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Computational Sustainability for Climate-Resilient Materials: AI-Driven Decarbonization Pathways for Cement and Industrial Systems

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Abstract

Cement production remains a major industrial source of anthropogenic CO_2 because emissions arise from both limestone calcination and high-temperature fuel combustion. This review examines how computational sustainability can support climate-resilient and low-carbon cement production by integrating artificial intelligence (AI), machine learning (ML), digital twins, optimization, life cycle assessment (LCA), techno-economic analysis, and industrial systems modeling. An interdisciplinary scoping review was conducted using Preferred Reporting Items for Systematic Reviews and Meta-Analyses Extension for Scoping Reviews (PRISMA-ScR) informed procedures to synthesize evidence across materials discovery, cement and concrete mix optimization, plant operations, LCA integration, and system-level decarbonization planning. The review identifies computational sustainability as a multi-scale decision-support framework that links materials design, plant operations, supply-chain coordination, and policy/system planning. The synthesis shows that supervised learning, ensemble models, physics-informed neural networks, explainable AI, multi-objective optimization, digital twins, and system dynamics can support low-carbon binder screening, SCM optimization, kiln control, predictive maintenance, environmental-impact assessment, and infrastructure planning. SCM-based clinker substitution and energy-efficiency improvements are the most mature near-term options, while alternative binders, electrification, hydrogen integration, and cement-specific carbon capture, utilization, and storage (CCUS) require further validation, cost reduction, infrastructure development, and alignment with standards. Critical gaps remain in open and representative datasets, external model validation, uncertainty quantification, long-term durability evidence, multi-plant field trials, and integrated prospective LCA–techno-economic–system modeling. The review concludes that computational sustainability can accelerate cement-sector decarbonization when data-driven prediction, physical constraints, environmental assessment, economic evaluation, and policy-aware systems planning are integrated into transparent and validated decision frameworks.

Keywords: *Computational sustainability, Cement decarbonization, Artificial intelligence, Machine learning, Life cycle assessment, Carbon capture and storage.*

1. Introduction

Sustainable technologies contribute not only to industrial performance but also to wider social and environmental objectives, consistent with global agendas such as the United Nations Sustainable Development Goals (SDGs) [1]. In the cement sector, structured decarbonization frameworks enable systematic evaluation and prioritization of carbon dioxide (CO_2) mitigation options, supporting evidence-based pathways toward net-zero commitments [2]. Cement decarbonization is difficult to achieve because CO_2 arises from fuel combustion for high-temperature heat and from process emissions during limestone calcination, which together

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lead to emissions even with a low-carbon electricity supply [3], [4]. The challenge is increased by sector scale, with cement and clinker among the largest industrial CO_2 sources globally, motivating urgent mitigation action [3], [5]. Global emissions remain material in gigatons per year, reflecting historical growth in cement output and its contribution to carbon budgets [6]. Several strategies are being proposed to reduce cement-related CO_2 emissions by lowering clinker use in cement production [7], [8]. Among these, partial replacement of Portland cement with supplementary cementitious materials (SCMs) is consistently identified as a high-impact and readily deployable option, enabling meaningful reductions in embodied carbon while maintaining performance when appropriately formulated [9], [10]. Emissions are also geographically concentrated, implying that feasible mitigation portfolios and enabling infrastructure depend strongly on regional production structure and policy context [11]. Collectively, these features justify integrated portfolios combining clinker reduction, efficiency gains, low-carbon heat options, and carbon capture to meet mid-century climate targets.

1.1. The climate imperative for cement decarbonization

The global cement industry is currently at a critical stage in addressing climate change, given its anthropogenic CO_2 emissions, and cement has been used since ancient times [6], [12]. Cement and clinker production remains one of the most carbon-intensive industrial processes, emitting approximately 2.8 gigatons of CO_2 per year, accounting for about 8% of global anthropogenic CO_2 emissions [13]. Unlike other industries, cement production has two sources of CO_2: energy use and raw materials. Limestone calcination ($CaCO_3 \rightarrow CaO + CO_2$) accounts for about 60% of total emissions [3], [4]; this chemical reaction is stoichiometric and occurs during the normal production of Portland cement, with the remaining 40% generated by fuel combustion (coal, petroleum coke, natural gas) [5], [14], [15], [16], [17], [18], [19]. This fundamental chemistry makes cement a hard-to-abate sector that cannot be decarbonized solely with renewable energy, with a substantial fraction of emissions stemming from process CO_2 emitted during limestone calcination, in addition to fuel CO_2. Therefore, renewable electricity or renewable heat alone cannot fully decarbonize the cement industry [4], [15], [20], [21], [22]. So, a comprehensive mitigation strategy generally requires reducing the clinker factor through clinker substitution and applying CO_2 capture to the remaining process and combustion emissions.

Global cement production totaled approximately 4.1 billion tons in 2020, with China accounting for more than 50%, followed by India, Vietnam, and the United States [5], [11]. The reported cement carbon intensity varies substantially by region and technology, typically ranging 0.5–0.9 tons CO_2 per ton of cement, with a representative average of about 0.65 tons CO_2 per ton, implying on the order of a minimum 2.8 $GtCO_2$ per year and underscoring cement as a major industrial CO_2 source [3], [4], [13], [19]. Consistent with this production structure, CO_2 emissions from cement in 2024 are highly concentrated in China (617.75 Mt), which is almost 3.3 times higher than India (185.97 Mt), followed by a secondary group including Vietnam (44.49 Mt), Türkiye (42.18 Mt), the United States (37.27 Mt), and Iran (36.96 Mt), as shown in Figure 1. Also, Indonesia (30.02 Mt), Saudi Arabia (29.38 Mt), Egypt (27.59 Mt), and Brazil (25.38 Mt) show high concentrations and emission disparities relative to the rest of Asia, with emission gaps between the leading producers and others.

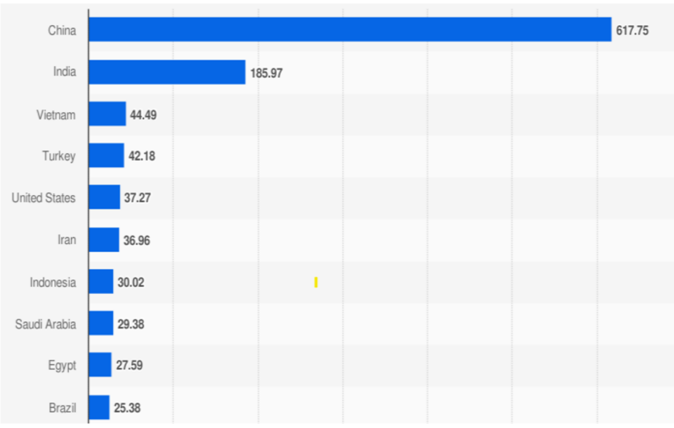

Figure 1. Annual CO_2 emissions from cement by country, 2024 [23].

An estimated increase in global cement demand has heightened the urgency of addressing CO_2 emissions from cement. Urbanization in developing economies, particularly in Asia and Africa, is expected to drive cement consumption to over 5 billion tons annually by 2050, potentially doubling current emission levels without transformative interventions [24], for example, scenario analysis for developing countries (excluding China) projects cement emissions rising from about 0.7 Gt (2018) to about 1.4–3.8 Gt (2050) depending on development paths, i.e., potentially doubling or more without strong interventions [15], [25]. Achieving the Paris Agreement goal of limiting global warming to 1.5–2°C requires the cement industry to reach near-zero emissions by mid-century. This shift demands a fundamental change in materials, production processes, and plans to address the sector's carbon intensity at the system level [3], [13]. Recent research identified opportunities for decarbonization, including material efficiency, clinker substitution, alternative fuel use, electrification, and carbon capture technologies [5], [19], [26]. The environmental impact of cement production extends beyond carbon emissions; it also includes resource depletion, particulate matter emissions, and ecosystem disruption. According to Habert, et al. [3], these multifaceted environmental challenges require integrated methods that consider the entire value chain, ie, from the extraction of raw materials to end-of-life recycling. The decarbonization of the cement industry is a climate necessity but also a broader sustainability challenge that requires systemic change [27], [28].

Artificial Intelligence (AI) and Machine Learning (ML) technologies are already being used to optimize energy systems, manage natural resources and reduce carbon emissions, thereby making methods more sustainable and overcoming environmental disputes [29]. AI-driven technologies help improve energy efficiency, use available resources more effectively, and support more sustainable decision-making. AI can contribute to global sustainability by offering innovative solutions across sectors such as energy optimization, environmental conservation, and waste management [30]. System-level optimization and digitalization of operations, as highlighted in a study, are necessary to make cement production climate-neutral, aligning with the research focus on AI-based whole-value-chain decarbonization of cement production [31], [32].

1.2. Sustainability: prospects and potential

Computational sustainability integrates computer science, operations research, and sustainability science to address complex environmental challenges [24], [33]. In the cement sector, it enables computational capabilities that can accelerate the transition to low-carbon production systems by linking materials innovation, plant operations, life-cycle evidence, and transition planning within a unified decision framework [18], [34].

In this review, computational sustainability is conceptualized as a multi-scale decision framework that connects AI/ML, digital twins, optimization, life cycle assessment (LCA), and industrial systems analysis across materials, plant, supply chain, and policy/system levels. AI and ML provide predictive capabilities, pattern recognition, surrogate modeling, and decision support for binder discovery, SCM optimization, hydration modeling, process monitoring, and property prediction. Digital twins connect sensor data, process models, and simulation environments to support dynamic representation of physical assets, real-time diagnostics, predictive maintenance, and operational decision-making. Optimization methods identify feasible low-carbon solutions subject to constraints on cost, emissions, strength, durability, energy use, resource availability, and infrastructure readiness. LCA provides the environmental accounting framework needed to evaluate impacts across the cement value chain and to avoid burden shifting between life-cycle stages and impact categories. Industrial systems analysis extends the analysis beyond individual plants by examining material flows, circularity, resource efficiency, inter-industry coordination, and system-wide interactions. Together, these components define computational sustainability as an integrative framework linking materials design, plant-scale control, supply-chain coordination, and system-level decarbonization planning.

Table 1 presents computational sustainability capabilities across materials design, plant operations, life cycle assessment, and system-level planning. It summarizes the key capability areas through which computational sustainability can accelerate decarbonization in the cement sector. It shows how AI/ML physics-informed neural networks (PINNs), digital twins, prospective life cycle assessment (pLCA), coupled with Integrated assessment models (IAM), optimization, and system dynamics (SD), support cement decarbonization by linking prediction, control, environmental assessment, and decision support.

Table 1. Computational sustainability in cement decarbonization.

Capability Area	**Core Computational Methods & Technologies**	**Cement Decarbonization Decision Function**	**Cement Decarbonization Value**	**Expected Outcomes**	**References**
Accelerated Materials Discovery	AI/ML screening, PINNs	Screens low-carbon binder formulations and optimizes SCM replacement levels under performance and durability constraints	Reduces experimental burden and accelerates identification of feasible low-clinker binders	Faster screening of large formulation spaces; shorter development timelines; optimized SCMs replacement while maintaining mechanical and durability performance	[24], [33], [35], [36].
Process Optimization & Intelligent Manufacturing	Real-time optimization, predictive maintenance, adaptive control, digital twins, Industry 4.0 (IoT sensors, edge computing, ML)	Converts high-frequency plant data into operational setpoints for kiln control, maintenance planning, and quality stabilization	Reduces kiln energy intensity and CO_2 emissions while preserving clinker quality under operational disturbances	Lower fuel and electricity consumption; improved process stability; potential 10–15% energy reduction and 8–12% CO_2 reduction through optimized operations	[18], [34], [37], [38]
Life Cycle Assessment Integration & Multi-Objective Decision Support	ML models, pLCA, IAMs	Evaluates environmental impacts across life cycle stages and supports multi-objective comparison under alternative future conditions	Reduces burden shifting and supports balanced decisions across carbon, cost, performance, and resource efficiency	Faster environmental screening; scenario-consistent pathway comparison; improved selection of low-carbon cement options	[36], [39].
System-Level Planning & Transition Design	AI-driven scenario analysis, SD modeling, Optimization	Identifies coordinated intervention portfolios across materials, processes, infrastructure, and policy instruments	Supports sector-wide planning under technical, economic, and policy constraints	Improved policy and infrastructure planning; robust intervention portfolios; stronger alignment between plant-scale decisions and net-zero targets	[39], [40], [41], [42], [43].

