology [30] to quantify the environmental impacts throughout a products life cycle. However, EPD information is typically presented as deterministic values, and, due to confidentiality concerns, the specific input data used for the calculations is not disclosed. Consequently, architects and designers face an arduous challenge when attempting to compare EPDs across different products, as there is a lack of reference scenarios and harmonization [163]. This challenge extends to product designers, who in turn struggle to define precise and accountable environmental targets, thereby hindering the transition towards more sustainable construction materials and practices. In addition, there is an absence of a standardised environmental design methodology that incorporates the inherent uncertainty in the environmental performance of different construction products.

Considering uncertainty in LCA is not new. Weidema and Wesnaes [84] presented a framework for the inclusion of data quality indicators (DQIs) to account for the reliability of the information. This approach was further developed by Coulon et al. [85] and Canter et al. [86]. The former called for improved transparency in LCA studies, while the latter presented a stochastic model to strengthen the LCA inventory phase, emphasising key processes in the final output. Uncertainties in LCA are divided into parameter, scenario, and model uncertainties, and all of them have a direct influence on the LCA results [42, 82]. Sugiyama et al. [164] suggested using statistical inputs to reveal uncertainty-related information in industry-based Life Cycle Inventory (LCI), enhancing transparency while preserving data confidentiality. Recent developments, such as the probabilistic-based framework for EPD comparison suggested by AzariJafari et al. [43], have aimed to provide a more comprehensive and robust comparison of different products by including the uncertainty of different sources. However, as the authors acknowledged, the selection of the LCI database plays a vital role in the comparison.

Examining the cement environmental footprint, Geng et al. [100] demonstrated considerable variability in the clinker carbon footprint in China, ranging from 750 to 840 kg CO_2/t. This variability manifests as a variable embodied footprint at the building level later on [95]. Moreover, Zhu et al. [92] showed that using standard CO_2 emission factors could overestimate China's national emissions by as much as 40% when compared to the ones derived from the stochastic analysis on carbon content, heating value, and oxidation value of hard coal fuel. This suggests that the use of stochastic analysis could yield much more accurate results. In the United States, DeRousseau et al. [101] disclosed that the cement carbon footprint ranges between 640 and 1000 kg CO_2/t, with a higher frequency observed between 755 and 820 kg CO_2/t. However, details regarding the variability of additional environmental burdens were overlooked and remain limited in numerous LCA studies, stressing out the need for comprehensive assessments beyond the carbon footprint.

Interest is growing in fostering closer collaboration between construction materials manufacturers and building designers by incorporating Key Environmental Performance Indicators (KEPIs) in the form of EPDs. This aligns with Europes strategic focus on developing sustainable construction materials. However, realising this goal demands two critical components, currently missing in the European context: i) establishing a reference benchmark to facilitate a comprehensive environmental performance comparison; and ii) implementing stochastic analysis for robust reliability studies.

This research aims to introduce an LCA-based probabilistic benchmark of the environmental impact of clinker and cement manufacturing in Europe. This novel methodology intends to overcome traditional deterministic LCA study limitations by covering the full spectrum of expected environmental impact frequencies and indicators. The multi-step approach integrates diverse data sources, including industry reports (IRs), environmental databases (EDBs) and EPDs to generate and validate the stochastic benchmarks. Different KEPIs are studied on a country level, extending beyond the current climate change focus and improving the granularity of data availability in the European context. A holistic environmental study of 300 existing EPDs is conducted, and an extensive database is generated and disclosed, serving as a reference for different stakeholders and future developments, including net-zero concrete materials.

3.3.3 Methodology

In this study, a stochastic LCA is conducted to analyse the manufacturing of clinker and cement in Europe at the country level. The framework developed for this research is illustrated in Fig. 3.21. Three different sources of information are used and statistically compared. First, IRs are analysed (Level 1). The most recent industry report from *Getting the Numbers Right* (GNR) [165] is employed for clinker and cement, providing statistical insights into fuel and electricity consumption during their production in Europe. This information is complemented with background environmental data from Ecoinvent v3.9 to translate it into KEPIs. Then, Ecoinvent v3.9 is used as EDB (Level 2), where relevant activities and emissions are stochastically transformed into KEPIs. A preliminary comparison is made between Level 1 and Level 2 data. Finally, over 300 current EPDs (Level 3) are analysed, contributing to a conclusive comparison and validation.

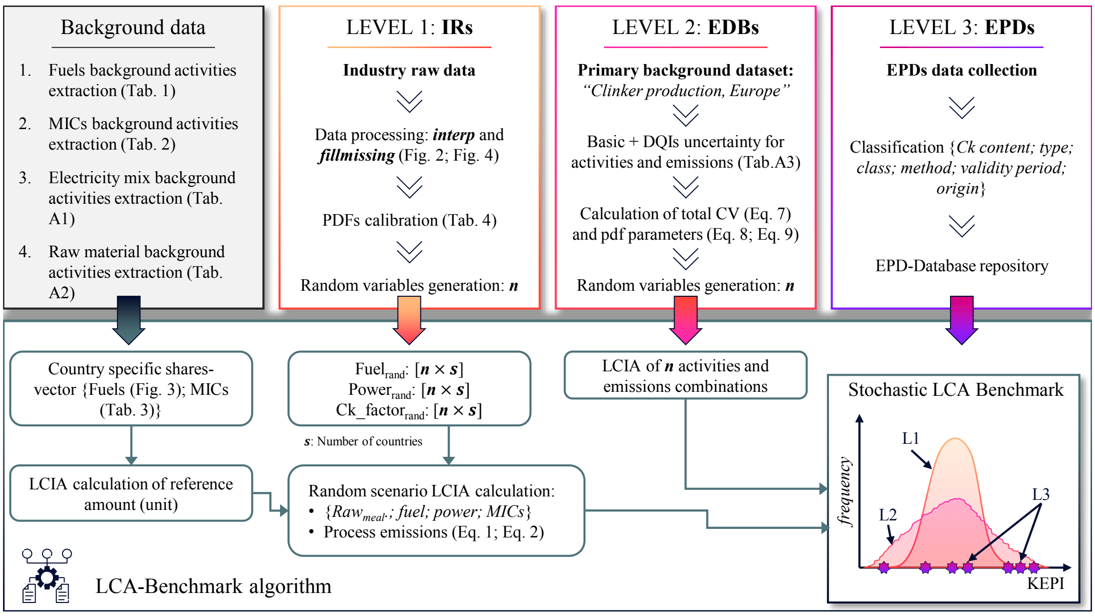


Figure 3.21: Methodology framework for the generation of LCA-based environmental benchmarks.

LCA methodological approach

This study aims to statistically analyse the variability of KEPIs during clinker and cement manufacturing in Europe. To this end, the cradle-to-gate approach is employed, and one tonne (1 t) of material is considered the functional unit. The environmental impact associated with clinker production is controlled by three main processes: i) the fuel consumption in the kiln during combustion; ii) the electricity consumption in the plant for operation (crushing, milling, and sieving) and buildings; and iii) the decomposition of carbonates during calcination [166]. The concept of cement equivalent is used. This means that the clinker-to-cement ratio is statistically simulated, representing country-specific distributions, and a representative national mix of supplementary cementitious materials is added accordingly. The Life Cycle Impact Assessment (LCIA) is performed using the EN15804 reference package 3.1 from the European Platform on LCA [167] because it is the framework used for the generation of EPDs. The impact categories selected for the comparison were total Global Warming Potential (GWP), Human Toxicity Carcinogenics (HT-Cancer) and Non-Carcinogenics (HT-NonCancer), Ozone Depletion Potential (ODP), Particulate Matter (PM), Photochemical Ozone Creation Potential (POCP), Acidification Potential (AP), Ecotoxicity (ET), Eutrophication Potential (EP), abiotic depletion potential of Non-Renewables (NR), Metals and Minerals Depletion (MMD), and Water Deprivation (WD).

LCI data sources

In this work, the data sources used for the LCI are categorised into three levels, as shown before, spanning from the industry to consumers. Firstly, up-to-date industry-related information [165] is used for clinker and cement manufacturing. The data encompasses 75% of total cement manufacturing in Europe from 2005 to 2020, with coverage exceeding 95% of total cement production in some countries, such as Germany, France, Poland, and the UK. Aggregated figures in the form of statistical distributions are utilised for non-linear regression of Probability Density Functions (PDFs), representing the stochastic nature of these processes. Secondly, the clinker manufacturing activity dataset from Ecoinvent v3.9 [149] is used, as this is normally considered for generating EPDs. An uncertainty analysis is performed for all upstream activities and emissions within the main product. Thirdly, a thorough analysis is conducted on over 300 open-access EPDs, covering cement products in Europe. These are classified based on the reported clinker-to-cement ratio, type and class of cement, country of origin, validity period, and the methodology applied during calculation. A comprehensive database is presented in the supplementary file and is available in an online repository.

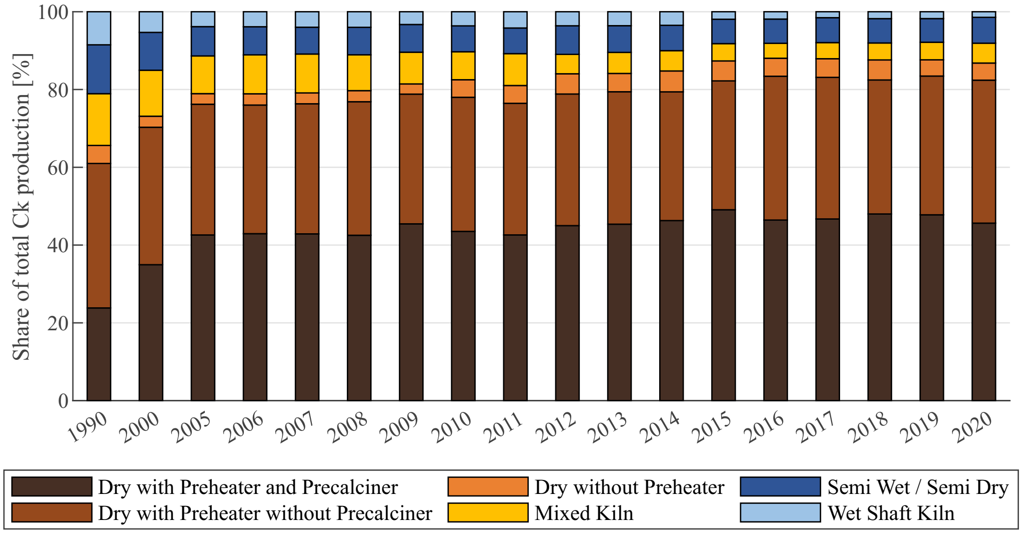
Stochastic analyses

Clinker and cement production: industry reports

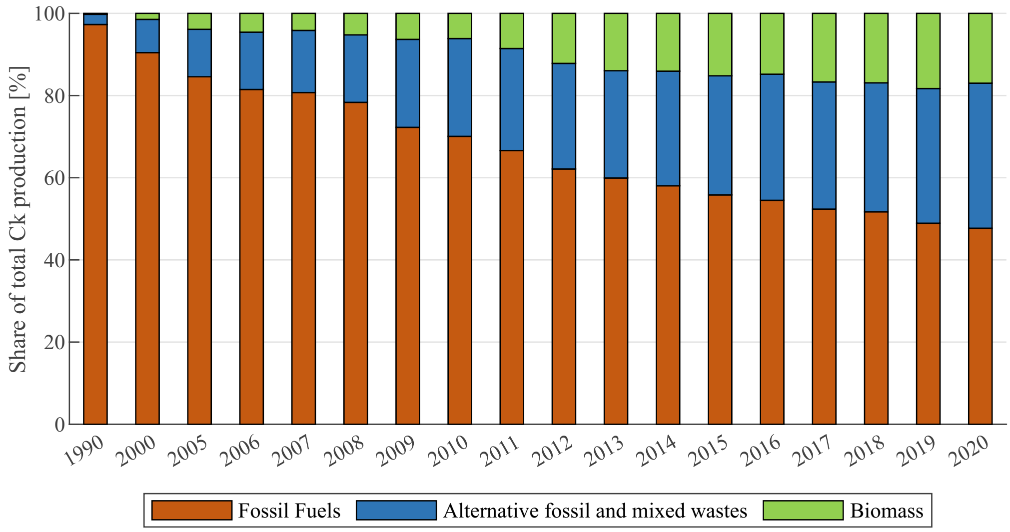
Clinker: The production of clinker consists of calcining around 1.52 t of raw materials per tonne of clinker, usually a mix of limestone and clay, at about 1450 °C of temperature [21, 23]. The environmental burdens of this process are highly influenced by the kiln technology and fuels used during combustion. The use of pre-heaters increases the efficiency of the calcination, requiring between 3000 and 4200 MJ/t of energy for a dry process, although some studies suggest even lesser amounts [168]. In contrast, semi-dry/semi-wet process consumption, also known as Lepol kilns, can range between 3300 and 5400 MJ/t, while wet processes can reach up to 6400 MJ/t clinker [169]. Over the last decades, Europe has pursued a transformation towards the use of more efficient kilns and consistently increased the use of alternative fuels, as shown in Fig. 3.22. Today, over 80% of the clinker is produced in dry kilns with preheaters, while less than 50% of direct fossil fuels are consumed [165].

A methodology to analyse the variability of energy and electricity in clinker production is developed. First, the variability in terms of fuel and electricity consumption per tonne of clinker is analysed for each country from the reported data, as shown in Fig. 3.23. Both the upper and lower tales of the distributions are truncated to the extreme values (dashed lines) to fill up the missing data from the reported series, thus covering 100% of clinker production. To evaluate the influence of this approach on the overall outcome, a sensitivity analysis is performed by contrasting the results with two alternative methods. Both linear and cubic interpolation are utilised between the datasets' amounts and the minimal and maximal expected engineering values, derived from the limits of the 95% confidence interval of the global distribution. The analysis is detailed in the Annex section. Then, interpolation from the data is conducted, and PDFs are fitted using the MATLAB *fitdist* function. Log-normal distributions are adopted because they fit best into the actual data and avoid unrealistic negative values that may be encountered when using normal distributions. The actual fitting against the raw data can be seen in the Appendix section. After that, a sample of 10000 points is randomly generated using the previously fitted PDFs for each country with the distribution parameters declared in Table 3.17. Once the vectors containing randomly generated amounts of fuel and electricity are created, the environmental impact of each scenario is calculated using a MATLAB-based algorithm developed by the authors [13]. To this end, the unitary KEPI of 1 MJ and 1 kWh for energy and electricity, respectively, in each country is calculated and then scaled to the randomly generated inventory amount.

As stated in GNR [165, 170], there are three main types of fuel: fossil, alternative fossils, and biomass. While fossil fuels are commonly known and used in LCA studies, datasets regarding alternative fossil fuels and biomass are scarce. The former includes the use of industrial wastes



(a)



(b)

Figure 3.22: Clinker manufacturing in Europe between 1990 and 2020: (a) per type of kiln; (b) per type of fuel.