To complement the capability-based summary in Table 1, Figure 2 presents the proposed computational sustainability framework for cement decarbonization. The Figure synthesizes the main computational methods reviewed in this study, including AI/ML, physics-informed neural networks, digital twins, multi-objective optimization, prospective LCA, techno-economic analysis, and system dynamics. These methods are mapped to four decision scales: materials design, plant operations, supply-chain coordination, and policy/system planning. The framework further links these decision scales to major cement decarbonization pathways, including SCM substitution, alternative binders, process optimization, alternative fuels and low-carbon heat, carbon capture, utilization, and storage (CCUS), and integrated mitigation portfolios. The final layer identifies measurable performance and deployment outputs, including CO_2 intensity, energy intensity, cost, durability, scalability, technology readiness, and evidence confidence.

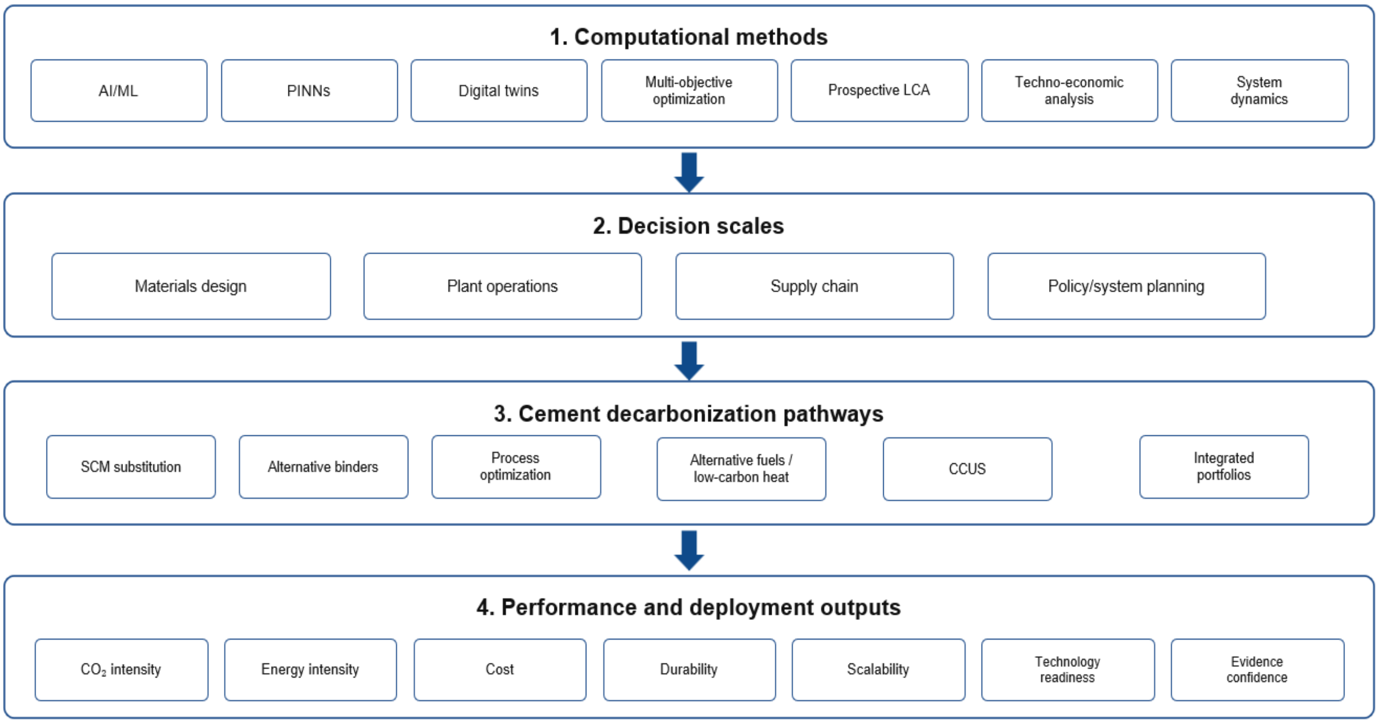

Figure 2. Computational sustainability framework for cement decarbonization.

Table 1 links computational sustainability capability areas to their underlying methods, cement-sector functions, decarbonization value, expected decarbonization contributions and implementation outcomes, clarifying how these capabilities support materials innovation, process optimization, life-cycle integration, and system-level planning.

More broadly, combining AI with domain expertise in materials science, chemical engineering, and industrial systems analysis strengthens sustainability problem-solving by aligning mechanistic understanding with data-driven prediction and optimization [34], [44]. Evidence indicates that AI-supported intelligent manufacturing of green cement is moving from conceptual development to implementation, with pilot activities reporting both environmental and economic gains [34]. The study focuses on four related areas, including (1) the discovery of materials and mix optimization, (2) optimization of the processes and intelligent manufacturing, (3) LCA integration, and (4) industrial-scale decarbonization planning. The review covers recent peer-reviewed journals, industry reports, and case studies from leading research institutions and cement producers.

Despite the growing literature on cement decarbonization, a specific gap remains. Existing reviews have made important contributions by examining cement-sector sustainability and material-efficiency pathways [3], socio-technical and policy options for cement and concrete decarbonization [5], low-carbon binder and concrete technologies [26] and AI/LCA-based assessment of cementitious materials [36]. However, these studies generally focus on individual technology groups, material pathways, environmental assessment methods, or transition challenges. They do not fully synthesize computational sustainability as an integrative framework that links AI/ML, digital twins, optimization, LCA, and industrial systems analysis across material design, plant operations, supply chain coordination, and policy- and system-level transition planning. This review addresses that gap by organizing the evidence on how computational methods support prediction, dynamic process representation, constrained optimization, environmental impact assessment, and system-level decarbonization decisions in the cement sector.

The unique contribution of this review is its multi-scale computational sustainability framing for cement-sector decarbonization. Rather than reviewing AI, low-carbon materials, process optimization, LCA, and transition planning as separate topics, the manuscript synthesizes them into connected decision-support tools across material, plant, supply chain, and policy/system levels. This framing clarifies how AI/ML, digital twins, optimization, LCA, and industrial systems analysis jointly support prediction, dynamic process representation, constrained decision-making, environmental assessment, and system-level decarbonization planning.

Abbreviations and Acronyms

Acronym	Full Term
AI	Artificial Intelligence
ML	Machine Learning
SCMs	Supplementary Cementitious Materials
GGBFS	Ground Granulated Blast-Furnace Slag
LCA	Life-Cycle Assessment
pLCA	Prospective Life-Cycle Assessment
IAMs	Integrated Assessment Models
SHAP	SHapley Additive exPlanations
CCUS	Carbon Capture, Utilization, & Storage
CCS	Carbon Capture & Storage
PINNs	Physics-Informed Neural Networks
SD	System Dynamics
RL	Reinforcement learning
ExAI	Explainable Artificial Intelligence
SCADA	Supervisory Control & Data Acquisition
IoT	Internet of Things
TEA	Techno-Economic Analysis
SDGs	Sustainable Development Goals
ANNs	Artificial Neural Networks
CAPEX	Capital Expenditure
MOO	Multi-Objective Optimization
SEM	Scanning electron microscopy
SVM	Support Vector Machine
MPC	Model predictive control
WHR	Waste heat recovery
LIME	Local Interpretable Model-agnostic Explanations
PSO	Particle Swarm Optimization
GA	Genetic Algorithms
UHPC	Ultra-High-Performance Concrete
RMSE	Root Mean Square Error
CSA	Calcium sulfoaluminate
BF–BOF	Blast furnace–basic oxygen furnace
R^2	Coefficient of determination

2. Literature Review

2.1. Cement production and carbon emissions

The production of Portland cement involves several energies and carbon-intensive stages, beginning with the extraction of raw materials (primarily limestone and clay), followed by crushing, grinding, and homogenization to form raw meal. The raw meal is processed in a rotary kiln, where calcination and high-temperature reactions (typically up to ~1450°C) produce clinker, which is subsequently cooled and blended with gypsum and other additives to produce finished cement [4], [19]. The clinker is then cooled, mixed with gypsum and other additives, and transported as finished cement [3]. Barbhuiya, et al. [4] outlined an extensive analysis of the decarbonization strategies in the cement industry, dividing it into five fundamental pathways: (i) materials efficiency provided by lowered clinker to cement ratios and optimized concrete mixes designs, (ii) alternative fuels such as biomass, waste derived fuels, and hydrogen, (iii) substituting clinker with SCMs, such as fly ash, slag, and calcined clays, (iv) energy efficiency improvement in either grinding, kiln operations, and heat recovery, and (v) CCUS technologies [4], [19], [45]. Each pathway offers distinct emission-reduction potential, with clinker substitution and CCUS identified as the most impactful strategies for achieving deep decarbonization [5], [26].

2.2. Computational sustainability model

Computational sustainability is a broad field that uses computational methods, such as AI, optimization, simulation, and data analytics, to address sustainability issues at environmental, economic, and social dimensions [33]. The field emerged in the late 2000s to address complex systems characterized by nonlinear dynamics, multiple stakeholders, and competing objectives that are difficult to resolve with conventional analytical approaches [44]. In industrial decarbonization, computational sustainability has many advantages, including (i) it enables multi-scale modeling that connects molecular-scale phenomena, e.g., cement hydration chemistry to system-scale dynamics, e.g., regional supply chains [35], [39]; (ii) it facilitates multi-objective optimization (MOO) to balance carbon reduction, cost minimization, performance, and resource efficiency within a unified decision framework [24], [36]; and (iii) it supports scenario analysis and uncertainty quantification to evaluate the robustness of decarbonization strategies under alternative futures and parameter uncertainty [39], [40]. Its application in cement decarbonization aligns with industrial digitalization and Industry 4.0, where intelligent manufacturing integrates cyber-physical systems, cloud computing, the Internet of Things (IoT), and AI to support real-time tracking of energy consumption, emissions, and product quality, thereby enabling continuous improvement and rapid response to operating disturbances [18], [34], [38], [46].

2.3. AI and ML in materials science

AI and ML have accelerated materials discovery and optimization by efficiently learning composition-processing-property relationships from experimental and computational datasets [35], [36]. Table 2 summarizes AI/ML methods most relevant to cementitious materials by linking representative algorithms to application targets, benefits, and deployment considerations, thereby clarifying how these tools support property prediction, hydration modeling, mix optimization, and interpretability under realistic constraints. Interpreted as a methodological progression from property prediction to physically constrained modeling, decision-oriented mix design, and transparent deployment. Supervised learning enables rapid screening on well-represented datasets, while PINNs improve physical consistency with limited data. MOO converts the mix design into a structured decision problem that balances emissions, cost, strength, workability, and durability.

Table 2. AI/ML methods in cementitious materials science

AI & ML Approach	Representative Methods	Application In Cementitious Materials	Key Benefits	Deployment Consideration	References
Supervised Learning	artificial neural networks (ANNs), Support Vector Machines, random forests, gradient boosting	Predicts compressive strength, durability indicators, workability, and other material properties from mix composition, curing conditions, and processing parameters	Enables rapid property prediction and screening of cementitious formulations within the training domain	Requires high-quality labeled datasets and may perform poorly outside the range of training data	[24], [33], [36], [47].
Physics-informed Neural Networks	Physics-informed Neural Networks incorporating domain knowledge (conservation laws, thermodynamics, kinetics)	Models cement hydration, heat evolution, phase assemblage, and mechanical property development.	Improves physical consistency, reduces data requirements, and supports extrapolation beyond purely empirical models	Requires correct formulation of governing equations, boundary conditions, and physically meaningful loss functions	[35].
Multi-Objective Optimization	Genetic Algorithms, Particle Swarm Optimization, Bayesian Optimization	Optimizes cement and concrete mix design under multiple objectives, including carbon footprint, cost, strength, workability, and durability	Identifies Pareto-optimal mix designs that balance sustainability and performance requirements	Requires well-defined objective functions, constraints, and validation of selected optimal mixtures	[13], [24], [33], [36].
Explainable Artificial Intelligence	SHapley Additive exPlanations Local Interpretable Model-agnostic Explanations	Interprets black-box model predictions and identifies influential variables affecting cementitious material performance	Improves transparency, supports expert validation, and strengthens confidence in AI-assisted material design	Explanations must be interpreted with domain knowledge and should not be treated as proof of causality.	[47]

ExAI further supports expert validation by identifying influential variables and thereby strengthening confidence in the design of low-carbon cementitious materials.

Combining AI with high-throughput experimentation and computational materials science, e.g., density functional theory and molecular dynamics, supported by cement hydration, enables a robust ecosystem for accelerated materials discovery [35], [36]. In this model of materials informatics, data-driven models learn composition-property relations and processing structures, and provide guided simulations or experiments, thereby reducing the search space and minimizing development cycles. This has been demonstrated across multiple material classes, including alloys, polymers, catalysts, and cementitious materials, thereby enabling quick screening, performance- and sustainability-based ranking, and refinement [36].

3. Methodology

An interdisciplinary scoping review was conducted to map and synthesize evidence at the intersection of cement and concrete decarbonization, computational sustainability, AI/ML, optimization, LCA, and industrial systems transformation. A scoping review design is appropriate because the evidence base spans heterogeneous study types and validation contexts (materials experiments, plant-level case studies, optimization and control studies, and prospective assessment), which are not sufficiently comparable for pooled quantitative synthesis [48]. The review is reported using Preferred Reporting Items for Systematic Reviews and Meta-Analyses Extension for Scoping Reviews (PRISMA-ScR) conventions to ensure transparency and reproducibility of evidence identification, screening, eligibility assessment, and thematic synthesis [3], [49]. The methodological structure was also informed by Making Future Floating Cities Sustainable: A Way Forward, which illustrates transparent reporting of database selection, search period, PRISMA-guided study selection, factor categorization, questionnaire-based prioritization, and stage-wise synthesis procedures [50].

3.1. Review objectives, questions, and analytical framework

This scoping review is designed to map computational sustainability approaches that enable cement and concrete decarbonization and to identify evidence maturity and deployment constraints across application contexts. The objectives are to (i) characterize computational method classes applied to cement decarbonization, (ii) document reported outcomes and validation approaches, (iii) identify recurring barriers to industrial scaling, and (iv) synthesize research gaps and implementation priorities. The review addresses four questions:

- Which computational methods (AI and ML, physics-informed and hybrid models, optimization, digital twins, system dynamics, and prospective assessment) are applied to cement and concrete decarbonization across materials, process operations, and system planning?
- Which decarbonization functions are targeted (materials design and SCM substitution, process control and energy efficiency, life-cycle and scenario assessment, and system-level transition planning) and what outcomes are reported (e.g., CO_2 reduction, energy reduction, property prediction performance, durability indicators)?
- What validation approaches support these outcomes (laboratory validation, cross-validation, industrial pilot evidence, scenario-based modeling), and what limitations are reported?
- Which constraints and gaps limit scalability and adoption (data limitations, legacy-system integration, operator adoption, policy and infrastructure dependence) and what research and implementation priorities follow?

To operationalize these questions, an analytical framework is used to classify each included study along two axes: computational method class (prediction, physics-constrained modeling, optimization, digital twin/control, dynamics/scenarios, prospective assessment) and application domain (materials, plant operations, assessment, system planning). Outcomes are charted using decision-relevant metrics (e.g., property prediction performance, reported energy/CO_2 reductions, life-cycle impacts, and cost indicators where reported), together with validation type and deployment readiness.

Accordingly, the analytical framework maps each study to a decision-scale material, plant, supply chain, or policy/system level. It identifies the corresponding computational function, including prediction, dynamic representation, optimization, environmental assessment, or system integration.

The analytical framework was further informed by AI-for-sustainable-engineering perspectives that emphasize system-level integration, ethical safeguards, low-carbon computing, local-context adaptation, and the interconnections among predictive modeling, optimization, assessment, and system-planning tools [51].

3.2. Information sources and temporal coverage

Evidence was retrieved from peer-reviewed journal articles and peer-reviewed conference proceedings indexed in Scopus, Web of Science, and Google Scholar. These sources were used as the primary indexing and discovery platforms, with iterative expansion through backward and forward citation chasing to capture influential and emerging studies relevant to hard-to-abate industrial decarbonization [3], [48], [49], [52]. The primary publication coverage targeted 2015–2026, selected to capture rapid growth in AI/ML, digital twins, optimization, prospective LCA, and industrial decarbonization assessment, while allowing earlier seminal sources where necessary for conceptual grounding.

3.3. Search strategy and keywords

Search strings combined three concept groups: (i) cement and concrete decarbonization, (ii) computational methods, and (iii) application domains, including materials, plant operations, LCA/prospective LCA, carbon capture, and system planning. Representative keyword families included: "cement decarbonization," "low-carbon cement," "net-zero cement," "clinker substitution," "supplementary cementitious materials (SCMs)," "calcined clay" OR "LC3," "alkali-activated materials," "AI cement production," "machine learning concrete," "physics-informed neural networks," "cement hydration modelling," "mix design optimization," "Bayesian optimization," "multi-objective optimization," "digital twin cement," "smart cement plant," "intelligent manufacturing," "Industry 4.0 cement," "kiln optimization," "predictive maintenance," "process control cement," "cement life cycle assessment," "prospective LCA clinker," "integrated assessment model cement," "techno-economic cement decarbonization," "carbon capture cement," "CCUS cement," "cement electrification," "hydrogen cement," and "system dynamics cement emissions" [5], [26], [39], [52], [53], [54], [55], [56]. Search strings were iteratively refined and adapted for database-specific syntax to ensure coverage across interdisciplinary outlets.

The database searches were performed from December 2025 to March 2026, with a final verification search completed in April 2026. The master Boolean search string was: ("cement decarbonization" OR "low-carbon cement" OR "net-zero cement" OR "clinker substitution" OR "supplementary cementitious materials" OR "alternative binders") AND ("artificial intelligence" OR "machine learning" OR "physics-informed neural networks" OR "digital twin" OR "multi-objective optimization" OR "system dynamics") AND ("life cycle assessment" OR "prospective LCA" OR "techno-economic analysis" OR "carbon capture" OR "CCUS" OR "industrial decarbonization"). The string was adapted only for database-specific syntax in Scopus, Web of Science, and Google Scholar.

3.4. Eligibility criteria

Inclusion criteria were: (i) peer-reviewed publications in English; (ii) direct relevance to cement and concrete decarbonization pathways or computational methods, including AI, hybrid modelling, LCA, SD, and digital twins within the cement–concrete system or closely coupled hard-to-abate systems; (iii) clear methodological transparency and sufficient bibliographic identifiability, including DOI where available; and (iv) studies addressing materials, process, system-level, or policy dimensions of decarbonization. Exclusion criteria included non-scholarly commentary, editorial opinions, vendor reports, blog materials, and non-peer-reviewed preprints, to ensure methodological rigor and the reliability of the evidence synthesis [52].

3.5. Screening and PRISMA-ScR reporting

A complete PRISMA-ScR flow diagram with numerical values is provided in Figure 3. Records retrieved from searches were consolidated and deduplicated before screening, n = 99 unique records for title and abstract screening. Following screening, 78 records were excluded, leaving 21 full texts assessed for eligibility. All full texts assessed met the inclusion criteria, yielding n = 21 studies for the final synthesis.

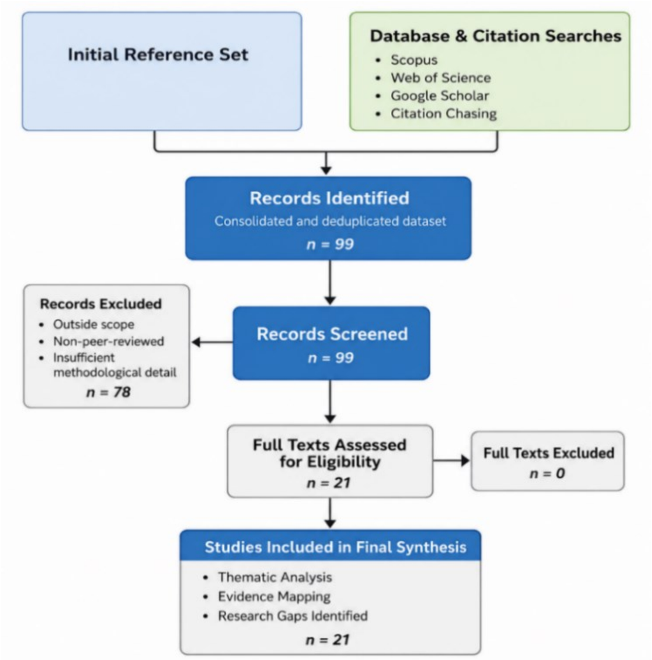

Figure 3. PRISMA-ScR flow diagram for study identification and selection.

The screening procedure involved four stages: duplicate removal, title and abstract screening, full-text eligibility assessment, and final evidence selection. The lead author conducted the initial screening, while both authors discussed uncertain or borderline records until agreement was reached. Records were excluded when they did not directly address cement and concrete decarbonization, computational sustainability methods, AI/ML, LCA, digital twins, system dynamics, CCUS, or closely related industrial decarbonization applications.

3.6. Evidence charting and appraisal approach

For each included study, evidence was charted using a structured extraction template capturing publication metadata; computational method class (e.g., supervised learning, physics-informed/hybrid models, optimization, digital twins, SD, prospective assessment); application domain (materials, process operations, assessment, system planning); input data type; output variables and reported performance metrics; validation approach (experimental validation, cross-validation, field trial, scenario analysis); and stated limitations. Evidence strength was appraised by recording validation type and context, including laboratory experimental validation, cross-validation, pilot or field evidence, scenario-based modeling, and prospective assessment. This approach supports critical interpretation of evidence maturity and deployment readiness without imposing appraisal tools designed for clinical or intervention-effect studies.

The final set of 21 studies represents the core evidence base used for structured scoping synthesis and evidence charting. These studies were selected because they directly addressed computational sustainability methods for cement and concrete decarbonization across materials design, plant operations, life-cycle assessment, techno-economic assessment, and system-level planning. The complete reference list contains 125 sources because additional references were used to provide contextual background, cement-sector emissions data, theoretical framing, methodological guidance, technical definitions, policy context, and comparisons with the wider industrial decarbonization literature. Therefore, the 21 studies should be interpreted as the structured synthesis sample, while the broader reference list provides supporting scholarly and contextual evidence for the full review.

3.7. Thematic synthesis

The included studies were synthesized using a cross-scale thematic structure aligned with the analytical framework: AI-enabled materials discovery and mix optimization; process optimization and intelligent manufacturing; LCA integration and prospective pathway assessment; and industrial-scale pathway planning [48], [49]. Within each theme, synthesis emphasized decision-relevant outcomes, validation strength, deployment constraints and research gaps to ensure critical interpretation [57]. This analytical structure was informed by review approaches that evaluate opportunities and risks, implementation constraints, and short- and long-term uncertainties in built-environment transitions [58]. To strengthen analytical depth, the synthesis was structured to distinguish established evidence, conditional findings, implementation constraints, and unresolved uncertainties across materials design, plant operations, life-cycle assessment, and industrial-scale decarbonization planning. Accordingly, the synthesis prioritizes cross-study interpretation over sequential study description by identifying what is established, what remains conditional, where implementation constraints persist, and which evidence gaps limit industrial deployment.