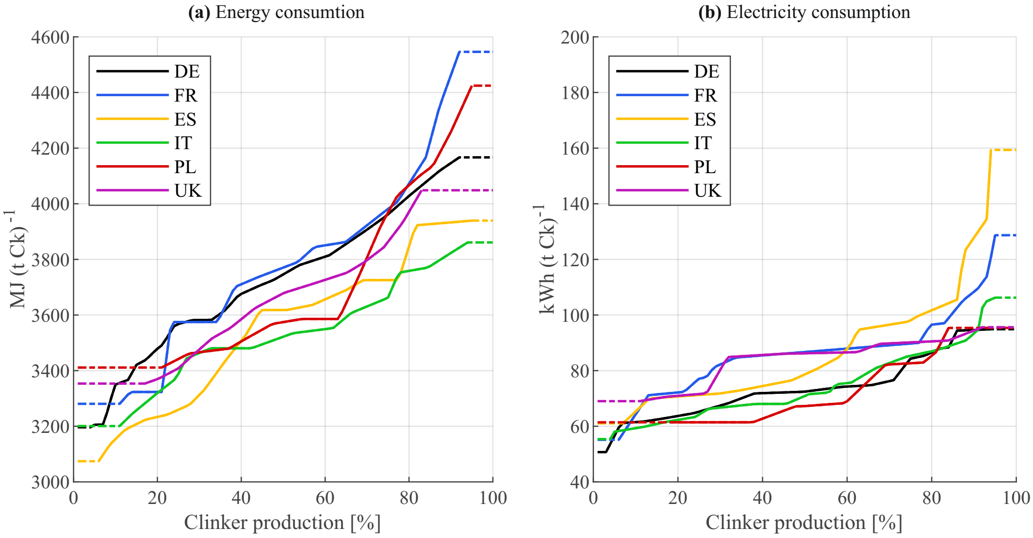


Figure 3.23: Statistical distribution of energy and electricity consumption during clinker manufacturing per country: (a) energy intensity; (b) electricity intensity. Dashed lines indicate truncated values.

such as plastics, solvents, and tyres, while the latter predominately consists of animal bone meal, sewage sludge, and wood-based waste. In total, 22 different background activities were selected from Ecoinvent v3.9 for the generation of representative fuel mixes. The total share of each fuel considered in the analysis is shown in Fig. 3.24 and Table 3.14, also available in the supplementary material file. For the case of alternative fuels, previous studies are considered for the calculation of the average net calorific value needed for the conversion to the mass unit of the reference product [171, 172]. Regarding the generation of electricity, national mixes are used for each country based on market activities, which are detailed in the supplementary file.

Cement The cement environmental benchmark is built upon the cement equivalent concept. For this, information regarding the statistical distribution of the clinker-to-cement ratio in the different countries is used; see Fig. 3.25a. The data is treated similarly to the fuel requirement in the clinker plant. The power consumption per unit of cement equivalent was used instead of the one calculated for clinker manufacturing, based on the statistical distribution shown in Fig. 3.25b. It should be highlighted, that the fly ash used as a supplementary Mineral Component (MIC) is commonly not milled since it has a relatively small particle size distribution and is therefore mixed directly in the cement. Thus, this is considered implicitly in the calculation of the electricity consumption per unit of cement equivalent, because of the stochastic approach.

Table 3.14: Background fuel consumption activities.

Name	Type	CV [MJ/kg]	Activity Name	Geography	Reference Product Name	Unit	Ref. Amount
Coal + Anthracite	Fossil		heat production, at hard coal industrial furnace 1-10MW	Europe	heat, district or industrial, other than natural gas	MJ	1
Petrol Coke	Fossil		heat production, heavy fuel oil, at industrial furnace 1MW [a]	Europe	heat, district or industrial, other than natural gas	MJ	1
(Ultra) Heavy Fuel	Fossil		heat production, heavy fuel oil, at industrial furnace 1MW	Europe	heat, district or industrial, other than natural gas	MJ	1
Diesel Oil	Fossil		heat production, light fuel oil, at industrial furnace 1MW	Europe	heat, district or industrial, other than natural gas	MJ	1
Natural Gas	Fossil		heat production, natural gas, at industrial furnace >100kW	Europe	heat, district or industrial, natural gas	MJ	1
Lignite	Fossil		heat and power co-generation, lignite	DE	heat, district or industrial, other than natural gas	MJ	1
Shale	Fossil		heat production, light fuel oil, at industrial furnace 1MW	Europe	heat, district or industrial, other than natural gas	MJ	1
Rdf Including Plastics	AF	32.4	treatment of waste plastic, mixture, municipal incineration	RoW	waste plastic, mixture	kg	-1
Other Fossil Based Wastes And Mixed Fuels	AF	38.3	treatment of waste mineral oil, hazardous waste incineration	Europe	waste mineral oil	kg	-1
Mixed Industrial Waste	AF	38.3	treatment of waste mineral oil, hazardous waste incineration	Europe	waste mineral oil	kg	-1
Solvents	AF	22.7	treatment of spent solvent mixture, hazardous waste incineration	Europe	spent solvent mixture	kg	-1
Tyres	AF	28.4	treatment of used tyre	GLO	used tyre	kg	-1
Waste Oil	AF	38.3	treatment of waste mineral oil, hazardous waste incineration	Europe	waste mineral oil	kg	-1
Impregnated Saw Dust	AF		heat production, wood chips from industry, at furnace 1000kW	RoW	heat, district or industrial, other than natural gas	MJ	1
Sewage Sludge	Biomass	4.1	treatment of raw sewage sludge, municipal incineration	RoW	raw sewage sludge	kg	-1
Wood, Non Impregnated Saw Dust	Biomass	15.5	heat production, untreated waste wood, at furnace 1000-5000 kW	RoW	waste wood, untreated	kg	-1
Paper, Carton	Biomass	13.0	heat production, untreated waste wood, at furnace 1000-5000 kW	RoW	waste wood, untreated	kg	-1
Animal Meal	Biomass		heat, from municipal waste incineration to generic market for heat district or industrial, other than natural gas	RoW	heat, district or industrial, other than natural gas	MJ	1
Animal Bone Meal	Biomass		heat, from municipal waste incineration to generic market for heat district or industrial, other than natural gas	RoW	heat, district or industrial, other than natural gas	MJ	1
Animal Fat	Biomass		heat, from municipal waste incineration to generic market for heat district or industrial, other than natural gas	RoW	heat, district or industrial, other than natural gas	MJ	1
Agricultural, Organic, Diaper Waste, Charcoal	Biomass		heat, from municipal waste incineration to generic market for heat district or industrial, other than natural gas	RoW	heat, district or industrial, other than natural gas	MJ	1
Other Biomass	Biomass	15.5	heat production, untreated waste wood, at furnace 1000-5000 kW	RoW	waste wood, untreated	kg	-1

[a] Used as a proxy, heavy fuel oil is replaced by petroleum coke using a CV of 35 MJ/kg.

Table 3.15: Background MICs activities.

Name	Activity Name	Geography	Reference Product Name	Unit	Reference Amount
Gypsum	market for gypsum, mineral	RER	gypsum, mineral	kg	1
Limestone	market for limestone, crushed, for mill	RoW	limestone, crushed, for mill	kg	1
Pozzlana	market for limestone, crushed, for mill	RoW	limestone, crushed, for mill	kg	1
Slag	market for ground granulated blast furnace slag	RoW	ground granulated blast furnace slag	kg	1
Fly Ash	electricity production, hard coal	RoW	electricity, high voltage	kWh	1

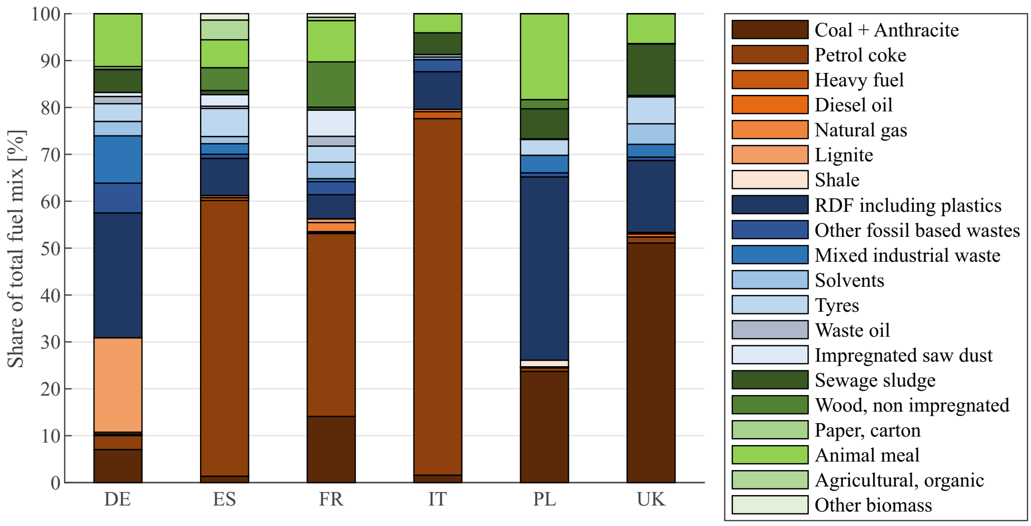


Figure 3.24: Shares fuel types consumed per country.

Table 3.16: Country-specific MICs distribution.

Country	Gypsum	Limestone	Pozzlana	Slag	Fly Ash	Price [euros/kWh]	Allocation FA
DE	20.5%	21.6%	0.5%	56.3%	1.1%	0.106	0.98%
FR	18.6%	35.5%	1.2%	43.1%	1.5%	0.134	0.78%
ES	23.6%	46.1%	10.2%	7.0%	13.2%	0.110	0.95%
IT	19.3%	62.0%	6.5%	5.7%	6.5%	0.123	0.85%
PL	20.7%	14.4%	0.2%	37.1%	27.7%	0.124	0.84%
UK	42.8%	49.8%	0.0%	0.5%	6.9%	0.092	1.13%

After generating the random variables, which comprise the clinker content in the cement equivalent binder mix, the country-specific MICs mix obtained from GNR [165] is added. Background data sets are selected from Ecoinvent and are displayed in Table 3.15. These activities correspond directly to the declared functional unit, so no allocation is needed. For the case of fly ash, the hard coal electricity production activity is used as a proxy, since this is the main activity from which fly ash is generated as a by-product. It is assumed that, on average, 0.052 kg of fly ash is generated for every kWh produced [173]. Then, economic allocation factors are derived for each country [23] based on actual local price data [174]. The total shares and allocation factors used are displayed in Table 3.16.

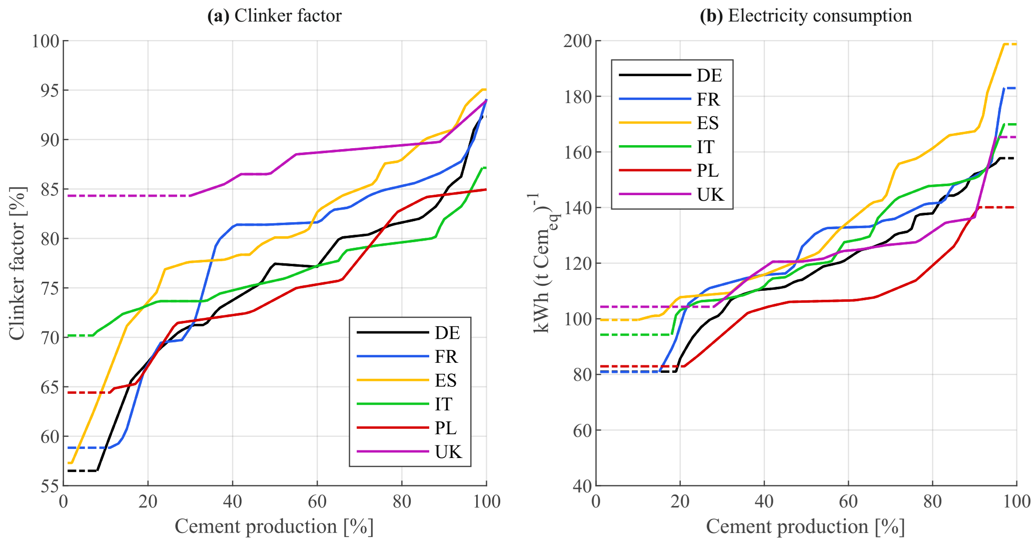


Figure 3.25: Statistical distribution for cement equivalent manufacturing. (a) clinker factor; (b) electricity intensity. Dashed lines indicate truncated values.

Temporal evolution Following the European goals, it is expected that most of the KEPIs will be considerably reduced over the years. Therefore, the temporal evolution of the selected KEPIs is analysed in the case of Germany. Input parameters for the years 2008, 2012, 2016, and 2020 are selected, and the previously described methodology is applied. To analyse the evolution of the KEPIs quantitatively and qualitatively, the results are compared in terms of relative performance against the reference year of 2008, as follows:

$$Ck_{KEPI_{i,j,norm}} = \frac{Ck_{KEPI_{i,j}}}{Ck_{KEPI_{i,2008}}}, \tag{3.10}$$

and

$$CEM_{KEPI_{i,j,norm}} = \frac{CEM_{KEPI_{i,j}}}{CEM_{KEPI_{i,2008}}}, \tag{3.11}$$

where $Ck_{KEPI_{i,j,norm}}$ and $CEM_{KEPI_{i,j,norm}}$ are the normalised ith KEPI corresponding to the jth year of the clinker and cement equivalent manufacturing, accordingly, and $Ck_{KEPI_{i,j}}$ and $CEM_{KEPI_{i,j}}$ are the absolute values.

Figs. 3.26a and 3.26b show the statistical evolution of both energy and electricity consumption during clinker manufacturing over the years. Additionally, Figs. 3.26c and 3.26d illustrate the parameters for the cement equivalent evolution in Germany. Specific information regarding the fuel mixes and MIC shares can be found in the supplementary material.

Ecoinvent

The uncertainty of the Ecoinvent dataset *Clinker production* is considered for comparison with industry-related information. As stated in the Ecoinvent documentation [149], the uncertainty is classified into basic and additional. The former is related to the intrinsic variability and stochastic error of the parameters and depends on the type of intermediate activity or elementary exchange and the type of process considered. The latter represents the deficiency of the used data and is quantified through the use of DQIs in the form of a pedigree matrix.

The original dataset is used as a proxy and modified to generate a fair comparison. Infrastructure-related activities, such as the cement plant, refractory materials, and machines, were omitted. For each activity and emission, basic and additional uncertainty are accounted for. Using Eq. (3.12), the information in the form of the variance of the underlying log-normal distribution is transformed into the coefficient of variation (CV). This allows the use of any PDF later on [88] because it is a dimensionless measure of dispersion independent of the PDF considered. Assuming that the DQIs used in the pedigree matrix are independent of each other, the total additional uncertainty is calculated based on each CV, as shown in Eq. (3.13). Then, the total uncertainty CV_t is obtained from Eq. (3.14).

$$CV = \sqrt{exp(\sigma^2) - 1} \tag{3.12}$$

$$CV_a = \sqrt{\prod_{i=1}^{5} exp(CV_i^2 + 1) - 1} \tag{3.13}$$

$$CV_t = \sqrt{CV_b^2 + CV_a^2} \tag{3.14}$$

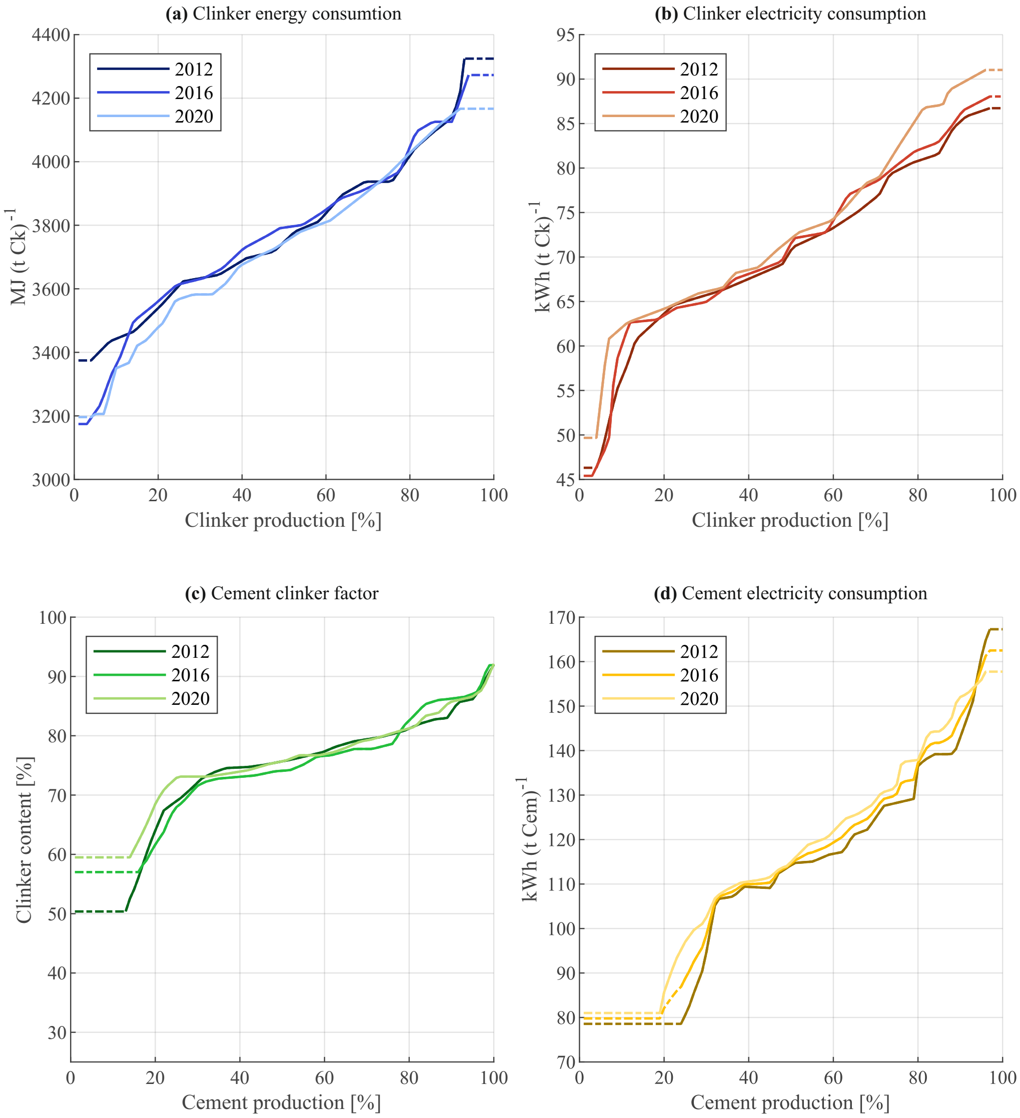


Figure 3.26: Statistical evolution for clinker and cement manufacturing in Germany. (a) clinker energy intensity; (b) clinker electricity intensity; (c) cement clinker factor; (d) cement electricity intensity.