4. Artificial Intelligence-Enabled Materials Discovery and Mix Optimization

AI-enabled materials informatics and optimization can be interpreted as a decision layer that links formulation space, performance constraints, and decarbonization outcomes across cementitious systems. The evidence consistently supports computational approaches that (i) reduce experimental burden through data-efficient screening, (ii) incorporate physics and constraints to improve credibility outside narrow training domains, and (iii) couple performance metrics to environmental indicators to prevent emissions reductions from being offset by durability or constructability [35], [36], [39]. Within this scope, the central contribution of AI is not merely faster prediction, but improved feasibility-aware design under raw-material variability and deployment constraints.

4.1. Supplementary cementitious materials

SCMs are the most immediately deployable decarbonization lever because they directly reduce clinker demand, and clinker production accounts for the majority of CO_2 emissions in the cement sector [56], [59]. Across the SCM literature, the evidence converges on two robust conclusions: (i) clinker substitution with SCMs can substantially lower cement carbon intensity while meeting performance requirements when mixture design and curing are appropriately managed, and (ii) the practical limit on substitution is increasingly determined by SCM availability, quality variability, and standards acceptance, rather than by fundamental material feasibility [60], [61], [62]. Reported reductions in cement carbon intensity of approximately 20–60% are achievable under suitable conditions, but the realizable benefit is region-specific and depends on feedstock continuity and requirement protocols [3], [4], [36].

Mature SCM practice includes widely standardized materials such as fly ash, ground granulated blast-furnace slag (GGBFS), silica fume, limestone, and natural pozzolans, which have extensive field history and are already used commercially where supply chains and codes permit [3], [4], [5], [19]. The evidence also indicates an emerging structural constraint: coal power phase-down reduces fly ash availability, and steel-sector transitions reduce conventional slag supply, increasing the need for alternative SCM streams and for more stringent quality-control and performance-based requirements [3], [4], [5]. Consequently, wide-scale SCM deployment is shifting from a material substitution problem to a qualification-under-variability problem, where adoption depends on consistent characterization, mix re-optimization, and procurement and standards frameworks that accept performance-based substitution pathways.

Within this constraint space, AI/ML contributions are most defensible when they enhance decision quality under uncertainty by linking SCM type and replacement ratio, water-to-binder ratio, curing conditions, and age to both performance and environmental outcomes, thereby enabling rapid exploration of feasible design spaces without exhaustive testing [36]. Evidence from LCA-integrated artificial neural network (ANN) studies supports the role of ML surrogates in predicting compressive strength and durability indicators, alongside environmental metrics such as global warming potential (GWP), which are essential for screening options without burden shifting [36]. Optimization workflows that combine structured experimental design with ML models further demonstrate how multi-criteria objectives can be reconciled in practice, including high-strength, low-carbon binder systems [24]. Finally, explainable ML approaches strengthen industrial relevance by identifying dominant drivers, often the SCM replacement ratio, water-to-binder ratio, and curing age, that support quality assurance and performance requirements for scale deployment under variable SCM supply [47].

SCM optimization is comparatively mature because it builds on established blended-cement practice, but the evidence is conditional on regional material availability, feedstock consistency, durability validation, and performance-based standards. The main unresolved issue is not whether SCMs can reduce clinker-related emissions, but how reliably optimized mixtures can be scaled under changing fly ash and slag availability, variable SCM quality, and different regulatory contexts.

4.2. Physics-informed neural networks for cement hydration

Cement hydration governs early-age heat evolution, setting, and strength development, and it also controls microstructural evolution that determines long-term durability; consequently, hydration modeling is a core enabling capability for low-carbon binder and SCM design [35]. Across the evidence base, the central limitation of conventional approaches is a credibility burden tension: mechanistic and thermodynamic models (e.g., Powers–Brownyard, Jennings–Tennis, and thermodynamic frameworks implemented in GEMS or PHREEQC) can be physically grounded but often require extensive parameterization and computational effort, whereas purely data-driven models may fit the training data but fail to generalize across changing binder compositions and curing conditions [35]. PINNs address this gap by directly embedding conservation laws and thermodynamic/kinetic constraints into the learning process, thereby improving physical consistency and robustness when empirical datasets are limited or the operating domain shifts.

From a decarbonization perspective, the most important implication is that PINNs support not only forward prediction (e.g., heat evolution and phase assemblage) but also inverse design, thereby enabling performance-constrained identification of feasible SCM replacement ratios and curing strategies that meet application-specific requirements. For example, EcoBlendNet integrates mass and energy balances and thermodynamic equilibrium constraints to produce physically admissible hydration predictions, demonstrating low prediction error for heat evolution and phase assemblage under experimental validation and enabling inversion from targets such as 28-day strength and allowable heat release to candidate low-carbon formulations [35]. The broader evidence indicates that PINN credibility is strengthened when coupled with microstructural characterization and multi-scale modeling, such as X-ray computed tomography, scanning electron microscopy (SEM), nanoindentation, lattice Boltzmann methods, and phase-field models, because these tools extend prediction from bulk properties to durability-relevant microstructural features, e.g., porosity, pore-size distribution, and interfacial transition zone behavior that govern service-life performance.

In general, PINNs offer stronger physical consistency than purely data-driven models, but their maturity in cement applications remains emerging. Their reliability depends on the correct governing equations, boundary conditions, and hydration constraints, as well as validation against independent experimental and durability datasets. Current evidence supports PINNs as promising tools for screening and inverse design, but large-scale industrial use remains limited by data availability, model complexity, and incomplete long-term field validation.

4.3. Multi-Objective Optimization (MOO) approaches

Concrete mix design is inherently multi-criteria, requiring simultaneous minimization of the carbon footprint and cost while meeting requirements for strength development, durability, workability, pumpability, and project constraints [13], [24], [33]. MOO becomes practically useful when coupled with (i) predictive surrogate models that approximate performance responses over the design space and (ii) feasibility constraints that encode constructability and specification compliance; without these elements, optimization outputs risk being mathematically optimal but operationally impracticable [13], [24]. Illustrative results show that combining machine-learning surrogates with a metaheuristic search can identify high-performance, low-carbon mixtures across multiple objectives. For example, ANN-based performance models coupled with particle swarm optimization (PSO) and genetic algorithms (GA) have been used to optimize ultra-high-performance concrete (UHPC) with recycled fine aggregates and SCM substitution, yielding Pareto sets that balance strength, carbon footprint, cost, recycled content, and workability, with reported designs achieving high compressive strengths and meaningful carbon reductions relative to conventional UHPC [13]. Method selection is driven by problem structure rather than preference: GA is suited to discrete design decisions and non-convex multimodal landscapes, PSO is efficient for continuous variables such as water-to-binder ratio and SCM replacement ratio, and Bayesian optimization is advantageous when objective evaluations are expensive because it manages exploration and exploitation efficiently [13], [33]. Finally, integrating MOO with LCA strengthens decision credibility by broadening optimization from single-metric carbon minimization to multi-impact sustainability, enabling mixtures that reduce GWP while also managing burdens of acidification, eutrophication, and resource depletion alongside technical and economic constraints [36], [39].

4.4. Alternative binders and novel cements

Beyond SCM-blended Portland cement, alternative binders expand the mitigation space by reducing or replacing clinker formation, but the evidence indicates that scalability is governed as much by standardization, durability validation, and supply-chain readiness as by the intrinsic emissions potential of these binders [4], [19], [26], [41]. In the literature, alkali-activated materials (AAMs), calcium sulfoaluminate (CSA) cements, magnesium-based systems, and bio-based binders are consistently highlighted as promising classes, yet their deployment readiness varies substantially across chemistries, precursor dependence, and regulatory acceptance [4], [19]. AAMs (geopolymers) can achieve reported carbon reductions of approximately 40–80% relative to Portland cement, depending on precursor selection and activator chemistry, but widespread adoption remains constrained by specification pathways, long-term durability evidence, and reliable precursor and activator supply chains [4], [26], [41]. SD evidence further suggests that achieving meaningful market penetration greater than 20% of the cement market requires coordinated interventions that combine targeted R&D to improve performance and reduce costs, policy incentives such as carbon pricing, and industry collaboration to establish standards and robust supply networks.

CSA cements offer a comparatively nearer-term pathway in specific applications because their production requires lower kiln temperatures (approximately 1250–1300°C) and reduced limestone demand relative to Portland cement, yielding reported CO_2 reductions of about 20–35% while providing rapid strength and sulfate resistance in appropriate exposure conditions [4], [19]. Magnesium-based systems can enable CO_2 uptake through carbonation curing and therefore offer a potential route toward carbon-negative concrete; however, the net benefit is highly sensitive to magnesium sourcing and upstream impacts (e.g., seawater extraction or magnesite mining), which must be assessed using life-cycle evidence rather than laboratory performance alone[4], [26]. Bio-based binders, including microbially induced calcite precipitation and enzymatic mineralization, remain in the early stages of research; their credibility depends on reproducible validation of durability and feasibility of scale-up in real construction environments.

From a critical synthesis perspective, AI and ML are most defensible as accelerators of requirement and scale-up, rather than as stand-alone predictors of isolated strength metrics. In particular, rapid screening of formulation spaces, prediction of performance under precursor variability, and identification of feasible processing windows can reduce the experimental burden and support standardization pathways for alternative binders [35], [36]. As datasets broaden across diverse binder chemistries, ML models can also help identify transferable structure–property relationships that guide formulation design toward durable, application-ready low-carbon cement systems.

Across materials-focused studies, deep cement decarbonization requires coordinated portfolios, and the most deployable near-term reductions are consistently associated with clinker reduction through SCM substitution, low-clinker binders and formulation optimization, subject to performance and durability constraints. The achievable substitution depends on SCM availability and regional supply dynamics, motivating LC3 and data-driven optimization linking mix variables to performance and environmental endpoints. Evidence on the long-term durability and standardization protocols for emerging SCM feedstocks and alternative binders remains insufficient, limiting large-scale adoption despite promising laboratory performance. Research and deployment should prioritize performance-based substitution frameworks and decision tools that integrate

AI-enabled mix optimization and physics-informed hydration modeling with prospective, scenario-consistent assessment to identify robust low-carbon formulations under future supply and policy conditions.

5. Process Optimization and Intelligent Manufacturing

The transition toward climate-neutral cement production requires a shift from isolated operational adjustments to intelligent, system-level manufacturing. While the literature demonstrates that AI-driven process optimization can yield substantial energy and emission reductions, a critical synthesis of recent studies reveals a distinct maturation in the field: research is moving beyond standalone predictive algorithms toward closed-loop control systems, hybrid physics-data models, and comprehensive digital twin architectures. However, bridging the gap between pilot-scale success and robust, fleet-wide industrial deployment remains a persistent challenge, heavily constrained by legacy infrastructure, process non-linearities, and the need for operator trust.

5.1. Smart cement plants and industry 4.0

The integration of Fourth Industrial Revolution (Industry 4.0) technologies, including cyber-physical systems, IoT sensors, cloud computing, and advanced process analytics, has fundamentally altered the operational landscape of cement plants [63], [64]. Recent research evaluated the implementation of AI in smart cement plants and demonstrated significant operational benefits compared to traditional manufacturing. The study reported that AI-driven systems achieved a 22.7% reduction in energy consumption, a 15.3% decline in CO_2 emissions, and an 11.8% improvement in clinker quality consistency [18]. Furthermore, AI-powered predictive maintenance reduced production downtime by 75% and lowered maintenance costs by 30%, while overall productivity increased by 20%. These results highlight the high potential of intelligent manufacturing for delivering simultaneous environmental and economic performance. The integration of AI and advanced sensor technologies allows unprecedented visibility into production processes. Through continuous IoT monitoring and digitalization, plants can capture high-dimensional, real-time data on the kiln's temperature profile, operational parameters, and material composition [18], [34], [38]. Also, AI can enable green, intelligent manufacturing in the cement industry through abnormal-condition detection, data-driven prediction of clinker and cement quality, early prediction of 28-day strength for proactive quality assurance, and digital-twin visualization that improves process understanding and operational decision-making [34].

Despite these promising outcomes, a critical evaluation of the literature indicates that these gains are highly contingent on the underlying digital infrastructure. The deployment of AI in existing facilities is frequently hindered by legacy control systems and outdated digital infrastructure that lack the computational capacity to process real-time, high-frequency data [18], [34]. To address this challenge, recent advancements emphasize distributed architectures. For example, edge computing is increasingly utilized for low-latency, sensor-level processing, while federated learning enables collaborative model training across multiple plants without compromising proprietary data privacy [18], [38]. Nevertheless, a recurring limitation across these studies is the assumption of stable operational baselines during model training. In reality, continuous equipment degradation, fluctuating raw material variability, and shifting environmental conditions require highly adaptive control strategies. Consequently, while digital twins and virtual replicas offer a risk-free environment for simulating and optimizing these complex processes, their widespread industrial adoption remains constrained by the need for robust, explainable AI frameworks that can secure operator trust and accommodate dynamic plant conditions.

5.2. Kiln optimization and predictive modeling

In cement production, the rotary kiln is the most critical node for process optimization because it accounts for the majority of thermal energy consumption and is a major source of CO_2 emissions. Kiln optimization is a high-impact route for process decarbonization because rotary-kiln operation simultaneously governs clinker quality, thermal efficiency, fuel demand, and direct emissions under strong nonlinearity, long residence times, delayed quality feedback, and variability in raw meal chemistry and fuel properties [4], [19], [37]. In practice, reliance on operator heuristics and delayed laboratory measurements can constrain achievable performance because key variables such as burning-zone temperature, oxygen level, feed rate, induced-draft fan current, and clinker mineral indicators interact dynamically [37]. Accordingly, recent work frames kiln operation as a constrained predictive optimization problem in which data-driven clinker-quality prediction is coupled with control actions that must satisfy operational and product constraints; for example, ML-based clinker-quality prediction integrated with non-linear model predictive control combines feed chemistry, operating variables, and heat input to maintain target quality while optimizing manipulated variables [65]. Explainable AI, such as Extreme Gradient Boosting (XGBoost) with Shapley Additive exPlanations (SHAP) analysis, strengthens industrial applicability by ranking influential variables and providing interpretable relationships between operating conditions and kiln responses, thereby supporting auditability and operator confidence responses [66]. In parallel, data-driven optimization studies in cement production show that user-defined objective functions, when combined with optimization, can improve performance relative to baseline settings when embedded within a validated decision framework [67]. Complementing these data-driven approaches, kiln expert systems provide rule-based or knowledge-driven decision support for real-time operational optimization, offering an additional pathway to improve stability and performance in practice continuously [64]. Despite methodological progress, adoption can still be limited by perceived model opacity, reinforcing the role of explainable methods in operator acceptance and compliance-oriented deployment.

5.3. Energy efficiency and electrification pathways

Energy efficiency improvement measures remain the most immediately implementable mitigation strategy because they typically require less capital and have shorter payback periods than transformative technology shifts, making them suitable for near-term deployment [19], [68]. The literature indicates that meaningful savings are achievable across raw material grinding, kiln operations, clinker cooling and finish grinding. Technological interventions in modern cement plants, such as waste heat recovery (WHR) systems, can capture 15–25% of kiln thermal energy for electricity generation thereby reduce net electricity consumption and related emissions, while high-efficiency grinding technologies, such as vertical roller mills and high-pressure grinding rolls, reduce electricity consumption by 30–40% compared to traditional ball mills supporting finer particle size distributions that can improve reactivity and enable higher SCM substitution [19], [46]. While energy efficiency provides essential near-term gains, achieving near-zero emissions ultimately requires electrifying cement production and integrating alternative fuels [44], [69].

Electrification of cement production, by replacing fossil-fuel combustion with renewable electricity for process heat, can reduce direct emissions; however, the net environmental benefit depends on grid carbon intensity, technology readiness, and electricity costs [44], [69]. Techno-economic analyses of electric kilns, plasma heating, and microwave-assisted calcination indicate that electrification can achieve approximately 40–60% CO_2 reduction, depending on the electricity mix, but would require substantial capital investment and access to low-cost renewable electricity [70].

For deep decarbonization, hybrid systems that combine electrification, alternative fuels, and carbon capture are consistently identified as the most credible route because they address both combustion- and process-related emissions while managing technology and infrastructure constraints [69], [71]. Comparative assessments of hydrogen and oxy-combustion pathways indicate that hydrogen-fueled kilns coupled with oxy-combustion and carbon capture can reduce emissions by exceeding 95%. However, the high cost of producing green hydrogen and oxygen remains a significant barrier [71]. In parallel, energy efficiency remains a pillar technology for decarbonizing industries, as efficiency measures typically offer shorter payback periods and lower implementation risks than transformative technologies, making them attractive for near-term implementation [68].

5.4. Digital twins for climate resilience

Digital twins and virtual models of physical assets, processes, or systems that are continuously updated with real-time data are becoming an effective tool for climate resilience and sustainability optimization in industrial settings [72]. In cement production, their practical value lies in providing a risk-free environment for scenario analysis, predictive maintenance, process optimization, and training of advanced control algorithms, thereby improving decision quality under disturbances and uncertainty [18], [72]. A multi-layer architecture includes asset-level twins that model individual equipment, such as kilns, mills, and conveyors; process-level twins that combine multiple assets to simulate production processes and system-level twins that model whole plants or supply chains [72]. This method supports optimization at different levels of granularity and coordination across organizational boundaries.

For climate resilience, digital twins enable systematic evaluation of adaptation strategies under alternative climate scenarios. A digital cement-plant twin can simulate the impacts of extreme heat on cooling-system performance, water availability constraints on wet grinding processes, and supply chain disruptions caused by climate-related disasters and inbound and outbound logistics, thereby informing robust operating policies and specific infrastructure investments [72]. The combination of digital twins with AI and ML forms a positive feedback loop in which operational data from the real world calibrates and improves the twin, and the twin produces high-fidelity synthetic data used to build and test AI models, further enhancing the development of an intelligent control system [18], [72].

Plant-level AI contributes to decarbonization mainly by improving constraint-aware monitoring, control, and reliability, thereby reducing energy intensity and stabilizing clinker and cement quality under disturbances. Kiln-centric interventions offer the highest potential for emissions reduction. Achievable performance improvements depend on high-quality data, reliable integration with legacy control architectures, operator trust and adoption, and the local energy and infrastructure context, especially grid carbon intensity for electrification and supply constraints for hydrogen and oxygen. Evidence for fleet-scale replication remains limited, with insufficient long-duration field validation and incomplete documentation of model drift, failure modes, and maintenance requirements for deployed systems. Therefore, emphasis should be placed on staged industrial pilots with clearly defined performance metrics, digital-twin-enabled safe testing, and deployment governance that incorporates uncertainty handling, safe fallback control strategy, and operator-in-the-loop decision support.

The digital twins are promising for plant-level monitoring, scenario testing, predictive maintenance, and operator decision support, but their maturity in cement manufacturing remains uneven. Evidence is strongest for diagnostic and simulation functions, while closed-loop optimization and autonomous control require stronger validation under real plant disturbances. Their deployment depends on sensor coverage, data quality, cybersecurity, integration with legacy control systems, operator trust, and continuous model maintenance.

6. Life cycle assessment integration with ML

The integration of ML with LCA is increasingly important for evaluating cement decarbonization options across multiple impact categories, life-cycle stages, and future operating conditions [18], [39], [73], [74]. LCA prevents narrow carbon-only interpretation by identifying burden shifting across raw material extraction, clinker production, grinding, transport, use, and end-of-life stages [18], [39]. ML improves this function by accelerating impact prediction, screening large design spaces, linking plant or mix-design variables to environmental outcomes, and supporting near-real-time decision-making. However, the evidence suggests that ML-enhanced LCA is only reliable when supported by transparent inventories, representative datasets, uncertainty analysis, and clearly defined system boundaries. Therefore, the value of ML–LCA integration lies not simply in faster computation, but in improving decision quality under technological, regional, and policy uncertainty.

6.1. Prospective LCA Frameworks

LCA is a standardized method for quantifying the environmental impacts of products and processes across all stages, from raw material extraction to end-of-life disposal [18], [39]. In cement decarbonization, LCA is essential because emission reductions in one stage may shift impacts to other life cycle stages or environmental categories [39], [43]. Traditional attributional LCA evaluates existing systems using current technologies and supply chains, whereas cement decarbonization requires assessing future technologies, evolving energy systems, and evolving policy conditions. Prospective LCA addresses this need by incorporating technological learning, market change, scenario uncertainty, and future background systems [27].

The recent study indicated that prospective LCA is most useful when it connects plant-level technology models with broader energy-system and policy scenarios. In cement, SCM-based clinker substitution can reduce emissions by about 20–40% by 2030, making it a strong near-term mitigation option, but the achievable benefit is constrained by regional availability and quality of SCMs [39]. Emission reductions above 80% generally require carbon capture and storage (CCS), but this depends on carbon pricing, CO_2 transport, storage infrastructure, and policy support. Electrification and hydrogen become more competitive as renewable electricity costs decline and carbon prices increase, but their performance remains highly context-dependent because energy costs, infrastructure readiness, and regional resource availability vary substantially [27], [39].

The critical implication is that no single decarbonization option can be ranked universally using static LCA results. Instead, prospective LCA shows that mitigation priorities depend on scenario assumptions, system boundaries, and regional constraints. ML can improve this process by enabling rapid exploration of large sets of scenarios, detecting sensitive parameters, and identifying strategies that remain environmentally favorable across multiple future conditions [39]. However, model outputs must be interpreted cautiously because uncertainty in future energy systems, policy design, and technology deployment can strongly affect comparative results. Therefore, prospective ML–LCA should be used as a decision-support framework for robust planning rather than as a fixed ranking tool.

6.2. AI-enhanced environmental impact assessment

ML enhances environmental impact assessment by automating data collection, improving prediction accuracy, and enabling real-time monitoring of environmental performance [36], [75]. In cement and concrete systems, this integration is important because environmental performance depends on interacting variables, including binder composition, SCM replacement level, aggregate source, admixture use, transport distance, electricity mix, and process energy demand.

A methodological framework couples artificial neural networks (ANNs) with LCA databases to optimize the inclusion of SCMs. This approach trains predictive models to estimate multiple impact categories, such as GWP, acidification, and eutrophication potentials, directly from mix design parameters [36]. Compared to traditional LCA, which is computationally intensive, ANN-LCA integration enables rapid evaluation of thousands of mix-design alternatives, facilitating near-real-time decision-making during procurement and production while minimizing the burden of exhaustive experimental testing [36]. This enables rapid screening of alternative cementitious composites and supports MOO, balancing environmental impacts with strength, durability, workability, and cost requirements. The main advantage is not merely faster LCA calculation, but the ability to embed environmental assessment directly into early-stage design and procurement decisions.

However, the reliability of AI-enhanced LCA depends strongly on inventory quality, dataset representativeness, system-boundary consistency, and validation against conventional LCA results. Poorly documented inventories or narrow training datasets can produce rapid but unreliable predictions. Therefore, ANN–LCA models should include uncertainty analysis, sensitivity testing, and transparent reporting of input assumptions before being used for material qualification or industrial decision support.

AI-enhanced assessment also improves plant-level emissions accounting by linking operational electricity use with time- and region-specific grid carbon intensity [75]. This matters because cement plants increasingly rely on electrical equipment, grinding systems, carbon-capture auxiliaries, and potentially electrified heat technologies. Static average-grid emission factors may obscure the real emissions impact of electricity consumption, whereas electricity–carbon coupling can identify lower-carbon operating windows and support demand-side management. Nevertheless, this approach is contingent on high-resolution plant data, reliable grid emissions information, and operational flexibility. The broader implication is that ML-enhanced LCA can shift environmental assessment from retrospective reporting to active operational decision support, but only when data governance, transparency, and uncertainty quantification are built into the assessment process.