where CV_t, CV_b, and CV_a are the total, basic, and additional uncertainty, respectively. The coefficients of basic uncertainty (CV_b) depend on the type of activity or emission and are obtained from Weidema et al. [175], while the additional component was derived from the pedigree matrix declared in the activity. As discussed by Zhang and Wang [94], the use of normal distributions can lead to unreasonable negative values, and log-normal distributions may cause bias because of the long tail. The latter was observed in the present study, and therefore a triangular distribution is adopted. The function parameters are obtained as follows:

$$a = 2 \times b - c \tag{3.15}$$

$$c = (1 + \sqrt{6} \times CV_t) \times b \tag{3.16}$$

where a, b, and c are the lower limit, peak location, and upper limit. Each activity and emission and their uncertainty information are available in the supplementary file, together with the DQI parameters used.

3.3.4 Results

This section describes and analyses the obtained simulation results. Firstly, the calibrated parameters for the PDFs of each country are showcased. Secondly, the benchmark derived from clinker and cement manufacturing is unveiled in the form of country-specific histograms, along with the main distribution parameters. Thirdly, a comparative analysis between the statistically generated scenarios and the EPD databank is conducted. Lastly, the temporal evolution of selected KEPIs in Germany is explored.

Clinker and cement PDFs for each country

Table 3.17 outlines the selected PDFs and their key parameters for each of the input domains used in this study. The Annex section provides further details on the calibration of simulated PDFs compared to the actual data. In addition, the sensitivity analysis results on the fill-up methodology used for data gaps are detailed. The results show that adopting extreme limits during the data gaps interpolation yields variations in the PDFs μ parameter under 0.2 %, 0.7 %, 0.9 %, and 0.5 % for the energy intensity, power intensities in clinker and cement, and the clinker ratio, respectively, across all countries except the UK. The latter exhibits a 2.2 % absolute relative difference regarding the clinker factor μ parameter when adopting linear interpolation, dropping to 1.2 % when cubic is used. The σ parameter exhibits much higher relative variation for all PDFs when compared to the original value, ranging from 11 % to over 400 %. However, when comparing the absolute difference against the original μ parameter, differences remain between 0.3 % and 2.9 %. Looking into the influence at the KEPI level, it is shown that the mean value across all KEPIs in all the countries analysed remains under 0.2 % variation. The effect on the standard deviation is analysed by comparing the 95% confidence interval minimal and maximal values on all KEPIs across each country compared to the original one. It is shown that almost all the indicators exhibit differences under 3 % in their limit values, highlighting the robustness of the current study. Only selected KEPIs in PL and UK, namely NRE and EP, show up to 13% difference.

On average, the energy intensity during clinker production varies from 3531 to 3799 MJ per tonne of clinker. Italy shows the lowest average value and variance, while France exhibits the highest average and variance. The power intensity for clinker manufacturing ranges from 72.8 to 89.0 kWh/t, with Poland having the lowest and Spain having the highest values. Similar to fuel, higher variance corresponds to higher average values, and vice versa. Electricity consumption in cement manufacturing follows a comparable pattern. It can be appreciated that it is, on average, 1.50 times higher than that associated with clinker. This is because of the additional grinding and milling of the clinker and other MICs. Poland shows the lowest average consumption at 105 kWh per tonne of cement equivalent. This is attributed to its higher use of fly ash, namely 27.7% of the total MIC distribution, as explained earlier. In contrast, Spain registers a 25% higher electricity demand, totalling 132.4 kWh/t. Variances follow the previously observed pattern. Regarding the clinker factor, the UK averages 87.3% content in their cement equivalent mix, nearly 10% more than the following Spain (ES) and 17% more than Poland, which has the lowest amount at 74.6%.

Table 3.17: PDF parameters obtained for clinker and cement in each country.

Input	Parameter	DE	FR	ES	IT	PL	UK
Energy intensity - clinker	Distribution	lognormal	lognormal	lognormal	lognormal	lognormal	lognormal
[MJ/t ck]	μ	8.224	8.238	8.172	8.168	8.214	8.207
	σ	0.077	0.099	0.080	0.058	0.086	0.068
Power intensity - clinker	Distribution	lognormal	lognormal	lognormal	lognormal	lognormal	lognormal
[kWh/t ck]	μ	4.299	4.445	4.455	4.303	4.273	4.420
	σ	0.159	0.197	0.257	0.180	0.171	0.112
Clinker factor - cement	Distribution	lognormal	lognormal	lognormal	lognormal	lognormal	lognormal
[% ck]	μ	4.307	4.340	4.375	4.336	4.308	4.469
	σ	0.126	0.138	0.120	0.053	0.091	0.030
Power intensity - cement	Distribution	lognormal	lognormal	lognormal	lognormal	lognormal	lognormal
[kWh/t cem]	μ	4.732	4.788	4.864	4.799	4.647	4.794
	σ	0.216	0.224	0.209	0.181	0.168	0.129

LCA probabilistic results

Table 3.18 presents the mean and standard deviation of the different KEPIs for both clinker and cement equivalent production across different countries, including the clinker manufacturing activity from the Ecoinvent dataset. Examining the results reveals that, except for ET, EP, and MMD, clinker generally performs poorly, indicating its higher environmental impact per tonne of material. The performance of ET and EP depends on the specific country under analysis, while for MMD, this is not the case. The MMD impact of cement equivalent is, on average, 7 to 8 times higher than that of clinker. This substantial difference is attributed to the relative impact on mineral additions, a point that will be elaborated on later. Furthermore, the standard deviation, representing variability, is consistently higher for cement than for clinker at the country level. Notably, the Ecoinvent dataset exhibits maximal variability in six out of twelve KEPIs, with the rest distributed among FR, DE, and ES, which aligns with expected results. France and Spain demonstrate high standard deviations in terms of clinker energy intensity, cement power intensity, and clinker factor, as previously explained. Germany exhibits notable variability in cement electricity intensity, particularly influencing the ET indicator. A detailed analysis of these findings is conducted in the subsequent subsections for each material.

Clinker Environmental Performance

Fig. 3.27 illustrates the benchmark through histograms focusing on clinker KEPIs, while Fig. 3.28 showcases the average relative contribution of fuel, electricity, process, raw materials, and MICs to each environmental indicator for both clinker and cement. Process-related emissions emerge as the most relevant for GWP, while playing a less significant role in terms of PM, AP, and ET and being irrelevant in the rest of the indicators. Fuel-related emissions predominantly control most KEPIs, except GWP, MMD, and, in some cases, WD. Electricity-related emissions play a significant role in non-renewable resource depletion, with their impact on other categories varying by the country analyzed. Notably, in Poland, they produce a substantial impact on many KEPIs due to the countrys reliance on hard coal for electricity generation.

Fig. 3.27 reveals good agreement between histograms generated from industry-reported inventories and those derived from the Ecoinvent database. The latter exhibits higher standard deviations in most KEPIs compared to individual countries, with consistently more variability than the lowest standard deviation. The PM, AP, and EP indicators show less variation in the Ecoinvent activity. However, the clinker carbon footprint standard deviation is notably 3 to 4 times higher than those for each country, representing almost 10% of its mean value (86.9 kg CO_{2eq}/t vs. 923 CO_{2eq}/t). This KEPI aligns with Ecoinvent industry data, but discrepancies exist in other

Table 3.18: KEPIs obtained for clinker and cement equivalent in Europe, 2020.

Impact Category	Unit		Clinker DE	FR	ES	IT	PL	UK	Ecoinvent	Cement equivalent DE	FR	ES	IT	PL	UK
GWP	kg CO2 eq	μ	851.5	862.7	870.2	921.3	896.8	941.4	923.4	684.6	685.2	718.2	736.6	741.4	838.6
		σ	20.0	29.4	23.5	19.9	25.6	24.2	86.9	70.6	84.6	77.4	39.0	54.9	32.0
HT-Cancer	CTUh	μ	7.92E-08	1.17E-07	1.16E-07	1.28E-07	9.75E-08	1.02E-07	1.27E-07	7.31E-08	9.79E-08	1.00E-07	1.06E-07	9.74E-08	9.29E-08
		σ	3.78E-09	9.01E-09	7.04E-09	5.81E-09	5.96E-09	4.93E-09	2.66E-08	5.28E-09	1.17E-08	1.08E-08	6.69E-09	7.40E-09	5.01E-09
HT-NonCan.	CTUh	μ	2.04E-06	2.34E-06	1.95E-06	2.15E-06	3.37E-06	3.59E-06	6.23E-06	1.94E-06	2.00E-06	1.74E-06	1.81E-06	3.53E-06	3.23E-06
		σ	1.14E-07	1.90E-07	1.20E-07	9.81E-08	2.49E-07	2.10E-07	2.25E-06	1.46E-07	2.25E-07	1.68E-07	1.11E-07	3.07E-07	2.04E-07
ODP	kg CFC-11 eq	μ	1.59E-06	3.28E-06	3.93E-06	4.92E-06	1.31E-06	2.68E-06	2.84E-06	1.71E-06	2.89E-06	3.52E-06	4.37E-06	1.39E-06	3.06E-06
		σ	8.08E-08	2.68E-07	2.75E-07	2.54E-07	7.14E-08	1.56E-07	4.18E-07	1.13E-07	3.12E-07	3.86E-07	3.07E-07	8.08E-08	2.42E-07
PM	DI	μ	1.64E-05	3.05E-05	2.56E-05	2.79E-05	2.19E-05	3.50E-05	1.05E-05	1.40E-05	2.49E-05	2.11E-05	2.22E-05	1.80E-05	3.09E-05
		σ	6.17E-07	2.22E-06	1.37E-06	1.14E-06	1.12E-06	1.81E-06	6.23E-07	1.06E-06	3.14E-06	2.41E-06	1.37E-06	1.41E-06	1.81E-06
POCP	kg NMVOC eq	μ	0.63	1.17	1.13	1.25	0.93	1.21	1.70	0.60	0.98	1.00	1.07	0.92	1.11
		σ	2.75E-02	9.23E-02	6.86E-02	5.66E-02	5.41E-02	6.29E-02	1.29E-01	3.46E-02	1.16E-01	9.68E-02	6.44E-02	5.91E-02	6.18E-02
AP	mol H+ eq	μ	1.57	2.80	2.73	3.12	2.51	3.20	1.76	1.37	2.28	2.34	2.53	2.44	2.85
		σ	4.65E-02	1.88E-01	1.41E-01	1.25E-01	1.29E-01	1.52E-01	1.09E-01	9.74E-02	2.82E-01	2.35E-01	1.51E-01	1.60E-01	1.54E-01
ET	CTUe	μ	1020.2	1543.9	1765.0	2060.7	1040.5	1100.6	983.5	1610.2	1734.7	1540.6	1705.2	1448.4	992.0
		σ	47.3	119.7	111.2	98.9	55.3	50.1	115.4	200.8	123.8	145.3	101.6	103.3	50.8
EP	kg P eq	μ	2.30E-01	6.31E-02	2.92E-02	3.98E-02	1.82E-01	1.84E-01	6.70E-02	2.18E-01	5.27E-02	2.92E-02	3.61E-02	2.02E-01	1.63E-01
		σ	1.51E-02	4.90E-03	1.49E-03	1.52E-03	1.61E-02	1.15E-02	8.21E-03	2.47E-02	6.23E-03	1.88E-03	2.03E-03	2.13E-02	1.11E-02
NRE	MJ	μ	2005.6	4017.0	3697.5	4256.7	2426.2	3475.6	2860.0	2205.3	3934.2	3483.8	3742.5	2654.7	3443.8
		σ	116.7	328.9	272.7	214.9	171.3	179.1	299.2	199.0	439.7	358.9	252.4	209.5	199.7
MMD	kg Sb eq	μ	2.82E-04	3.02E-04	2.94E-04	2.93E-04	2.65E-04	3.01E-04	2.32E-04	2.18E-03	1.82E-03	1.98E-03	1.88E-03	2.17E-03	2.24E-03
		σ	6.32E-06	9.48E-06	9.28E-06	6.15E-06	5.55E-06	6.09E-06	2.53E-05	6.86E-04	6.80E-04	7.69E-04	2.70E-04	5.04E-04	3.99E-04
WD	m3 world eq	μ	97.90	64.32	58.66	67.04	72.71	68.95	46.45	82.84	60.38	54.66	66.47	68.36	63.64
		σ	4.00	2.60	2.62	2.95	2.95	1.67	8.06	7.71	5.49	5.05	5.12	4.75	2.31

categories, as discussed in the EPD analysis. Specifically, the PM indicator shows a lower impact in Ecoinvent due to its inclusion of actual measured data, potentially leading to an overestimation in our study.

Fig. 3.27 also highlights a connection between the worst-performing countries in terms of human health-related impacts and the use of fossil fuels. This is particularly evident in carcinogenic substance emissions, where all fossil fuels generate a similar unitary impact (1.14 to 1.30 CTUh per MJ, except for lignite, whose impact is around 0.6 CTUh per MJ). Germanys lower reliance on fossil fuels explains its 2040% lower cancerogenic footprint compared to other countries.

Italy, Spain, France, and the United Kingdom primarily source more than half of their fuel mix from fossil sources (Fig. 3.24). Nevertheless, it can be appreciated that the UK differentiates from the former three countries in carcinogenic emissions and ODP, particularly due to the choice of coal (UK) versus petrol coke (IT, ES, and FR). Germany outperforms other countries in almost all impact categories due to its lower reliance on fossil fuels in clinker manufacturing, except for the EP indicator, which exhibits a higher average impact (33% more kg Peq than the second worst country) possibly linked to the use of lignite (20% of Germanys total fuel mix, with associated spoil leachate from lignite mining). Despite similar fossil fuel consumption in the UK and France (50% to 55%), differences in KEPIs such as ODP, PM, and POCP underscore the influence of fuel types and additional factors, such as impregnated sawdust use in France.

Cement Environmental Performance

Fig. 3.29 displays the KEPIs for cement equivalent, with deterministic values from Ecoinvent v3.9 for various cement types included for comparison and validation. Remarkably, there is a good agreement among all indicators.

Examining the cement carbon footprint, similar value ranges are observed for the generated histograms and cement types CEM I, CEM II, and CEM IV. However, CEM III B/C and CEM V/B fall outside the histogram boundaries (discussed in the next section). CEM I, which contains at least 95% clinker, aligns with the upper boundaries of the histogram, consistent with clinker results.