6.3. Circular economy and resource efficiency

Circular economy strategies complement LCA and ML by shifting decarbonization attention from production efficiency alone to material substitution, lifetime extension, recycling, reuse, and end-of-life recovery design [3], [76], [77]. In cement and concrete systems, the most relevant strategies include the use of waste-derived materials as SCMs or alternative fuels, recycled concrete aggregates, durability-oriented design, selective demolition, and higher-value recovery of construction and demolition waste [13], [76]. These strategies can reduce demand for virgin raw materials and lower emissions, but their performance depends on material quality, contamination levels, transport requirements, regulatory acceptance, and whether recycled inputs deliver equivalent technical performance.

The evidence indicates that digital tools can strengthen circular cement and concrete systems by improving material identification, quality prediction, and matching between waste generators and users [13], [76]. ML models can classify waste-derived materials according to composition, contamination risk, and expected performance, while digital product passports, blockchain-based material tracking, and AI-supported sorting can improve transparency across construction and demolition systems [76]. However, the benefits of the circular economy should not be assumed automatically. Recycling or reuse can be environmentally weak if processing energy, transport distances, or quality losses outweigh the avoided production of virgin material. LCA is therefore necessary to verify whether circular strategies reduce total impacts rather than shifting burdens to logistics, processing, or durability performance.

Material-efficiency evidence further suggests that design, reuse, and lifetime-extension strategies can substantially reduce material demand and associated emissions, with reported global savings of 20–40% in material use and 30–50% in related emissions by 2050 under system-based material-efficiency scenarios [77]. For cement, this means decarbonization should not be limited to lower-carbon binders or plant technologies; it should also include demand-side strategies that reduce unnecessary use of cement and concrete while preserving performance and service life. The critical implication is that circular economy 4.0 can support cement decarbonization only when digital systems are connected to LCA-based verification, performance standards, and regional material markets. Without these conditions, circular strategies may remain fragmented and difficult to scale into reliable industrial practice [76].

ML–LCA integration, prospective assessment, and circular economy tools are strongest when used together. LCA provides environmental accounting, ML accelerates prediction and optimization, prospective scenarios account for future uncertainty, and circular economy strategies reduce material demand and improve resource productivity. The key evidence gap is the limited integration of these components into transparent, validated, and region-specific decision frameworks. Future work should therefore prioritize open-source inventory datasets, uncertainty-aware ML models, dynamic electricity and material-supply assumptions, and LCA-verified circular-economy platforms for the decarbonization of cement and concrete.

7. Industrial-Scale Decarbonization Strategies

Industrial-scale decarbonization requires integrating technologies whose feasibility is determined more by infrastructure, investment conditions, and policy credibility than by plant-only decisions [5], [19], [70]. Across the evidence base, achieving deep decarbonization in the cement sector requires moving beyond plant-level operational optimizations to implement sector-wide strategies. These include deploying CCUS, integrating hydrogen and renewable energy, and conducting system dynamics–based pathway analysis treating the portfolio as interdependent, with regional constraints on CO_2 transport and storage capacity, electricity and hydrogen costs, and cross-sector material flows determining which pathways are implementable at scale [78], [79]. CCUS addresses residual process emissions, while hydrogen and renewable electrification mainly reduce combustion emissions but are constrained by energy costs and infrastructure availability. SD–based pathway analysis adds critical value by explicitly representing feedbacks, delays, and learning effects, showing that outcomes depend strongly on timing, coordination, and policy stability rather than technical feasibility alone. Industrial symbiosis interactions are therefore critical: cement–steel coupling affects SCM availability as steelmaking routes change, while shared CO_2 transport and storage networks and hydrogen infrastructure can lower costs but require coordinated investment and governance [80].

7.1. Carbon Capture, Utilization, and Storage (CCUS)

Carbon Capture, Utilization, and Storage (CCUS) is consistently identified as an essential mitigation method to achieve deep decarbonization in the cement sector by addressing unavoidable process emissions from limestone calcination [5], [19], [70], [78], [79]. The key synthesis outcome is that capture performance alone is not the binding constraint; the decisive barriers are energy penalty, integration complexity, and access to CO_2 transport and geological storage infrastructure. The literature categorizes cement capture routes into post-combustion capture with amine solvents or solid sorbents, oxy-fuel combustion of fuel in pure oxygen to form a concentrated CO_2 stream, and calcium looping via $CaO/CaCO_3$ cycles to capture CO_2 [70], [78], [79]. These technologies have advantages and challenges regarding capture efficiency, energy penalty, capital cost, and integration complexity [79]. Recent critical evaluations indicate that while calcium looping aligns well with existing calcination infrastructure, it can achieve high capture efficiencies and net emission reductions of 68–76% when appropriately integrated, with residual emissions depending on remaining fuel and electricity emissions and thus requiring low-carbon energy to approach near-zero outcomes [78].

Beyond capture, AI and ML are increasingly deployed to accelerate CCUS deployment through surrogate modeling, process prediction, and materials screening. For example, ANN and Support Vector Machine (SVM) models combined with nonlinear optimization have been used to identify operating regions that improve capture performance and reduce energy demand in MEA-based systems, illustrating how data-driven optimization can support deployable decision rules under multi-variable constraints [81]. Data-driven approaches significantly reduce the computational burden of simulating complex solvent-based capture systems, enabling real-time process optimization and improved decision-making for industrial flue-gas treatment [81], [82], [83]. Furthermore, carbon utilization pathways, such as co-production of cement and methanol, offer dual benefits by converting captured CO_2 into valuable chemical feedstocks [42]. However, the economic viability of these utilization and storage networks remains heavily constrained by the need for substantial infrastructure investment, favorable carbon pricing, and access to low-cost renewable hydrogen [42], [79]. Accordingly, CCUS deployment is best framed as an infrastructure-coupled strategy that must be co-developed with low-carbon power/heat and enabling CO_2 networks [5], [19], [79].

Therefore, CCUS is the most technically relevant option for residual calcination emissions, but its deployment maturity differs across capture routes and regions. Post-combustion capture is comparatively easy to retrofit but incurs energy and solvent-management penalties; oxy-fuel and calcium-looping options may improve capture performance but require deeper process integration and a higher capital commitment. The evidence consistently supports CCUS for deep emissions reduction, but real-world deployment remains constrained by cost, energy penalty, CO_2 transport and storage infrastructure, policy support, and public acceptance.

7.2. System dynamics modeling of decarbonization pathways

SD modeling has emerged as a critical framework for evaluating long-term decarbonization strategies because industrial decarbonization transitions involve complex interactions, feedback loops and time delays [39], [40], [41]. This model integrates subsystems, including production demand, which captures the growth of cement consumption driven by urbanization and infrastructure development; technology adoption, which models the adoption of low-carbon technologies depending on the costs, performance and policy incentives; emission and carbon pricing, which keeps track of the total emissions and the impact of carbon taxes or cap-and-trade systems; investment and finance, where the cement producers make capital allocation and policy and regulation that includes emissions standards, green procurement requirement and subsidies, to simulate the co-evolution of the cement sector under various climate targets [40]. A critical synthesis of these scenario analyses reveals three main requirements for sector-wide planning:

- The Cost of Delay: Delaying decarbonization investments by a decade can increase cumulative emissions by 30–40% and raise the economic cost of achieving net-zero targets by up to 70%.
- Portfolio Superiority: Integrated portfolio strategies that combine clinker substitution, alternative fuels, energy efficiency, and CCS consistently outperform single-technology pathways in both cost-effectiveness and overall emissions reduction.
- Policy Credibility: Durable, long-term policy signals are essential, as regulatory volatility and uncertain carbon-price pathways frequently reverse capital-intensive investments in decarbonization technologies.

SD modeling also exposes potential unintended consequences of isolated interventions. For example, aggressive promotion of SCM-blended cements without ensuring adequate SCM supply can lead to market disruptions and price spikes, quality issues and backlash from construction stakeholders, whereas the early withdrawal of coal-based fuels without the identification of low-carbon substitutes can increase production costs and loss competitiveness [40].

7.3. Hydrogen and renewable energy integration

Green hydrogen is best interpreted as a conditional fuel-side mitigation option for cement kilns rather than a complete deep-decarbonization solution. Its main value lies in reducing combustion-related CO_2 emissions when hydrogen is produced from low-carbon electricity, but its deployment depends on the cost of delivered hydrogen, the availability of infrastructure, flame stability, kiln heat-transfer requirements, and compatibility with existing burner systems [69], [71], [84], [85]. Evidence from hydrogen-enriched kiln combustion shows that partial coal substitution can reduce kiln-related CO_2 emissions by about 15–19.6%, while a 5% hydrogen thermal fraction can provide CO_2 reductions of up to 26.4%, depending strongly on the hydrogen production route [85], [86]. These results indicate that hydrogen can support near- to medium-term fuel decarbonization, especially where natural-gas blending, on-site hydrogen production, and waste-heat recovery can reduce integration barriers.

However, hydrogen substitution alone remains structurally limited because it does not directly address calcination emissions, which constitute a major share of cement-sector CO_2 output. Comparative evidence indicates that natural-gas oxyfuel combustion can reduce total energy input by about 35%, while hydrogen-based configurations reduce energy demand by 11–33%; nevertheless, indirect calcination can require about 8% more hydrogen than direct calcination, and hydrogen accounts for only 27.6% of total CO_2 reduction relative to the reference plant [71]. This suggests that hydrogen is most effective when integrated into broader plant redesigns rather than treated as an isolated fuel replacement.

The stronger deep-decarbonization case emerges when hydrogen-related systems are combined with oxy-combustion and CCS. Oxy-combustion with CCS can reduce direct CO_2 emissions by 96–99% and total emissions by about 90%, but this performance is accompanied by higher energy demand, including a 7% increase in thermal energy use and substantial electricity penalties for oxygen supply [84], [86]. Electrolytic oxygen can reduce dependence on conventional air separation, but its benefits depend on abundant, low-carbon electricity and integration with hydrogen production. Therefore, hydrogen should be positioned as an enabling component within an integrated mitigation package that includes oxy-combustion, CCS, renewable electricity, waste-heat recovery, and raw-material innovation, rather than as a stand-alone route to deep cement decarbonization.

7.4. Cross-sectoral synergies: steel, cement, and beyond

Industrial decarbonization increasingly depends on intersectoral coordination, in which actions in one industry can create mitigation opportunities, resource benefits, or infrastructure advantages in another [43], [87]. The cement and steel industries are closely connected through SCM supply, especially GGBFS from blast-furnace slag, as well as through waste-heat recovery, CO_2 transport and storage networks, and potential carbon-storage infrastructure. This linkage creates important decarbonization opportunities: cement can support wider industrial decarbonization by acting as a CO_2 mineralization platform in concrete products, an absorber of industrial by-products such as slag and fly ash, and a participant in shared CO_2 transport and storage systems [43]. However, this coupling also creates vulnerability, as future changes in steelmaking, particularly reduced blast-furnace operations, may limit slag availability and weaken one of the cement sector's most established clinker-substitution routes.

Cement–steel collaboration offers important opportunities for industrial symbiosis, but its value depends on coordinated planning rather than simple material exchange. Regional clustering of cement and steel facilities can support the use of steel slag in cement production, enable waste-heat exchange, and reduce the cost of shared carbon-capture infrastructure [88]. However, the transition in steelmaking from blast furnace–basic oxygen furnace (BF–BOF) routes toward electric arc furnace and direct reduced iron processes creates a major constraint for cement decarbonization because electric arc furnace production generates less slag, thereby reducing the future supply of GGBFS as a mature SCM [43], [88]. This supply risk strengthens the case for alternative SCM development, performance-based standards, and coordinated inter-industry planning.

Life-cycle and circular-economy evidence further indicates that deeper decarbonization requires an integrated assessment across the steel and cement value chains to avoid shifting environmental burdens and improve material efficiency and infrastructure use [88]. Therefore, cement–steel collaboration should be assessed not only as an emissions-reduction opportunity, but also as a resource-security and infrastructure-planning challenge requiring coordinated investment, standards alignment, and regional planning.

Deep decarbonization of the cement sector is most credible when CCUS, low-carbon heat options, and system-level planning are deployed as a coordinated portfolio rather than as isolated technologies. Deployment outcomes depend on infrastructure availability, CO_2 transport and storage, hydrogen supply chains, grid readiness, investment conditions, and durable policy signals that support capital-intensive transitions. Evidence remains limited on large-scale integration performance across regions, particularly regarding infrastructure build-out timing, cross-sector competition for low-carbon electricity and hydrogen, and governance models for shared CO_2 networks. Priority should be given to infrastructure-aware pathway assessment combining SD and prospective evaluation, coupled with coordinated planning across cement, steel, and energy systems to align material flows, shared CO_2/hydrogen networks, and policy mechanisms that sustain long-horizon investment.

7.5. Specific future research directions

Future research should shift from broad claims of digitalization toward validated computational tools that address identifiable data, modeling, and governance challenges in cement decarbonization. Federated learning offers a practical approach to multi-plant model development by enabling cement producers to train shared models for kiln control, predictive maintenance, quality prediction, and emissions monitoring while keeping proprietary plant data local [89], [90]. This is particularly relevant where single-plant datasets are too narrow to support robust generalization across raw meal chemistry, fuel mix, kiln design, maintenance history, and control practices.

Generative AI should be developed as a constrained materials-discovery tool for low-carbon binders rather than as an unconstrained formulation generator. Generative and inverse-design models can propose candidate chemistries or mixture configurations under target property constraints, but cement applications require experimental validation, physics-based hydration constraints, durability screening, and LCA filtering before proposed binder systems can be considered technically credible [91], [92]. High-performance computing (HPC) provides a complementary foundation by enabling large-scale simulation of hydration, microstructure development, transport properties, carbonation, and process performance across wide formulation and operating spaces [93], [94][88, 89]. Coupling HPC simulations with ML surrogates could accelerate the multi-objective optimization of cement systems, in which strength, durability, cost, heat release, SCM availability, and embodied carbon must be evaluated together.

Digital product passports should be adapted for cement and concrete supply chains to improve traceability of clinker content, SCM origin, recycled input quality, embodied carbon, and end-of-life recovery potential [95], [96]. Such systems would strengthen circular economy implementation by linking material provenance with verified performance and environmental data, but their value depends on interoperable data standards, third-party verification, and alignment with procurement and carbon-reporting requirements. Explainable AI is also essential for industrial decision support because plant engineers, operators, regulators, and managers require transparent justification for AI-generated recommendations in kiln operation, mix optimization, emissions accounting, and maintenance planning [97]. Explainability should therefore be treated as a deployment requirement rather than a post-processing add-on.

AI-enabled carbon accounting should be integrated with LCA, plant monitoring, and environmental, social, and governance (ESG) reporting frameworks to improve the consistency, auditability, and timeliness of emissions data [98], [99]. In cement production, this requires linking operational data from kilns, mills, fuels, electricity use, SCM procurement, transport, and carbon-capture systems to verifiable estimates of Scope 1, Scope 2, and relevant Scope 3 emissions. The critical research need is not only more advanced algorithms but also validated governance structures that connect AI outputs to standards-compliant reporting, uncertainty documentation, human oversight, and regulatory assurance.

8. Challenges, Limitations, and Research Gaps

The evidence reviewed in this manuscript indicates that computational sustainability for cement decarbonization is advancing rapidly, but its practical value depends on the maturity, transferability, and deploy ability of each method. Across the literature, the strongest evidence supports AI and ML as decision-support tools for screening, prediction, monitoring, and optimization, while evidence is weaker for autonomous control, long-term durability prediction, large-scale deployment, and verified real-world emissions reduction. The following subsections, therefore, synthesize the major barriers that determine whether computational approaches can move from promising demonstrations to reliable industrial implementation. Key constraints on the real-world impact of AI-enabled cement decarbonization include data limitations, barriers to industrial validation, operator adoption requirements, and policy/economic uncertainties [100]. The gap clarifies the practical barriers that must be addressed to move from model development to operational practice.

8.1. Data availability and quality barriers

The effectiveness of AI and ML approaches depends critically on the availability of high-quality, representative datasets [36], [47]. Several data challenges continue to constrain AI-enabled progress in cement and concrete research and deployment. Table 3 synthesizes the main data-related barriers to AI/ML development and deployment in the cement and concrete industry. It links each barrier to its implications for model validity and practical mitigation actions. This structure clarifies that data limitations are not only availability problems but also affect model validation, reproducibility, and confidence in low-carbon cement and concrete applications. Table 3 shows that AI/ML progress in cement and concrete is constrained less by data volume than by representativeness, standardization, access, and time-horizon coverage.

Sparse and uneven experimental datasets limit generalization; inconsistent protocols introduce bias in aggregated data; proprietary industrial datasets restrict external validation; and the lack of evidence of multi-decade durability elevates uncertainty, motivating harmonized reporting, privacy-preserving collaboration, and physics-guided extrapolation for credible deployment.

Table 3. Data-related barriers affecting AI/ML reliability and deployment in cement research.

Barrier	Description	Impact on AI/ML	Deployment implication	Mitigation Strategy	References
Experimental Data Limitations	Comprehensive datasets covering diverse mix designs, curing regimes, alternative binders, recycled aggregates, and long-term performance remain limited. Most studies report a small number of mixtures or controlled laboratory conditions.	Reduces model robustness, increases the risk of overfitting, and limits prediction accuracy outside the training domain.	Weakens confidence in AI-based screening of low-carbon binders and mix designs under practical field conditions.	Develop open benchmark datasets, expand experimental coverage across material types and curing regimes, and standardize reporting of mix composition and performance metrics.	[36], [47].
Data Heterogeneity	Experimental protocols, measurement techniques, curing conditions, specimen geometries, and reporting formats vary across studies.	Introduces inconsistency, bias, and noise when datasets are combined for model training.	Limits cross-study comparability and reduces transferability of models across laboratories, regions, and material systems.	Establish harmonized data schemas, metadata requirements, and minimum reporting standards for cement and concrete datasets.	[36]
Proprietary industrial data	High-value plant and production data are often held in private databases and are not publicly accessible due to commercial and confidentiality concerns.	Restricts model training, external validation, and benchmarking using real operating data.	Limits multi-plant generalization and slows industrial adoption of AI-enabled monitoring, control, and optimization tools.	Apply federated learning, privacy-preserving ML, secure data-sharing agreements, and anonymized multi-site benchmarking.	[18], [38].
Long-term performance data gaps	Durability, aging, and lifecycle performance data over service-life periods are rarely available, particularly for emerging low-carbon cementitious systems.	Limits the validation of models predicting durability, degradation, and long-term service performance.	Constrains regulatory acceptance and market confidence in alternative binders, SCM-rich concretes, and recycled-material systems.	Combine accelerated testing, field monitoring, physics-informed extrapolation, and digital material passports to support long-term validation.	[3], [35], [36].
Data quality and completeness	Datasets may contain missing values, inconsistent units, incomplete metadata, measurement error, and unreported processing conditions.	Reduces reproducibility and can produce unstable or misleading model outputs.	Increases risk when AI outputs are used for material requirements, quality control, or plant decision support.	Implement data-quality checks, unit harmonization, uncertainty reporting, metadata documentation, and reproducible data-preprocessing workflows.	[36], [47].

8.2. Scalability and industrial validation barriers

While many AI-enabled models have proven effective at pilot scale, significant challenges emerge at the industrial level [18], [34]. Table 4 summarizes the main barriers to scaling AI-enabled cement technologies from pilot projects to industrial deployment, linking each barrier to its operational impact and the required mitigation measures. The Table shows that industrial deployment depends on more than algorithmic performance. Process complexity determines whether models remain reliable under changing plant conditions, while legacy infrastructure affects whether AI outputs can be integrated into operational control systems.

Table 4. Scalability and industrial validation barriers for AI Implementation in cement plants.

Barrier	Industrial challenge	Effect on deployment	Validation requirement	Implementation response	References
Process Complexity	Cement plants operate as highly coupled systems, subject to disturbances from raw material variability, fuel quality, equipment degradation, kiln stability, and safety constraints.	Models developed under laboratory or pilot conditions may fail under non-stationary plant conditions.	Multi-plant validation under variable feed chemistry, fuel blends, production rates, and operating constraints.	Develop robust hybrid models and adaptive control systems that combine process knowledge with real-time data.	[18], [37].
Legacy Systems Integration	Retrofitting AI-based control systems into existing plants with older, legacy control infrastructure	Minimal computational capabilities and communication protocols complicate the execution of real-time data flow and control.	Testing of interoperability, data latency, cybersecurity, and compatibility with existing plant control layers.	Address digital infrastructure gaps to enable compatible data flow and control.	[18], [34].
Operator Acceptance	Plant operators may be cautious about black-box AI recommendations, particularly when kiln stability, product quality, and safety are at stake.	Low trust can prevent sustained use of AI recommendations even when model accuracy is high.	Human-in-the-loop validation using interpretable outputs, uncertainty estimates, and operator feedback.	Apply explainable AI, decision dashboards, operator override options, and training programs to build confidence.	[47]
Economic Viability	AI deployment requires investment in sensors, data infrastructure, software integration, validation, cybersecurity, and staff training.	Adoption may be delayed where energy prices are low, carbon pricing is weak, or capital costs are high.	Techno-economic evaluation of payback period, energy savings, CO_2 reduction, maintenance savings, and implementation cost.	Prioritize high-value use cases such as kiln control, predictive maintenance, and energy optimization before wider deployment.	[18], [40]

Operator acceptance is equally important because model recommendations must be interpretable and actionable in safety-critical production environments. Economic viability ultimately determines whether digital upgrades are adopted beyond pilot scale, particularly when energy and carbon price signals are weak. Therefore, scalable AI implementation requires combined technical validation, human-centered design, and techno-economic justification.

8.3. Policy and economic barriers

Achieving deep decarbonization in the cement sector requires supportive policy frameworks and economic incentives [5], [19], [40].

Table 5 synthesizes the policy and economic barriers that govern the adoption of deep decarbonization technologies in the cement industry, linking each barrier to its mechanism, deployment constraint, and required policy response, thereby clarifying how market signals, standards, procurement, infrastructure, and international coordination influence the adoption of low-carbon cement technologies. The Table indicates that cement decarbonization depends not only on technology readiness but also on the credibility of policy and market conditions. Carbon pricing and procurement policies influence demand formation and investment incentives, while standards determine whether low-carbon binders can enter regulated construction markets.

Table 5. Policy and economic barriers to deep cement-sector decarbonization.