Country-specific performance mirrors the order seen in clinker manufacturing, but with a lower carbon footprint due to reduced clinker content. Poland is an exception, showing a higher mean and standard deviation than Italy, contrary to the clinker case. This can be attributed to two main reasons. On the one hand, the process-related emissions are diluted by the lower clinker content, making the other emissions more relevant. In addition, the cement manufacturing process consumes more electricity than the clinker. As it was shown before, on average, around 120

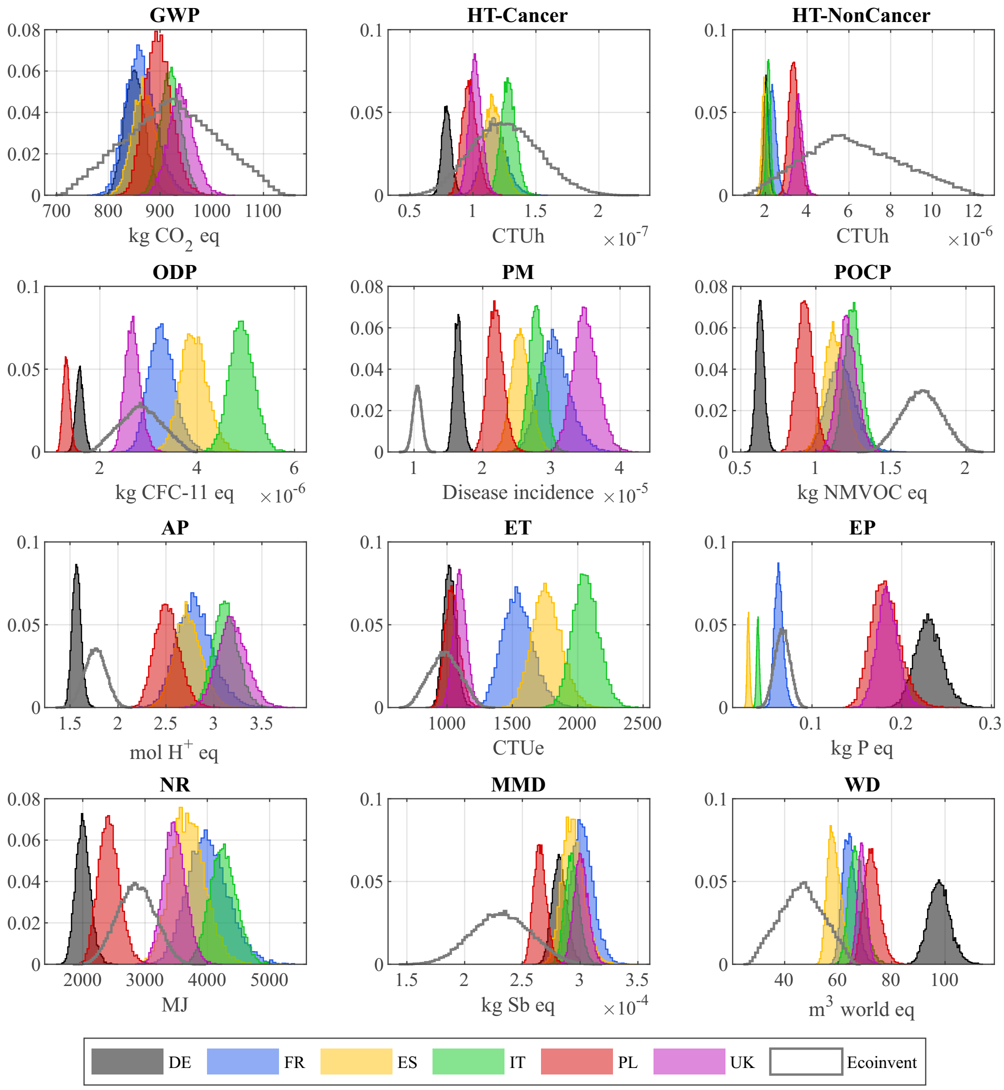


Figure 3.27: Histograms of clinker KEPIs in Europe, 2020.

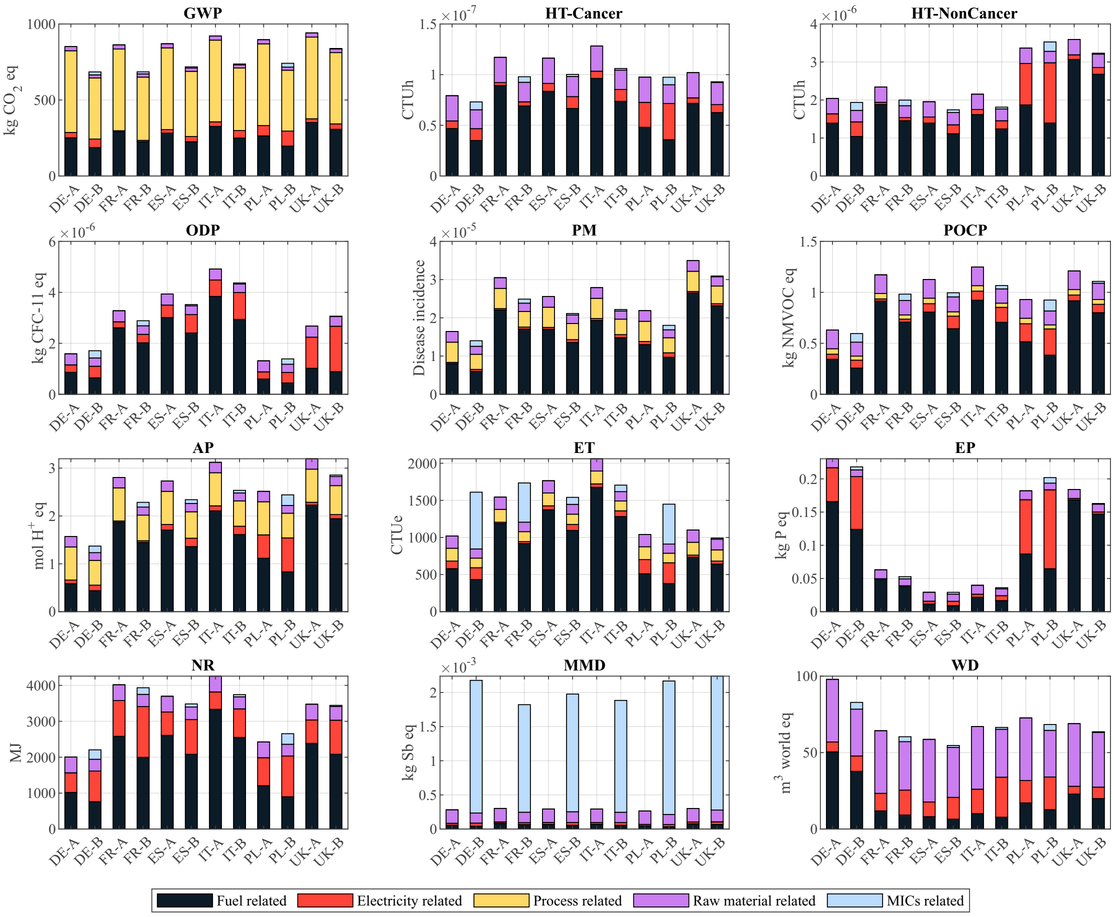


Figure 3.28: Contribution analysis to the clinker (A) and cement equivalent (B) average environmental footprint by country.

kWh of electricity per tonne of cement equivalent is needed, while the clinker consumes 80 kWh/t. On the other hand, Polands electricity mix uses high amounts of hard coal, making the unitary contribution of the electricity consumption to cement manufacturing 145% more than for the clinker. This fact also explains why Poland is the worst-performing country in terms of the non-carcinogenic human toxicity category.

For the rest of the human-related KEPIs, theres good agreement between the generated stochastic data and Ecoinvent deterministic values. The rule of higher clinker content leading to increased environmental burdens applies here, along with the impact of fossil fuels (both during calcination and the background electricity mix).

Ecosystem quality indicators exhibit reasonable agreement. The AP shows a difference between Germany and the rest of the countries. This disparity arises from variations in unitary acidification impact for different fuels. For example, 1 MJ of hard coal combustion generates almost twelve times more acidification impact (1.1E-3 $molH^{+}$) than lignite. Germany's reliance on the latter (over 2/3 of the fossil fuel mix), while other countries use a mix of hard coal, petcoke, and heavy fuel oil, explains the observed difference in AP. This pattern reverses in EP, where 1 MJ from lignite is 2.15 times worse than the second-highest source, hard coal.

Finally, resource depletion-related KEPIs show exceptional agreement between the calculated benchmark and the different cement types. In particular, the metals and minerals depletion potential exhibits all deterministic values in the central range of the generated histograms.

Clinker factor and EPDs benchmark

This section assesses the agreement between the simulated stochastic KEPIs and information from the EPD database. Using 10000 randomly generated cement equivalent compositions based on the calibrated model distributions for different countries (Table 3.17), KEPIs are calculated, and results are organised by decreasing clinker factor. The optimal front for each country, highlighting the best-performing result in each 1% interval, is presented in Fig. 3.30. Only EPDs generated with the same impact methodology and falling within a reasonable range are displayed for clarity.

Fig. 3.30 reveals a decreasing trend in most KEPIs with the reduction of the clinker factor. However, an optimal threshold exists where the benefits of reducing clinker are outweighed by the burdens of MICs. This threshold varies by country and the specific KEPI considered.

The climate change indicator benefits most from reduced clinker content, exhibiting a linearly decreasing trend across all countries. A 1% reduction in clinker reflects an abatement of 7 kg CO_{2eq} for DE, FR, ES, and PL and 8.5 to 9.3 kg CO_{2eq} for UK and IT, respectively. Notably, there is strong agreement between this study and EPDs within the 40% to 95% clinker content range. However, discrepancies below the 40% ratio may arise from data incompleteness in histogram

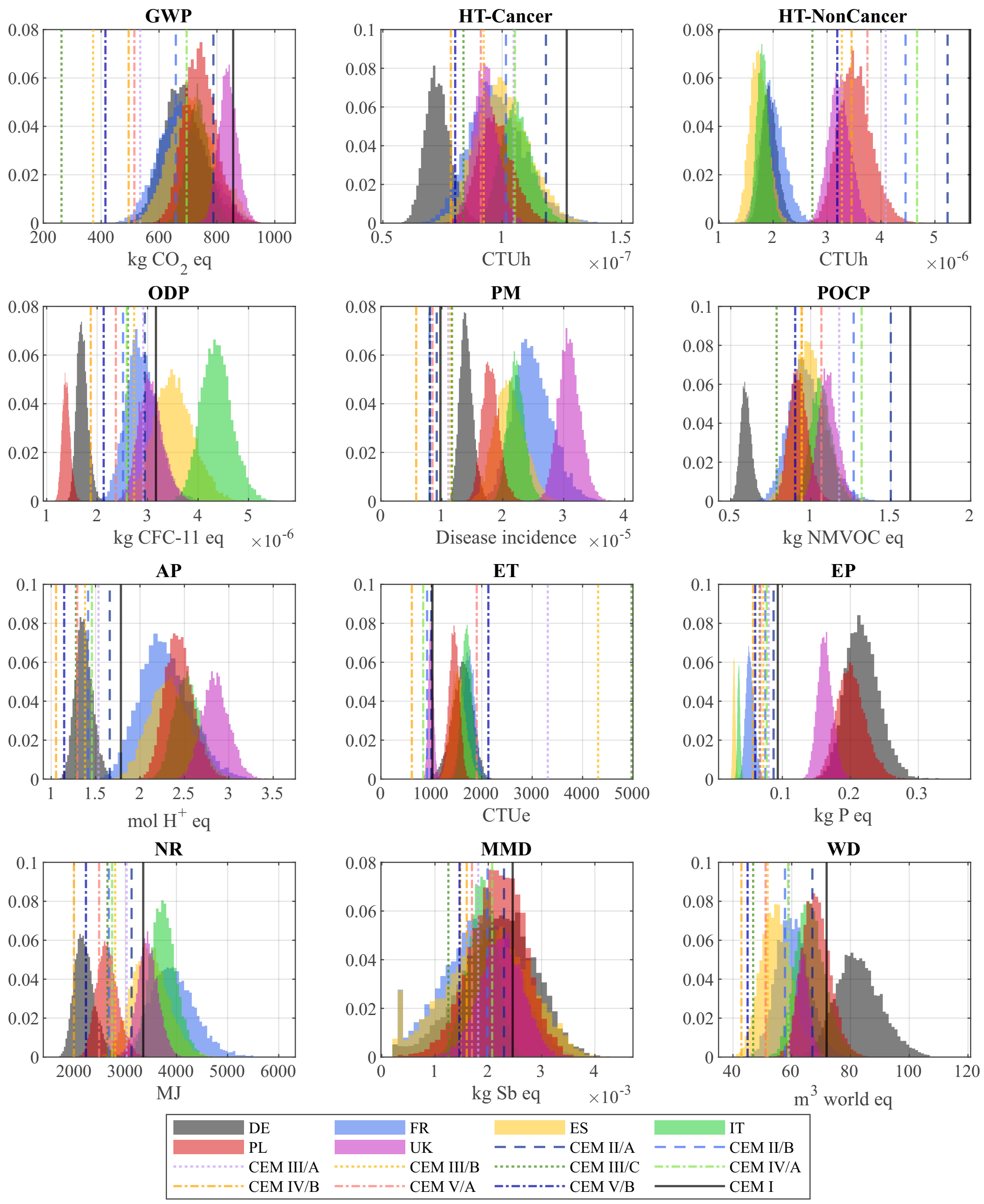


Figure 3.29: Histograms of cement equivalent KEPIs in Europe, 2020.

calculations or EPDs lack of representativeness for the current volume of cement manufacturing in Europe.

Concerning human health-related impacts, the advantages of reducing clinker content are not immediately evident. A critical point emerges where further clinker replacement by MICs becomes counterproductive. For instance, countries with high Ground Granulated Blast Furnace Slag (GGBFS) usage, such as Germany, France, and Poland, show a sharp increase in ET indicator with greater clinker replacement (in contrast to the decreasing trend in other countries using different MICs), related to the hydrogen sulphide emission during the quenching of the slag. The agreement between simulated values and EPDs is limited, with significant variability in the disclosed values.

Italy stands out with the most substantial decrease in impact slope among different indicators, signalling high improvement potential. These findings emphasise that clinker replacement with limestone is a highly efficient strategy for reducing the environmental footprint of cement.

Similar to previous analyses, the non-renewable energy depletion indicator aligns well between this study and the disclosed data. Examining metals and minerals depletion reveals a seemingly linear relationship with clinker replacement, influenced by gypsum, fly ash, and, in a lesser amount, slag usage. Furthermore, the electricity mix also plays a significant role, as depicted in Fig. 3.28.

Temporal evolution

Fig. 3.26 shows the statistical evolution of Germany's clinker and cement manufacturing parameters. It can be seen that from 2008 until today, there has been a trend in the reduction of the clinker's energy intensity, probably linked to an increase in the efficiency of the kilns. However, it is also possible to see an increase in terms of both electricity consumption and mean clinker content.

Fig. 3.31 illustrates the temporal evolution of GWP, ET, and NR for clinker and cement equivalent manufacturing in Germany from 2008 and 2020. The complete data for other indicators is available in the supplementary file. The average histogram value is highlighted, and the relative performance against 2008 is displayed.

Notably, there is a higher degree of variability in cements environmental performance compared to clinker, consistent with observations in the previous section. This variability is attributed to fluctuations in electricity consumption and clinker content. The CO_2 footprint consistently improves over the years, reaching 4.6% and 7.2% reductions for clinker and cement, respectively, compared to 2008. This improvement is linked to the reduced energy requirements in clinker manufacturing and the decreased use of fossil fuels. The NR indicator exhibits clear improvement,

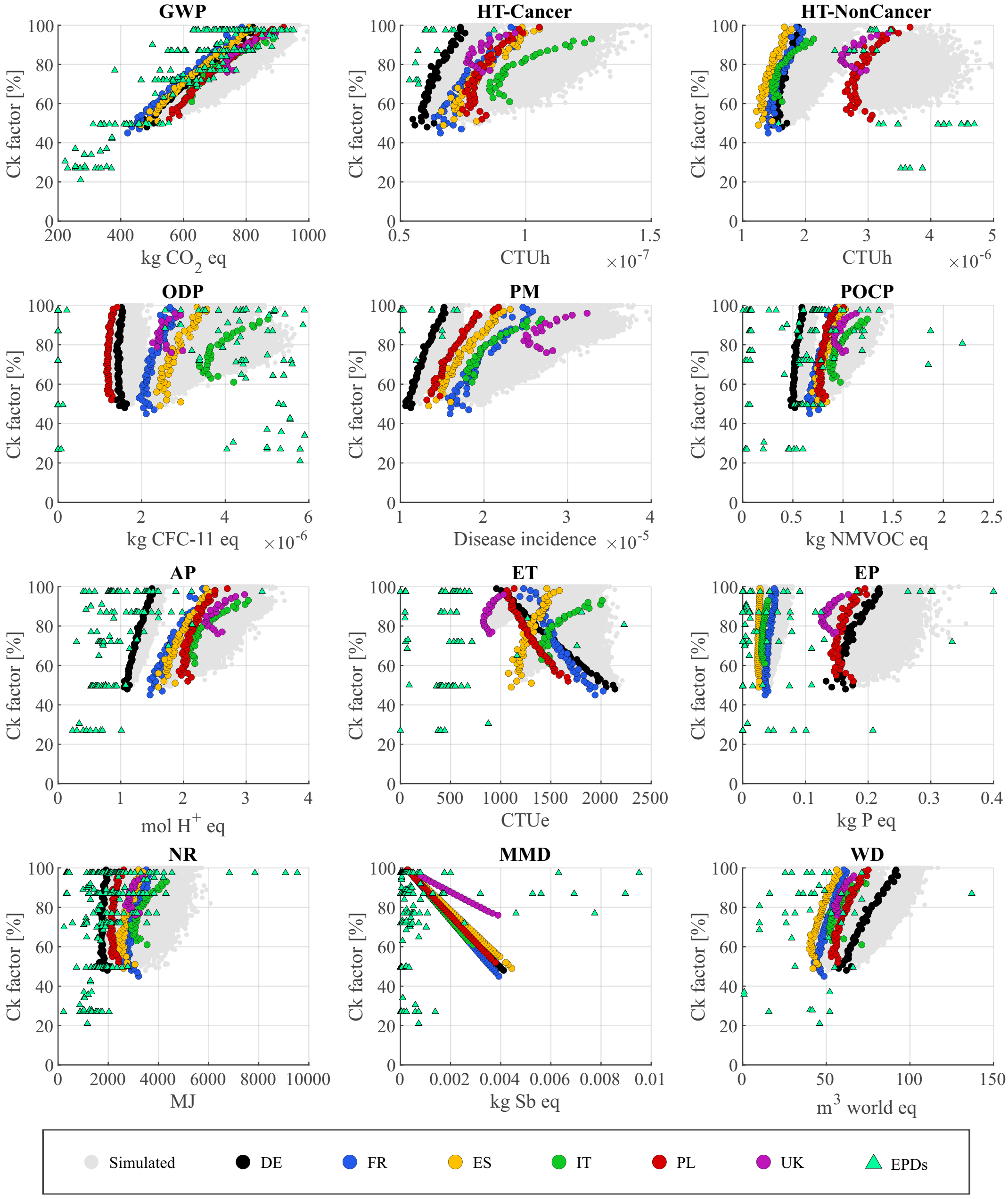


Figure 3.30: Comparison between LCA simulated results and EPDs for cement KEPIs as a function of the clinker factor.

with a total reduction of 24.5% and 22%, showing the highest cutback between 2008 and 2012, followed by a diminishing pace (6.5% and 5.9%). However, there is a growth in the variability of cement performance, mainly due to increased variability in clinker content.

The AP indicator, reflecting the ecosystem impact, shows a noticeable reduction in 2012, 2016, and 2020, potentially attributed to decreased use of slag and fossil fuels in cement and clinker manufacturing.

3.3.5 Limitations and future research

The established benchmarks are tailored to a specific subset of European countries, showcasing a remarkable depth of comprehensive data. When undertaking comparisons between the current research-involved countries and those on a European or even non-European scale, caution should be exercised. This entails ensuring that the completeness of the datasets being compared is equal, thus fostering a more accurate and meaningful analysis. Moreover, data gaps will inevitably introduce some degree of bias in the results. The benchmarks demonstrated robustness across all countries, except for PL and the UK in particular KEPIs indicators, as explained before, stressing the importance of data completeness.

The subsequent identification of research gaps serves as an initial foundation for future investigations. There is an imperative need for the creation of global stochastic benchmarks to facilitate the sustainable development of the cement industry. Nevertheless, it's crucial to acknowledge that the challenge persists in collecting comprehensive global data. A deeper investigation regarding the use of different mineral additions to clinker and their impact on the environmental benchmarks should be explored. Moreover, new performance-based KEPIs are needed for a comprehensive comparison of different cementitious materials. Economic assessment can also be included in combination with stochastic indicators. Additionally, the effect of emerging manufacturing technologies, such as carbon capture and storage or utilisation, needs to be further assessed. Finally, the development of a stochastic-based framework for the judgement of EPDs could greatly benefit the cement industry in its path towards more sustainable materials.

3.3.6 Conclusions

This study delves into the environmental footprints of clinker and cement in Europe, employing a robust LCA methodology. The investigation begins with industry-reported data, paving the way for the development of a stochastic benchmark encompassing six European countries that collectively contribute over 75% of European cement manufacturing. This benchmark undergoes

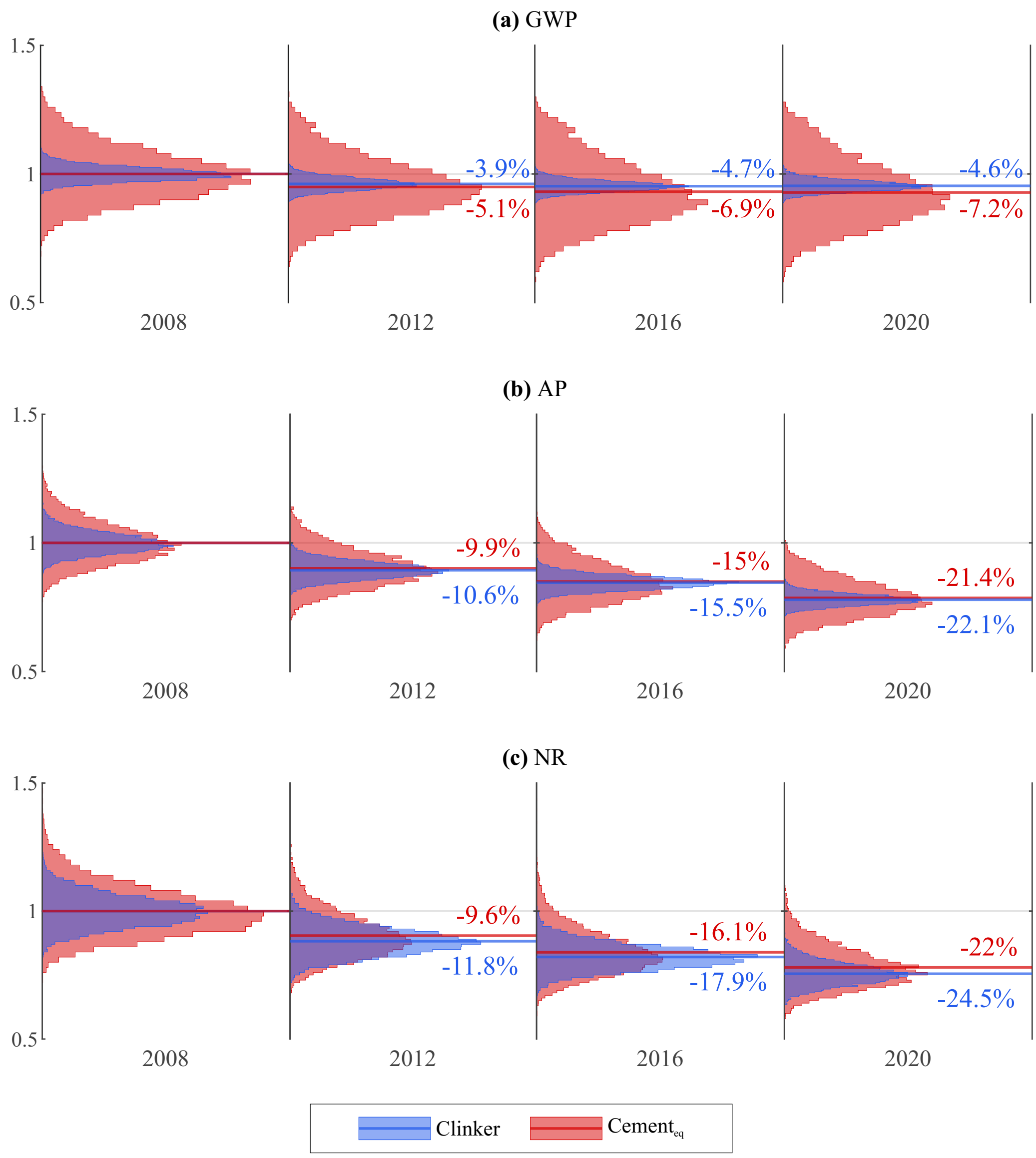


Figure 3.31: Time evolution LCA results for three clinker and cement KEPIs in Germany, 2008 to 2020. (a) GWP; (b) AP; (c) NR.

a meticulous validation process against background environmental datasets from Ecoinvent, supplemented by the analysis and comparison of over 300 EPDs. The culmination of these efforts yields a wealth of insights and significant conclusions across various dimensions.

Regarding clinker and cement manufacturing:

- In the realm of clinker and cement manufacturing, the study underscores the potency of clinker reduction or replacement as a highly effective measure for curbing cement-related GHG emissions. This reduction exhibits a notable pace, amounting to 7 to 9 kg CO_{2eq}/t for each 1% reduction. However, it can lead to an increase in other environmental burdens, depending on the mineral component used as a replacement. The search for low-carbon binder alternatives will need to account for a holistic environmental impact analysis. Calcine clays may, in this aspect, be a promising solution.
- A significant agreement is observed among the developed histograms, the Ecoinvent database, and producer-published EPDs concerning the CO_2 footprint of cements in Europe. However, the study acknowledges the need for sustained efforts to achieve a similar level of confidence across various Key Environmental Performance Indicators (KEPIs). Notably, the study exposes a considerable dispersion in results, particularly in terms of damage to ecosystems and biodiversity.
- The adoption of country-specific benchmarks, as opposed to industry averages from background environmental databases such as Ecoinvent, enhances accuracy and reliability. This approach demonstrates a remarkable reduction in result variability, ranging from 2 to 7 times the standard deviation across all KEPIs. The methodology's adaptability to any particular country or region positions it as a powerful tool for producers, manufacturers, and consumers to measure and track the environmental performance of construction products.
- The study identifies the reduction in energy intensity in cement manufacturing as a strategic pathway towards achieving overall enhanced environmental performance. A temporal analysis of Germany's industry substantiates the efficacy of this approach, suggesting potential exploration into low-energy binder production, such as belite cement.

From a country-specific perspectives:

- Italy and the UK stand out as beneficiaries of a 10 to 20% reduction in average clinker content in their cement equivalent mix. This reduction not only impacts the national Green House Gas (GHG) emissions profile positively but also mitigates damage to human health, ecosystems, and non-renewable resource depletion. However, the study cautions that the potential of this measure in the UK is contingent on a shift to a less fossil-intensive electricity mix.

- Poland emerges as a country with significant potential to reduce its cement environmental footprint through a shift to a renewable electricity mix, such as wind energy. However, this transformation is anticipated to decrease the availability of fly ash, leading to potential environmental impacts if replaced by slag.

- Germany showcases global leadership in both clinker and cement production, consistently exhibiting the lowest or second-lowest environmental impact across various indicators. Notably, Germany's performance in terms of CO_{2eq} emissions, human toxicity (HT), ozone depletion potential (ODP), particulate matter (PM), photochemical ozone creation potential (POCP), acidification potential (AP), ecotoxicity (ET), non-renewable resource depletion (NR), and metal depletion (MMD) outshines other countries. However, Germany faces challenges, particularly in terms of eutrophication potential (EP) and water depletion potential (WDP), indicating the need for targeted improvement strategies.

For designers of EPDs:

- The study highlights a scarcity of agreement between disclosed information and industry-related data, particularly for impact categories beyond climate change. The inclusion of variability-related information, such as the standard deviation of calculated values, is advocated to enhance designers' understanding of construction materials' impact.

- The study positions itself as a benchmark for various stakeholders, serving manufacturers, designers, and policymakers. It emphasises the importance of using supplier-specific information for intermediate consumers, highlighting its direct impact on product environmental performance. Additionally, the study underscores the pitfalls of relying on background data, which can introduce substantial variability in results, compromising assessment quality and reliability.

To wrap up, the research lends support to the use of stochastic information for EPD disclosure, drawing a parallel with specifying the compressive strength of concrete. Acknowledging and addressing uncertainty is deemed crucial for accurate building environmental assessments, aligning with the industry's quest for transparent and uncertainty-aware environmental evaluations.

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

For closer analysis (or reproduction), the research data collected and generated in this work can be found at https://doi.org/10.5281/zenodo .10362042.

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4 Conclusions and outlook

4.1 Conclusions

This thesis delves into the extended possibilities achieved through the development of an industry-specific LCA tool. Transitioning from the current status quo of LCA analysis to environmentally driven material design demands new tools capable of accurately predicting environmental impacts throughout the service life. In this regard, three main pillars were explored, beginning at the computational structure level and spanning over two main areas of research: LCA non-linearities and reliability analysis. Specific aspects of cement and lime-based materials systems were examined, such as the carbonation potential of lime-based renders, plasters and calcium-silicate bricks. Process-based LCIs were developed, and future-oriented scenarios were investigated. From all the aforementioned, the following conclusions can be drawn.

4.1.1 LCA algortihm

- An LCA modelling algorithm was successfully developed in Matlab, and validated against well established commercial software. Moreover, increased automation can be attained by integrating the scientific contributions of publication 1 [13] with the code listings provided in the annex section 5.1 of this thesis.
- The most commonly used LCA data structure was incorporated, enabling seamless integration with future database developments and other software systems.
- Bottom-up data structuring was achieved, facilitating the modelling of environmental impact contribution at an emission level. This approach proves to be a powerful tool in the scientific research community, as it allows for the modelling of new specific materials and processes.

- The current LCA algorithm was designed to accommodate further developments and additions. Indeed, publications 2 [5] and 3 [14] were built upon the foundational syntax presented in publication 1 [13]. This underscores the potential for future research within the team.

4.1.2 Non-linear LCA

- Non-linearities in LCA were modelled, by coupling the operational energy demand of a reference building with its material footprint defined by the construction system. A semi-automatic integration was achieved, calculating thousands of different combinations and, consequently, LCA outputs.
- The results indicate that traditional steady-state LCA analysis are insufficient for optimising the environmental footprint of buildings during the design stage. This inadequacy stems from their shortage to capture the interconnectivity among different design parameters.
- The current use phase of buildings emerges as the primary controlling stage in terms of environmental burdens. However, the future-oriented scenario analysis revealed that the role of materials in the overall LCA result will become increasingly relevant and potentially be the most influencing factor. This result underscores the near-future need of incorporating LCA tools during the design of new products.

4.1.3 Carbon uptake in lime-based construction systems

- The CO_2 uptake potential of lime-based construction systems was effectively analysed at a building scale. It was demonstrated that while the carbonation of a thin layer render can be significant, when studied independently, its contribution to reducing the overall carbon footprint of the entire building is less than 1%. In contrast, calcium-silicate bricks were found to contribute between 5% to 20% in current and future $low-CO_2$ energy carrier scenarios, respectively. This underscores the importance of exploring new methods to enhance the CO_2 capture potential in bricks.

4.1.4 LCA-based reliability design

- Stochastic benchmarks were successfully developed for the European cement industry. The country-specific KEPIs proved an advancement and up to 7 times more reliable method of comparing LCA results.

- An extensive EPD database was openly shared with the broad scientific community, displaying more than 160 downloads to the date.
- The reduction of clinker content was proven to be a main driver for decreasing the cement's carbon footprint along with other environmental indicators. However it was also demonstrated, that it can lead to an increase in some areas of damage depending on the mineral replacement used. This result supports the use of holistic environmental analysis instead of carbon accounting methods that could lead to a bias if used for decision making.
- There is a gap to be filled regarding the disclosure of variability-related information along with EPDs. This will enhance the quality of LCA results, particularly in the supply chain.

4.2 Limitations and future research

The following general limitations can be highlighted apart from the particular ones discussed in each publication:

- The dynamic response of the LCA study presented in publication 2 was not directly addressed in discrete time-steps. As discussed in chapter 2, the timing of emissions and the development of the inventory will have a direct influence on the outcome. The approach followed was scenario-based, suggesting that the real solution lies somewhere in between.
- Further investigation is needed regarding the role of carbonation in lime-based construction units in reducing a building's carbon footprint. The current analysis was based on a few studies published on this topic, with several boundary conditions that may not always be applicable to real structures.
- While the clinker environmental benchmark developed for the cement industry could potentially be used as a proxy for the lime industry, factors like the kiln type and efficiency, and fuels used, will significantly affect the results' reliability. Developing benchmarks for lime poses challenges due to confidentiality concerns related to market share distribution among companies in Europe. This could be overcome by developing a worldwide benchmark.

In addition, this thesis opens up the possibilities of future research comprising:

1. Developing a discrete time-steps modelling framework for both inventory and impact assessment methods, to enhance the accuracy of environmental modelling of construction materials throughout their lifecycle.

2. Addressing seasonal and daily user behavior for different time horizons in the use phase of buildings.
3. Developing an EPD labelling framework based on reliability analysis, facilitating communication at a business-to-business level while enhancing the robustness of LCA developments in the built environment.
4. Further research regarding CO_2 absorption in calcium-silicate bricks. Particularly, the development of methods for capturing CO_2 at cradle to gate level (i.e., during manufacturing) could potentially benefit the industry, by providing a transparent and traceable method for accounting the decarbonisation strategy.

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5 Annex

5.1 Programming syntax

Ecospold 2: Technology matrix

Listing 5.1: Matlab code for obtaining technology matrix for XML files on Ecospold 2 format.

```
folderPath = 'specify_folder';
spoldFiles = dir(fullfile(folderPath, '*.spold'));
Techno = cell(length(spoldFiles), 1);
for fileIdx = 1:length(spoldFiles)
% Construct the full file path
  filePath = fullfile(folderPath, spoldFiles(fileIdx).name);
  docNode = xmlread(filePath);
% Find all 'intermediateExchange' nodes
  intermediateNodes = docNode.getElementsByTagName('intermediateExchange');
% Get the name of the first 'intermediateExchange'
  firstExchangeName = char(intermediateNodes.item(0).getElementsByTagName('name').item(0).getTextContent());
  geographyNode = docNode.getElementsByTagName('geography').item(0);
  geography = char(geographyNode.getElementsByTagName('shortname').item(0).getTextContent());
% Initialize cell arrays to store extracted data
  intermediateExchangeId = cell(intermediateNodes.getLength-1, 1);
  activityLinkId = cell(intermediateNodes.getLength-1, 1);
  amount = cell(intermediateNodes.getLength-1, 1);
  name = cell(intermediateNodes.getLength-1, 1);
  unitName = cell(intermediateNodes.getLength-1, 1);
  meanValue = cell(intermediateNodes.getLength-1, 1);
  mu = cell(intermediateNodes.getLength-1, 1);
  variance = cell(intermediateNodes.getLength-1, 1);
  varianceWithPedigreeUncertainty = cell(intermediateNodes.getLength-1, 1);

```

```
for i = 1:intermediateNodes.getLength-1
  node = intermediateNodes.item(i);
% Extract values from attributes
  intermediateExchangeId{i+1} = char(node.getAttribute('intermediateExchangeId'));
  activityLinkId{i+1} = char(node.getAttribute('activityLinkId'));
  amount{i+1} = char(node.getAttribute('amount'));
% Extract values from child nodes
  nameNode = node.getElementsByTagName('name').item(0);
  name{i+1} = char(nameNode.getTextContent());
  unitNameNode = node.getElementsByTagName('unitName').item(0);
  unitName{i+1} = char(unitNameNode.getTextContent());
% Check if 'uncertainty' node exists
  uncertaintyNode = node.getElementsByTagName('uncertainty').item(0);
% Initialize uncertainty fields to 0
  meanValue{i} = '0';
  mu{i} = '0';
variance{i} = '0';
  varianceWithPedigreeUncertainty{i} = '0';
% If 'uncertainty' node exists, extract values from 'lognormal' child node
  if ~isempty(uncertaintyNode)
    lognormalNode = uncertaintyNode.getElementsByTagName('lognormal').item(0);
    meanValue{i} = char(lognormalNode.getAttribute('meanValue'));
    mu{i} = char(lognormalNode.getAttribute('mu'));
    variance{i} = char(lognormalNode.getAttribute('variance'));
    varianceWithPedigreeUncertainty{i} = char(lognormalNode.getAttribute('varianceWithPedigreeUncertainty'));
  end
end
dataTable = table(intermediateExchangeId(2:end), activityLinkId(2:end), name(2:end), amount(2:end), unitName(2:end), meanValue, mu, variance, varianceWithPedigreeUncertainty, ...
'VariableNames', {'intermediateExchangeId', 'activityLinkId', 'name', 'amount', 'unitName', 'meanValue', 'mu', 'variance', 'varianceWithPedigreeUncertainty'});
Techno{fileIdx} = dataTable;
end
```

Ecospold 2: Environmental matrix

Listing 5.2: Matlab code for obtaining environmental matrix for XML files on Ecospold 2 format.

```
  folderPath = 'specify_folder';
  spoldFiles = dir(fullfile(folderPath, '*.spold'));
  Element = cell(length(spoldFiles), 1);
  Info = cell(length(spoldFiles), 2);
  for fileIdx = 1:length(spoldFiles)
% Construct the full file path
  filePath = fullfile(folderPath, spoldFiles(fileIdx).name);
  docNode = xmlread(filePath);
  geographyNode = docNode.getElementsByTagName('geography').item(0);
  geography = char(geographyNode.getElementsByTagName('shortname').item(0).getTextContent());
% Find all 'intermediateExchange' nodes
  elementaryNodes = docNode.getElementsByTagName('elementaryExchange');
  intermediateNodes = docNode.getElementsByTagName('intermediateExchange');
% Get the name of the first 'intermediateExchange'
  firstExchangeName = char(intermediateNodes.item(0).getElementsByTagName('name').item(0).getTextContent());
% Initialize cell arrays to store extracted data
  elementaryExchangeId = cell(elementaryNodes.getLength-1, 1);
  amount = cell(elementaryNodes.getLength-1, 1);
  name = cell(elementaryNodes.getLength-1, 1);
  unitName = cell(elementaryNodes.getLength-1, 1);
  meanValue = cell(elementaryNodes.getLength-1, 1);
  mu = cell(elementaryNodes.getLength-1, 1);
  variance = cell(elementaryNodes.getLength-1, 1);
  varianceWithPedigreeUncertainty = cell(elementaryNodes.getLength-1, 1);
  compartment = cell(elementaryNodes.getLength-1, 1);
  subcompartment = cell(elementaryNodes.getLength-1, 1);

for i = 1:elementaryNodes.getLength-1
  node = elementaryNodes.item(i);
% Extract values from attributes
  elementaryExchangeId{i+1} = char(node.getAttribute('id'));
  amount{i+1} = char(node.getAttribute('amount'));
% Extract values from child nodes
  nameNode = node.getElementsByTagName('name').item(0);
  name{i+1} = char(nameNode.getTextContent());
  unitNameNode = node.getElementsByTagName('unitName').item(0);
  unitName{i+1} = char(unitNameNode.getTextContent());
  compartmentNode = node.getElementsByTagName('compartment').item(0);
  compartmentNode2 = compartmentNode.getElementsByTagName('compartment').item(0);
  compartment{i+1} = char(compartmentNode2.getTextContent());
  subcompartmentNode = compartmentNode.getElementsByTagName('subcompartment').item(0);
  subcompartment{i+1} = char(subcompartmentNode.getTextContent());
```

```
% Check if 'uncertainty' node exists
  uncertaintyNode = node.getElementsByTagName('uncertainty').item(0);
% Initialize uncertainty fields to 0
  meanValue{i} = '0';
  mu{i} = '0';
  variance{i} = '0';
  varianceWithPedigreeUncertainty{i} = '0';
% If 'uncertainty' node exists, extract values from 'lognormal' child node
if ~isempty(uncertaintyNode)
    lognormalNode = uncertaintyNode.getElementsByTagName('lognormal').item(0)
        ;
  if isempty(lognormalNode)
    lognormalNode = uncertaintyNode.getElementsByTagName('normal').item(0);
  end
    meanValue{i} = char(lognormalNode.getAttribute('meanValue'));
    mu{i} = char(lognormalNode.getAttribute('mu'));
    variance{i} = char(lognormalNode.getAttribute('variance'));
    varianceWithPedigreeUncertainty{i} = char(lognormalNode.getAttribute('
        varianceWithPedigreeUncertainty'));
  end
end
dataTable = table(elementaryExchangeId(2:end), name(2:end), compartment(2:end
    ), subcompartment(2:end), amount(2:end), unitName(2:end), meanValue, mu,
    variance, varianceWithPedigreeUncertainty, ...
'VariableNames', {'intermediateExchangeId', 'name', 'compartment', '
    subcompartment', 'amount', 'unitName', 'meanValue', 'mu', 'variance', '
    varianceWithPedigreeUncertainty'});
Elements{fileIdx} = dataTable;
Info{fileIdx,1} = firstExchangeName;
Info{fileIdx,2} =  geography;
end
```

5.2 Publication 3: Annex section

5.2.1 Calibrated distribution results

Figures 5.1 to 5.4 show the raw extracted data from the industry reports together with the calibrated PDFs shown in Table 3.17.

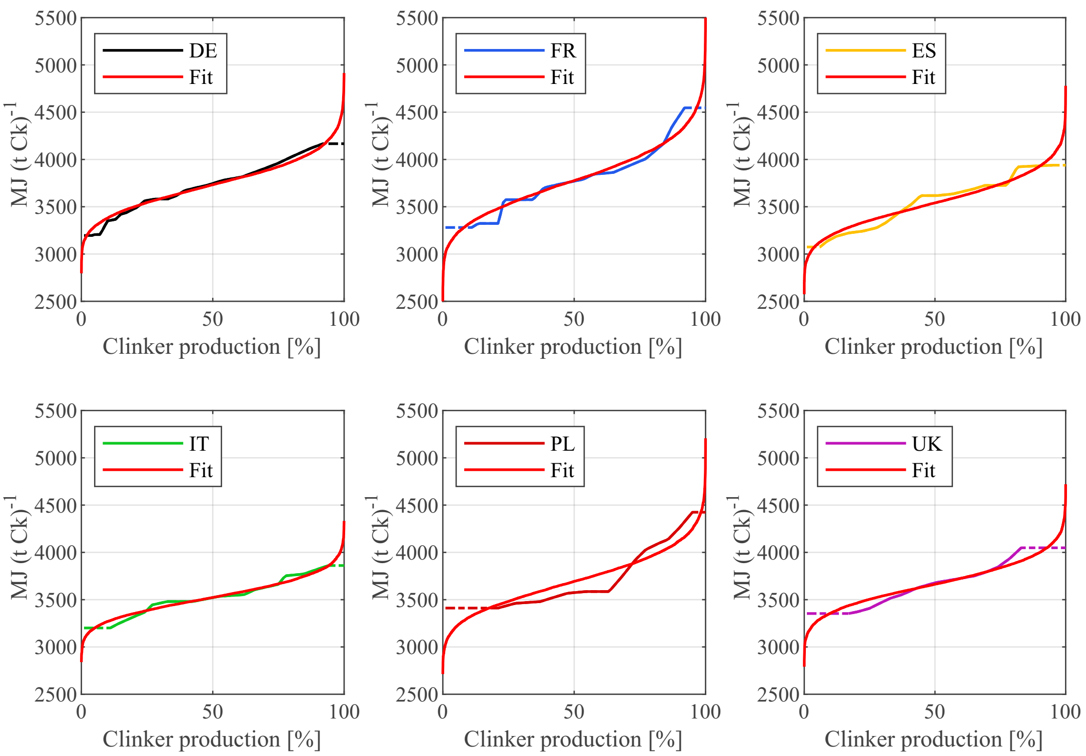

Figure 5.1: PDFs calibrated into raw data: Clinker energy intensity

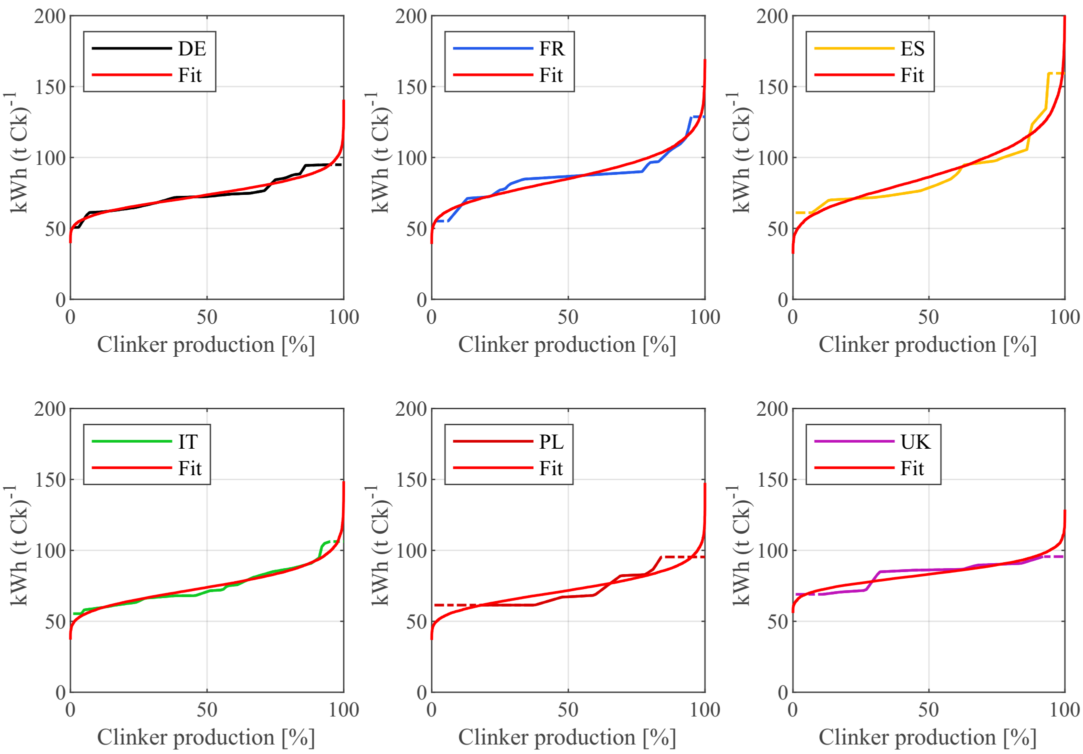

Figure 5.2: PDFs calibrated into raw data: Clinker power intensity

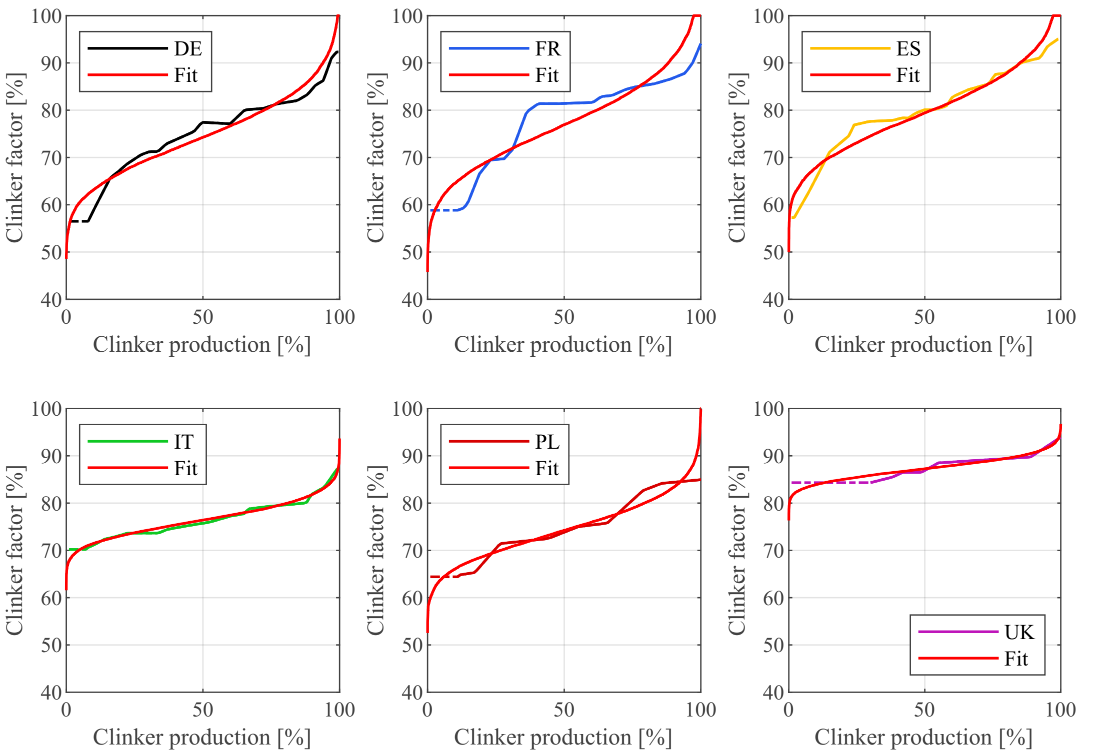

Figure 5.3: PDFs calibrated into raw data: Cem clinker factor

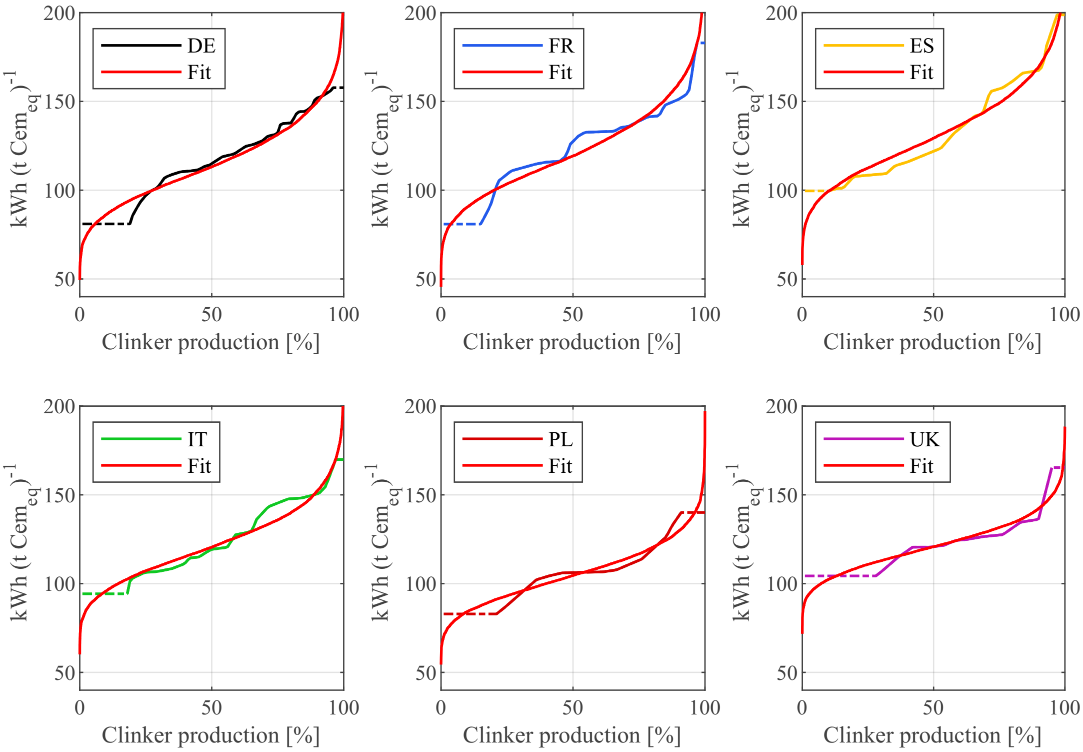

Figure 5.4: PDFs calibrated into raw data: Cem power intensity

5.2.2 Sensitivity of the parameter calibration

Figures 5.5 to 5.8 show the different fitting curves obtained when applying the filling methods described in the methodology section. Additionally, the influence of the different approaches in the PDFs parameters and the KEPIs is shown in Tables 5.2 and 5.3.

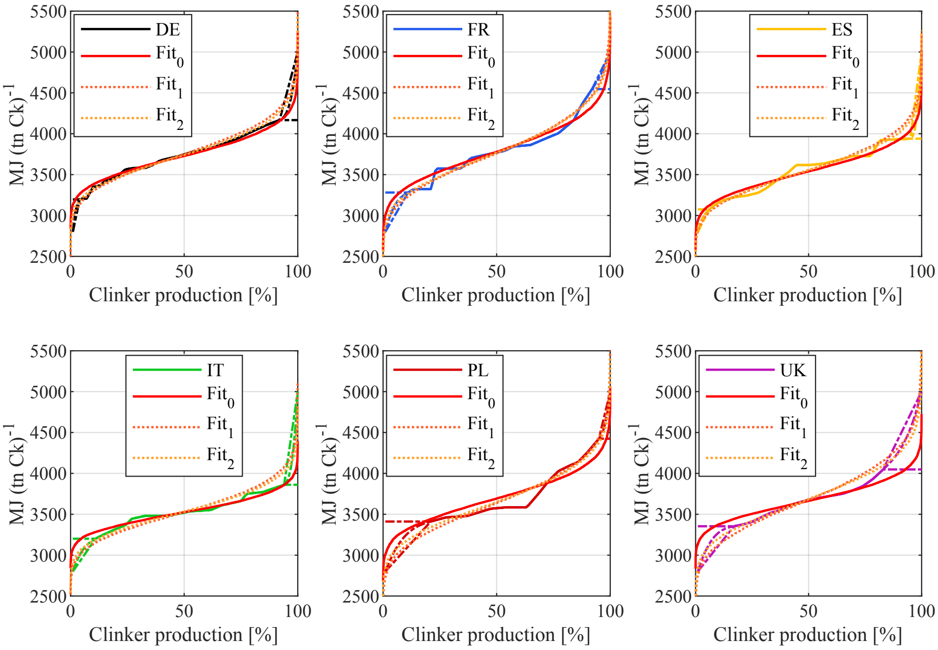

Figure 5.5: PDFs calibrated with different filling methods: Clinker energy intensity

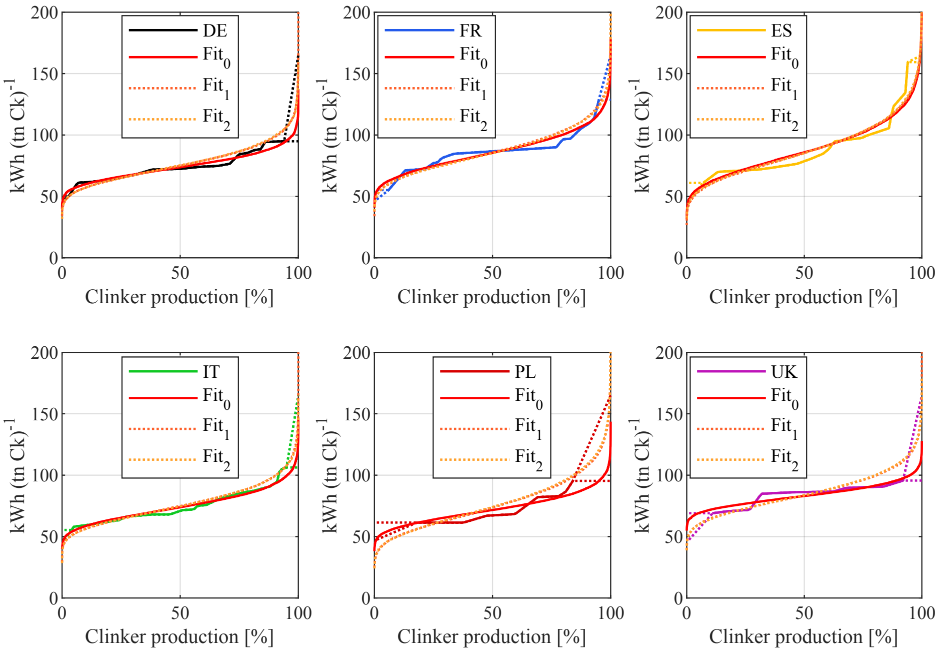

Figure 5.6: PDFs calibrated with different filling methods: Clinker power intensity

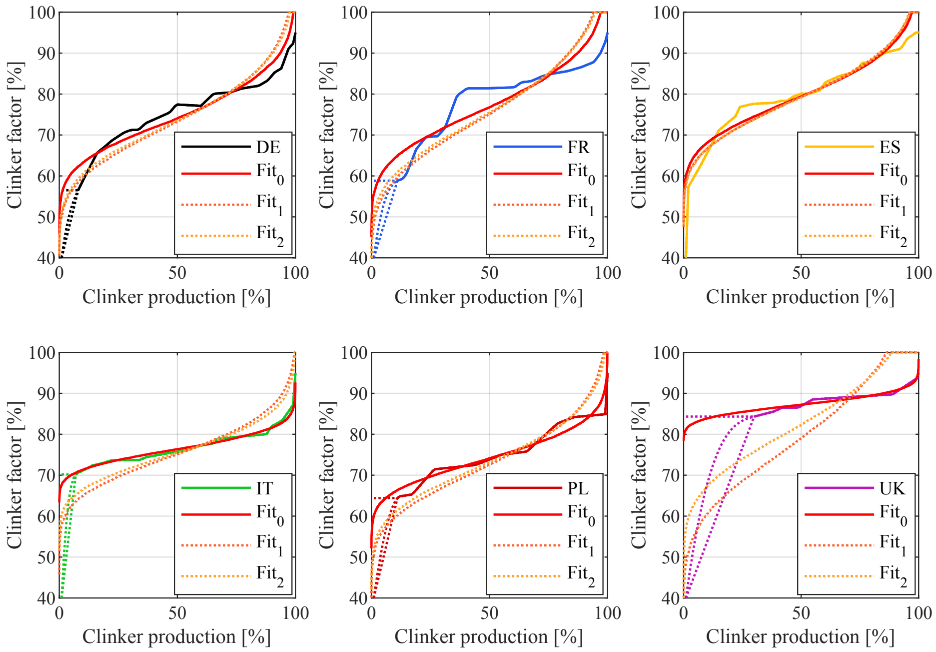

Figure 5.7: PDFs calibrated with different filling methods: Cem clinker factor

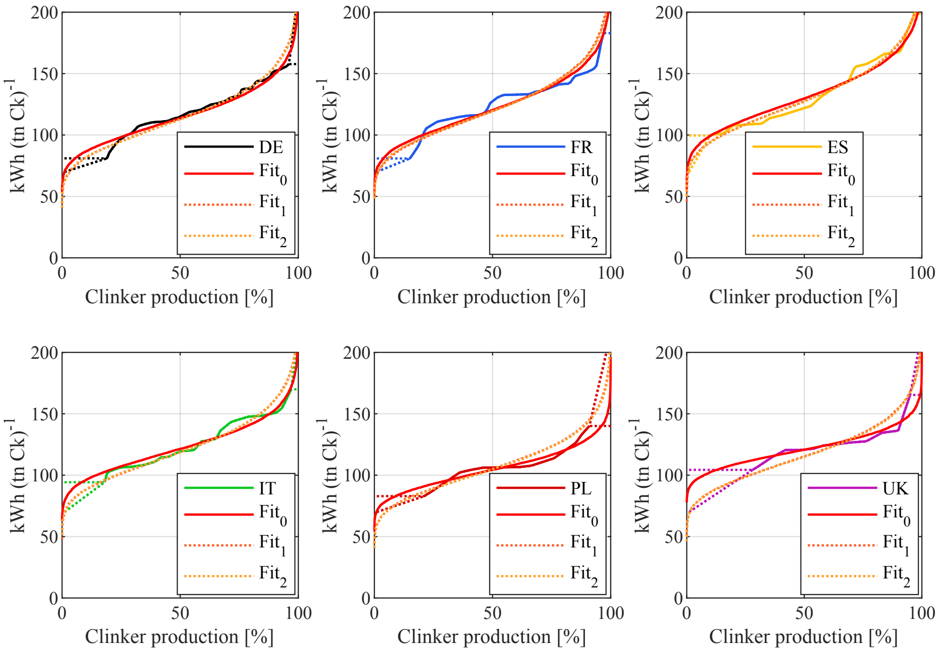

Figure 5.8: PDFs calibrated with different filling methods: Cem power intensity

Table 5.1: PDF parameters obtained for different filling methods.

		Fit_0: Original						Fit_1: linear interpolation						Fit_2: cubic interpolation					
Input	**Parameter**	**DE**	**FR**	**ES**	**IT**	**PL**	**UK**	**DE**	**FR**	**ES**	**IT**	**PL**	**UK**	**DE**	**FR**	**ES**	**IT**	**PL**	**UK**
Energy intensity - clinker	μ	8.224	8.238	8.172	8.168	8.214	8.207	8.230	8.233	8.177	8.170	8.198	8.212	8.228	8.236	8.175	8.169	8.204	8.213
[MJ/ton ck]	σ	0.0770	0.0992	0.0805	0.0579	0.0863	0.0678	0.0999	0.1229	0.1017	0.0946	0.1216	0.1263	0.0929	0.1176	0.0955	0.0841	0.1108	0.1105
Power intensity - clinker	μ	4.299	4.445	4.455	4.303	4.273	4.420	4.318	4.448	4.448	4.314	4.302	4.427	4.318	4.448	4.448	4.314	4.302	4.427
[kWh/ton ck]	σ	0.1585	0.1968	0.2574	0.1801	0.1706	0.1123	0.2118	0.2256	0.2742	0.2221	0.2969	0.2074	0.2118	0.2256	0.2742	0.2221	0.2969	0.2074
Clinker factor	μ	4.307	4.340	4.375	4.336	4.308	4.469	4.294	4.320	4.371	4.318	4.284	4.370	4.297	4.327	4.371	4.324	4.290	4.414
[% ck]	σ	0.1259	0.1383	0.1196	0.0525	0.0911	0.0305	0.1621	0.1866	0.1341	0.1144	0.1521	0.2129	0.1552	0.1716	0.1341	0.0987	0.1408	0.1582
Power intensity - cement	μ	4.732	4.788	4.864	4.799	4.647	4.794	4.726	4.780	4.849	4.778	4.652	4.750	4.726	4.780	4.849	4.778	4.652	4.750
[kWh/ton cem]	σ	0.2157	0.2239	0.2094	0.1813	0.1678	0.1295	0.2537	0.2506	0.2410	0.2341	0.2425	0.2257	0.2537	0.2506	0.2410	0.2341	0.2425	0.2257

Table 5.2: Clinker KEPIs for different filling methods.

		DE			FR			ES			IT			PL			UK		
		Fit_0	**Fit_1**	**Fit_2**	**Fit_0**	**Fit_1**	**Fit_2**	**Fit_0**	**Fit_1**	**Fit_2**	**Fit_0**	**Fit_1**	**Fit_2**	**Fit_0**	**Fit_1**	**Fit_2**	**Fit_0**	**Fit_1**	**Fit_2**
AP	μ	1.57E+00	1.58E+00	1.58E+00	2.81E+00	2.80E+00	2.80E+00	2.73E+00	2.74E+00	2.74E+00	3.12E+00	3.13E+00	3.13E+00	2.51E+00	2.53E+00	2.53E+00	3.20E+00	3.22E+00	3.22E+00
[mol H+ eq]	σ	4.68E-02	6.09E-02	5.73E-02	1.86E-01	2.31E-01	2.21E-01	1.40E-01	1.77E-01	1.67E-01	1.24E-01	2.03E-01	1.80E-01	1.28E-01	2.08E-01	2.00E-01	1.51E-01	2.87E-01	2.50E-01
GWP	μ	8.52E+02	8.55E+02	8.54E+02	8.63E+02	8.63E+02	8.63E+02	8.70E+02	8.72E+02	8.72E+02	9.21E+02	9.23E+02	9.23E+02	8.96E+02	8.98E+02	8.99E+02	9.41E+02	9.46E+02	9.46E+02
[kg CO2 eq]	σ	2.02E+01	2.63E+01	2.48E+01	2.90E+01	3.60E+01	3.44E+01	2.35E+01	2.94E+01	2.78E+01	1.98E+01	3.20E+01	2.85E+01	2.55E+01	3.87E+01	3.65E+01	2.40E+01	4.56E+01	3.99E+01
ET	μ	1.02E+03	1.03E+03	1.03E+03	1.55E+03	1.54E+03	1.54E+03	1.76E+03	1.77E+03	1.77E+03	2.06E+03	2.07E+03	2.07E+03	1.04E+03	1.05E+03	1.05E+03	1.10E+03	1.11E+03	1.11E+03
[CTUe]	σ	4.76E+01	6.21E+01	5.89E+01	1.18E+02	1.47E+02	1.40E+02	1.11E+02	1.41E+02	1.32E+02	9.80E+01	1.61E+02	1.43E+02	5.49E+01	8.76E+01	8.38E+01	4.99E+01	9.48E+01	8.26E+01
NRE	μ	2.01E+03	2.03E+03	2.03E+03	4.02E+03	4.03E+03	4.03E+03	3.70E+03	3.71E+03	3.71E+03	4.26E+03	4.28E+03	4.28E+03	2.42E+03	2.46E+03	2.46E+03	3.48E+03	3.52E+03	3.52E+03
[MJ]	σ	1.18E+02	1.57E+02	1.55E+02	3.24E+02	3.95E+02	3.80E+02	2.71E+02	3.19E+02	3.09E+02	2.14E+02	3.38E+02	3.04E+02	1.70E+02	2.93E+02	2.85E+02	1.78E+02	3.36E+02	3.03E+02
EP	μ	2.30E-01	2.33E-01	2.33E-01	6.31E-02	6.31E-02	6.31E-02	2.92E-02	2.93E-02	2.93E-02	3.98E-02	4.00E-02	3.99E-02	1.82E-01	1.86E-01	1.86E-01	1.84E-01	1.86E-01	1.86E-01
[kg P eq]	σ	1.52E-02	1.99E-02	1.92E-02	4.83E-03	6.00E-03	5.73E-03	1.48E-03	1.67E-03	1.64E-03	1.52E-03	2.33E-03	2.12E-03	1.59E-02	2.87E-02	2.81E-02	1.14E-02	2.17E-02	1.89E-02
HT-Cancer	μ	7.93E-08	7.98E-08	7.97E-08	1.17E-07	1.17E-07	1.17E-07	1.16E-07	1.17E-07	1.17E-07	1.28E-07	1.29E-07	1.29E-07	9.74E-08	9.85E-08	9.86E-08	1.02E-07	1.03E-07	1.03E-07
[CTUh]	σ	3.81E-09	4.96E-09	4.69E-09	8.90E-09	1.11E-08	1.05E-08	7.02E-09	8.78E-09	8.30E-09	5.77E-09	9.36E-09	8.33E-09	5.91E-09	9.89E-09	9.56E-09	4.90E-09	9.31E-09	8.13E-09
HT-NonCancer	μ	2.04E-06	2.06E-06	2.06E-06	2.34E-06	2.34E-06	2.34E-06	1.95E-06	1.96E-06	1.96E-06	2.15E-06	2.16E-06	2.16E-06	3.36E-06	3.41E-06	3.41E-06	3.59E-06	3.63E-06	3.63E-06
[CTUh]	σ	1.14E-07	1.49E-07	1.41E-07	1.87E-07	2.33E-07	2.22E-07	1.19E-07	1.48E-07	1.41E-07	9.74E-08	1.58E-07	1.41E-07	2.47E-07	4.21E-07	4.09E-07	2.08E-07	3.96E-07	3.45E-07
MMD	μ	2.82E-04	2.84E-04	2.83E-04	3.02E-04	3.02E-04	3.02E-04	2.94E-04	2.94E-04	2.94E-04	2.93E-04	2.94E-04	2.94E-04	2.65E-04	2.66E-04	2.66E-04	3.01E-04	3.03E-04	3.02E-04
[kg Sb eq]	σ	6.40E-06	8.47E-06	8.35E-06	9.34E-06	1.15E-05	1.10E-05	9.21E-06	1.03E-05	1.02E-05	6.16E-06	8.89E-06	8.32E-06	5.50E-06	9.11E-06	8.79E-06	6.03E-06	1.14E-05	1.04E-05
ODP	μ	1.59E-06	1.60E-06	1.60E-06	3.28E-06	3.28E-06	3.28E-06	3.93E-06	3.95E-06	3.95E-06	4.92E-06	4.95E-06	4.94E-06	1.31E-06	1.33E-06	1.33E-06	2.68E-06	2.72E-06	2.72E-06
[kg CFC-11 eq]	σ	8.16E-08	1.07E-07	1.04E-07	2.64E-07	3.28E-07	3.12E-07	2.74E-07	3.34E-07	3.19E-07	2.53E-07	3.96E-07	3.58E-07	7.08E-08	1.17E-07	1.13E-07	1.54E-07	2.89E-07	2.87E-07
PM	μ	1.64E-05	1.65E-05	1.65E-05	3.05E-05	3.05E-05	3.05E-05	2.56E-05	2.57E-05	2.57E-05	2.79E-05	2.80E-05	2.80E-05	2.19E-05	2.18E-05	2.18E-05	3.50E-05	3.53E-05	3.53E-05
[Disease incidence]	σ	6.20E-07	8.08E-07	7.55E-07	2.19E-06	2.73E-06	2.60E-06	1.37E-06	1.74E-06	1.63E-06	1.13E-06	1.85E-06	1.64E-06	1.13E-06	1.58E-06	1.46E-06	1.80E-06	3.42E-06	2.98E-06
POCP	μ	6.30E-01	6.34E-01	6.33E-01	1.17E+00	1.17E+00	1.17E+00	1.13E+00	1.13E+00	1.13E+00	1.25E+00	1.25E+00	1.25E+00	9.28E-01	9.34E-01	9.35E-01	1.21E+00	1.22E+00	1.22E+00
[kg NMVOC eq]	σ	2.77E-02	3.61E-02	3.40E-02	9.11E-02	1.13E-01	1.08E-01	6.84E-02	8.52E-02	8.07E-02	5.63E-02	9.06E-02	8.09E-02	5.38E-02	8.47E-02	8.07E-02	6.25E-02	1.19E-01	1.04E-01
WD	μ	9.79E+01	9.85E+01	9.84E+01	6.44E+01	6.44E+01	6.44E+01	5.87E+01	5.86E+01	5.86E+01	6.71E+01	6.74E+01	6.74E+01	7.27E+01	7.35E+01	7.34E+01	6.90E+01	6.94E+01	6.93E+01
[m3 world eq]	σ	4.03E+00	5.25E+00	4.94E+00	2.57E+00	3.04E+00	2.99E+00	2.61E+00	2.76E+00	2.75E+00	2.97E+00	3.78E+00	3.77E+00	2.92E+00	5.21E+00	5.10E+00	1.65E+00	3.13E+00	2.80E+00

Table 5.3: Cement KEPIs for different filling methods.

		DE			FR			ES			IT			PL			UK		
		Fit_0	Fit_1	Fit_2	Fit_0	Fit_1	Fit_2	Fit_0	Fit_1	Fit_2	Fit_0	Fit_1	Fit_2	Fit_0	Fit_1	Fit_2	Fit_0	Fit_1	Fit_2
AP	μ	1.37E+00	1.25E-01	1.19E-01	2.29E+00	3.55E-01	3.30E-01	2.34E+00	2.69E-01	2.65E-01	2.53E+00	2.86E-01	2.50E-01	2.44E+00	2.40E-01	2.32E-01	2.86E+00	4.73E-01	3.97E-01
[mol H+ eq]	σ	9.98E-02	1.25E-01	1.19E-01	2.84E-01	3.55E-01	3.30E-01	2.41E-01	2.69E-01	2.65E-01	1.51E-01	2.86E-01	2.50E-01	1.60E-01	2.40E-01	2.32E-01	1.54E-01	4.73E-01	3.97E-01
GWP	μ	6.86E+02	9.02E+01	8.62E+01	6.86E+02	1.08E+02	1.00E+02	7.19E+02	8.59E+01	8.57E+01	7.36E+02	7.88E+01	6.90E+01	7.42E+02	8.62E+01	8.13E+01	8.39E+02	1.33E+02	1.09E+02
[kg CO2 eq]	σ	7.24E+01	9.02E+01	8.62E+01	8.61E+01	1.08E+02	1.00E+02	7.83E+01	8.59E+01	8.57E+01	3.90E+01	7.88E+01	6.90E+01	5.48E+01	8.62E+01	8.13E+01	3.20E+01	1.33E+02	1.09E+02
ET	μ	1.61E+03	2.54E+02	2.45E+02	1.73E+03	1.55E+02	1.47E+02	1.54E+03	1.71E+02	1.66E+02	1.70E+03	1.86E+02	1.63E+02	1.45E+03	1.61E+02	1.52E+02	9.93E+02	1.56E+02	1.31E+02
[CTUe]	σ	2.04E+02	2.54E+02	2.45E+02	1.27E+02	1.55E+02	1.47E+02	1.49E+02	1.71E+02	1.66E+02	1.02E+02	1.86E+02	1.63E+02	1.03E+02	1.61E+02	1.52E+02	5.10E+01	1.56E+02	1.31E+02
NRE	μ	2.21E+03	2.35E+02	2.35E+02	3.94E+03	5.20E+02	5.03E+02	3.48E+03	4.12E+02	4.07E+02	3.74E+03	4.27E+02	3.85E+02	2.65E+03	3.10E+02	3.05E+02	3.44E+03	4.91E+02	4.28E+02
[MJ]	σ	1.98E+02	2.35E+02	2.35E+02	4.43E+02	5.20E+02	5.03E+02	3.64E+02	4.12E+02	4.07E+02	2.53E+02	4.27E+02	3.85E+02	2.09E+02	3.10E+02	3.05E+02	1.99E+02	4.91E+02	4.28E+02
EP	μ	2.18E-01	3.05E-02	2.96E-02	5.28E-02	7.78E-03	7.24E-03	2.92E-02	2.13E-03	2.13E-03	3.61E-02	3.36E-03	3.07E-03	2.02E-01	3.18E-02	3.14E-02	1.63E-01	3.04E-02	2.58E-02
[kg P eq]	σ	2.50E-02	3.05E-02	2.96E-02	6.26E-03	7.78E-03	7.24E-03	1.89E-03	2.13E-03	2.13E-03	2.04E-03	3.36E-03	3.07E-03	2.13E-02	3.18E-02	3.14E-02	1.11E-02	3.04E-02	2.58E-02
HT-Cancer	μ	7.32E-08	6.69E-09	6.40E-09	9.81E-08	1.46E-08	1.36E-08	1.00E-07	1.25E-08	1.22E-08	1.06E-07	1.23E-08	1.08E-08	9.74E-08	1.11E-08	1.08E-08	9.30E-08	1.50E-08	1.26E-08
[CTUh]	σ	5.38E-09	6.69E-09	6.40E-09	1.17E-08	1.46E-08	1.36E-08	1.11E-08	1.25E-08	1.22E-08	6.70E-09	1.23E-08	1.08E-08	7.38E-09	1.11E-08	1.08E-08	5.01E-09	1.50E-08	1.26E-08
HT-NonCancer	μ	1.94E-06	1.83E-07	1.76E-07	2.00E-06	2.80E-07	2.61E-07	1.74E-06	1.94E-07	1.90E-07	1.81E-06	2.01E-07	1.77E-07	3.53E-06	4.56E-07	4.47E-07	3.23E-06	5.67E-07	4.82E-07
[CTUh]	σ	1.48E-07	1.83E-07	1.76E-07	2.26E-07	2.80E-07	2.61E-07	1.72E-07	1.94E-07	1.90E-07	1.11E-07	2.01E-07	1.77E-07	3.06E-07	4.56E-07	4.47E-07	2.04E-07	5.67E-07	4.82E-07
MMD	μ	2.17E-03	8.74E-04	8.38E-04	1.81E-03	8.77E-04	8.16E-04	1.97E-03	8.42E-04	8.44E-04	1.89E-03	5.72E-04	5.01E-04	2.16E-03	8.05E-04	7.55E-04	2.24E-03	2.16E-03	1.73E-03
[kg Sb eq]	σ	7.01E-04	8.74E-04	8.38E-04	6.98E-04	8.77E-04	8.16E-04	7.68E-04	8.42E-04	8.44E-04	2.69E-04	5.72E-04	5.01E-04	5.04E-04	8.05E-04	7.55E-04	3.99E-04	2.16E-03	1.73E-03
ODP	μ	1.71E-06	1.35E-07	1.33E-07	2.89E-06	3.86E-07	3.62E-07	3.52E-06	4.45E-07	4.37E-07	4.37E-06	5.09E-07	4.63E-07	1.39E-06	1.19E-07	1.16E-07	3.06E-06	4.49E-07	4.29E-07
[kg CFC-11 eq]	σ	1.12E-07	1.35E-07	1.33E-07	3.14E-07	3.86E-07	3.62E-07	3.94E-07	4.45E-07	4.37E-07	3.08E-07	5.09E-07	4.63E-07	8.07E-08	1.19E-07	1.16E-07	2.41E-07	4.49E-07	4.29E-07
PM	μ	1.40E-05	1.37E-06	1.30E-06	2.49E-05	3.94E-06	3.67E-06	2.12E-05	2.75E-06	2.71E-06	2.22E-05	2.62E-06	2.29E-06	1.80E-05	2.15E-06	2.01E-06	3.10E-05	5.47E-06	4.60E-06
[Disease incidence]	σ	1.09E-06	1.37E-06	1.30E-06	3.16E-06	3.94E-06	3.67E-06	2.46E-06	2.75E-06	2.71E-06	1.37E-06	2.62E-06	2.29E-06	1.41E-06	2.15E-06	2.01E-06	1.82E-06	5.47E-06	4.60E-06
POCP	μ	5.96E-01	4.38E-02	4.19E-02	9.83E-01	1.44E-01	1.35E-01	9.97E-01	1.12E-01	1.10E-01	1.07E+00	1.15E-01	1.02E-01	9.24E-01	8.73E-02	8.43E-02	1.11E+00	1.74E-01	1.47E-01
[kg NMVOC eq]	σ	3.52E-02	4.38E-02	4.19E-02	1.16E-01	1.44E-01	1.35E-01	9.92E-02	1.12E-01	1.10E-01	6.46E-02	1.15E-01	1.02E-01	5.90E-02	8.73E-02	8.43E-02	6.19E-02	1.74E-01	1.47E-01
WD	μ	8.30E+01	9.86E+00	9.41E+00	6.05E+01	6.63E+00	6.38E+00	5.46E+01	5.55E+00	5.60E+00	6.65E+01	7.26E+00	7.11E+00	6.84E+01	7.28E+00	7.05E+00	6.36E+01	9.05E+00	7.44E+00
[m3 world eq]	σ	7.91E+00	9.86E+00	9.41E+00	5.55E+00	6.63E+00	6.38E+00	5.05E+00	5.55E+00	5.60E+00	5.14E+00	7.26E+00	7.11E+00	4.74E+00	7.28E+00	7.05E+00	2.30E+00	9.05E+00	7.44E+00