Barrier	Mechanism	Deployment constraint	Required Policy Actions	References
Carbon Pricing	Carbon pricing internalizes the climate cost of cement production through taxes, cap-and-trade systems, or emissions trading schemes.	Carbon prices in many jurisdictions remain below the level needed to justify capital-intensive mitigation options such as carbon capture, hydrogen, and electrification.	Establish credible, rising, and predictable carbon-pricing signals, supported by safeguards to protect competitiveness and prevent leakage.	[5], [19], [39], [40]
Green Procurement	Public procurement can create early demand for low-carbon cement and concrete by requiring embodied-carbon limits in infrastructure and building projects.	Weak or fragmented procurement rules may fail to create stable demand, while poorly designed mandates may increase costs or create supply constraints.	Introduce performance-based procurement standards, embodied-carbon thresholds, and phased market-development mechanisms for low-carbon cement products.	[19], [26], [28]
Standards & Regulations	Building codes and material standards determine which binders, SCM replacement levels, and alternative cement systems can be used in practice.	Prescriptive Portland cement-based standards can restrict the adoption of alternative binders, SCM-rich systems, and recycled-material formulations.	Shift toward performance-based standards that allow novel materials when strength, durability, safety, and environmental criteria are satisfied.	[4], [5], [19], [26], [41]
Infrastructure Investment	Technologies such as CCUS, hydrogen, and electrification require shared infrastructure, including CO_2 transport and storage networks, hydrogen supply chains, and grid upgrades.	Individual cement producers often cannot finance or coordinate infrastructure systems that extend beyond plant boundaries.	Use public-private partnerships, infrastructure planning, investment incentives, and regional industrial-cluster models to support shared assets.	[19], [43], [71], [79]
International Coordination	Cement is traded across regions, and uneven climate policies can shift production to jurisdictions with weaker emissions constraints.	A unilateral policy can create carbon leakage risks and weaken incentives for domestic producers to invest in low-carbon technologies.	Coordinate international standards, carbon border adjustment mechanisms, emissions accounting rules, and technology-support frameworks.	[5], [19]

Infrastructure requirements for CCUS, hydrogen, and electrification also exceed the capacity of individual firms, requiring coordinated planning and public-private investment. International alignment is also needed to reduce the risk of carbon leakage, maintain competitiveness, and accelerate low-carbon deployment.

8.4. Interdisciplinary integration barriers

Computational sustainability for cement decarbonization will require deep interdisciplinary collaboration among materials science, chemical engineering, computer science, industrial systems analysis, economics, and policy, but disciplinary silos, terminology differences, and misaligned incentives tend to hinder such collaboration [33], [34], [36]. Communication barriers arise because materials researchers and AI practitioners often use different conceptual frameworks, terms and validation models, which can hinder shared problem formulation, data standardization, and the interpretation of model outputs, thereby reduce efficiency of the research process and increase the risk of methodological misalignment [34], [36]. There is also an objective misalignment that complicates implementation: academic researchers are more interested in novelty and publication metrics, whereas industry practitioners are more interested in reliability, cost-effectiveness, and regulatory compliance.

A model of collaborative research is necessary to bridge this gap by redirecting incentives toward common interests [18], [34]. Lastly, educational barriers pose a major limitation, as few programs currently offer integrated education in computational sustainability, materials science, and industrial systems. It is thus crucial to implement interdisciplinary curricula to develop a workforce capable of translating decarbonization plans into practice [33], [44].

8.5. Comparative maturity and critical evidence gaps

The reviewed evidence shows that AI methods and cement decarbonization pathways differ substantially in maturity, data requirements, interpretability, and deployment readiness. ANNs are mature and useful for strength prediction, mix-design screening, and environmental-impact estimation, but they require large, representative labeled datasets and may perform poorly outside the training domain [101], [102]. PINNs improve physical consistency by embedding governing equations and hydration constraints, but their reliability depends on the correct formulation of physical laws, boundary conditions, and loss functions [35], [103]. Ensemble learning methods such as random forests, gradient boosting, and XGBoost often provide strong predictive performance and variable-importance information, but their transferability depends on representative plant or materials datasets [1], [102], [104]. Hybrid optimization frameworks are useful for balancing carbon, cost, strength, workability, durability, and process constraints, but optimized outputs still require experimental or industrial validation before practical deployment [7], [105].

The technological maturity of decarbonization pathways is also uneven. SCM optimization is the most mature near-term option because it directly reduces clinker demand and is already deployed in many markets. However, future availability of fly ash and slag may limit its expansion [3], [4], [56]. Alternative binders offer greater potential reductions but remain constrained by evidence on durability, standards acceptance, and precursor supply [106], [107]. Digital twins and AI-based kiln optimization are promising plant-level tools, but evidence remains concentrated in pilots and selected industrial contexts, with broader deployment depending on data quality, process integration, and operator acceptance [1], [3], [108]. Electrification and hydrogen-based production depend strongly on low-carbon electricity, cost, burner compatibility, and infrastructure availability, while CCUS remains essential for residual calcination emissions but faces capital, energy, transport, storage, and policy barriers [5], [84], [85], [86], [109].

The strongest evidence supports near-term use of AI for decision support, screening, monitoring, and optimization. Evidence remains limited or inconsistent for autonomous control, large-scale deployment, long-term durability prediction, and verified real-world emissions reductions [102], [104], [108]. Future studies should prioritize transferable datasets, explainable and physics-informed models, long-duration field validation, and transparent reporting of uncertainty and implementation constraints. AI-enabled decarbonization should therefore be evaluated not only by predictive accuracy or optimization performance, but also by explainability, data governance, fairness, computational energy demand, and suitability for local industrial contexts [51].

8.5.1. Comparative suitability of AI approaches under industrial conditions

The suitability of AI methods for cement decarbonization depends strongly on data availability, process complexity, physical understanding, and deployment context. Supervised learning methods, including ANNs, random forests, and gradient boosting, are most suitable when large labeled datasets are available, such as for strength prediction, mix-design screening, quality control, and routine process monitoring [101], [102], [104]. Their main limitation is limited transferability when raw materials, fuel mixtures, curing conditions, or plant operating regimes differ from those in the training data [102], [104]. PINNs and hybrid physics–ML models are more suitable in settings where data are limited but strong process knowledge exists, such as in hydration modeling, heat evolution, clinker chemistry, and thermochemical process representation; however, their application depends on correct physical constraints and careful validation [103].

Ensemble learning and explainable AI are especially relevant under industrial conditions where model transparency and operator confidence are required. These approaches can support variable ranking, fault diagnosis, emissions monitoring, and kiln-response interpretation, but their outputs must be interpreted with engineering judgment rather than treated as causal proof [1], [97]. Multi-objective optimization and Bayesian optimization are most useful where competing objectives must be balanced, including CO_2 reduction, energy use, cost, strength, durability, and production stability [105]. Digital twins are most appropriate for plants with sufficient sensor coverage, reliable data infrastructure, and integration with process-control systems, where they can support scenario testing, predictive maintenance, and operational decision support [108], [110]. Overall, no AI method is universally superior; the most promising approach depends on whether the industrial problem is data-rich, physics-constrained, control-oriented, multi-objective, or trust-sensitive.

8.6. Real-world implementation barriers

The deployment of computational sustainability tools in cement manufacturing is constrained by practical barriers that extend beyond model accuracy or technical feasibility. Data governance and ownership remain major concerns because high-resolution datasets on kiln, fuel quality, maintenance, and emissions are commercially sensitive and often controlled by individual plants or corporate groups. This limits data sharing, model benchmarking, and cross-plant validation. Strong data governance is therefore required to define decision rights, accountability, data quality responsibilities, access control, and lifecycle management for industrial data [111]. Industrial data availability is also uneven because manufacturing datasets often contain missing values, inconsistent labeling, heterogeneous sensor formats, and site-specific operating conditions, which can limit the transferability of ML models across plants [104], [112].

Cybersecurity is another critical implementation barrier because AI-enabled monitoring, digital twins, and advanced control systems increase connectivity between operational technology and information technology systems. Greater connectivity improves visibility and control but also expands the potential attack surface of industrial cyber-physical systems, requiring secure architectures, access control, anomaly detection, and continuous risk management [113], [114]. Explainability and trustworthiness are equally important because operators and managers are unlikely to rely on AI recommendations for kiln control, mix design, maintenance planning, or emissions reporting unless the models provide transparent reasoning, uncertainty estimates, and clear links to process knowledge [97]. Regulatory and organizational conditions also influence adoption, as cement plants must comply with product standards, environmental permits, health and safety requirements, and carbon reporting rules, which can slow AI-assisted process changes or new material formulations.

Workforce readiness is essential because engineers, operators, and managers require skills in data interpretation, model oversight, cybersecurity awareness, and human-in-the-loop decision-making. Industry 4.0 adoption studies show that skills shortages, organizational resistance, unclear implementation pathways, and weak digital readiness can restrict the adoption of advanced manufacturing technologies [115], [116]. Economic barriers further limit implementation, particularly where AI deployment requires new sensors, plant digitalization, cloud or edge-computing infrastructure, staff training, software integration, and long-term model maintenance.

These constraints indicate that successful implementation depends on an integrated technical, organizational, regulatory, and economic strategy rather than on algorithm development alone [115], [116]. Because the reported emission-reduction values are drawn from studies with different baselines, system boundaries, timeframes, regional contexts, and technology assumptions, the ranges should be interpreted as indicative rather than directly additive. Therefore, Table 6 provides a comparative synthesis of the reviewed decarbonization options, using reported CO_2-reduction potential alongside qualitative indicators of technology readiness, evidence strength, scalability, cost burden, and implementation confidence.

Table 6. Comparative synthesis of cement decarbonization pathways.

Decarbonization option	Reported emission reduction potential	Technology readiness	Evidence strength	Scalability	Cost and infrastructure burden	Main constraints	References
SCM-based clinker substitution	Approximately 20–60% cement-intensity reduction under suitable substitution levels	High for mature SCMs; medium for emerging SCMs	High	Medium to high	Low to medium	Regional SCM availability, quality variability, durability validation, and standards acceptance	[3], [4], [5], [11], [56], [117]
Alternative binders and novel cement systems	Approximately 20–80%, depending on binder chemistry, performance boundary, and allocation method	Medium for calcined-clay and CSA systems; low to medium for AAMs, magnesium-based binders, and bio-based systems	Medium	Medium	Medium	Long-term durability, precursor availability, activator-related impacts, standardization, cost uncertainty, and market acceptance	[3], [4], [5], [35], [36], [56]
AI-enabled process optimization and digital twins	Approximately 8–15% through improved kiln control, energy efficiency, predictive maintenance, and process stability	Medium to high in digitally mature plants	Medium	High in plants with strong sensors and automation infrastructure	Medium	Data quality, legacy-system integration, cybersecurity, operator acceptance, and model drift	[5], [36], [66]
Alternative fuels and low-carbon heat	Approximately 10–40%, depending on thermal substitution rate, fuel composition, biogenic fraction, and heat-system configuration	High for selected waste-derived fuels; medium for hydrogen and electrification	Medium	Medium	Medium to high	Fuel availability, chlorine and moisture control, burner compatibility, electricity supply, hydrogen availability, and combustion stability	[4], [5], [84], [117]

8.7. Review limitations

This review has several limitations. Publication bias may affect the evidence base because studies reporting successful AI applications, strong predictive accuracy, or positive decarbonization outcomes are more likely to be published than unsuccessful, negative, or inconclusive findings [118]. Database coverage is another limitation because the review relied primarily on Scopus, Web of Science, and Google Scholar; these databases differ in journal coverage, conference indexing, citation capture, and inclusion of non-journal sources, meaning that some relevant engineering, computer science, or industry-oriented studies may have been missed [119].

The use of English-language peer-reviewed literature may also introduce language bias and underrepresent regional studies published in other languages, particularly from major cement-producing countries [120]. The exclusion of non-peer-reviewed reports, vendor documents, and some forms of grey literature improves academic rigor but may omit recent industrial deployments, proprietary case studies, and emerging digitalization practices that have not yet appeared in peer-reviewed journals. This limitation is especially relevant for AI, digital twins, advanced process control, and industrial data platforms, where implementation can advance faster than academic publication. Finally, the AI literature is evolving rapidly; therefore, some methods, tools, and applications may become outdated or be superseded shortly after publication, a known limitation in fast-moving research fields [121]. These limitations mean that the review should be interpreted as a structured synthesis of available peer-reviewed evidence rather than a complete inventory of all industrial practice.

9. Future Directions and Recommendations

Future research and implementation priorities should be aligned to accelerate the transition from demonstration-scale studies to fleet-scale deployment. Emphasis should be placed on interoperable data infrastructure, explainable AI, validation-centered deployment pathways, and the enabling policy and infrastructure conditions required for net-zero-compatible cement systems.

9.1. Research priorities

Table 7 consolidates the priority research directions needed to translate advances in computational sustainability into scalable decarbonization practices in the cement sector. Open datasets and standardized reporting provide the foundation for reproducible AI/ML models, while physics-informed and explainable systems improve confidence under limited data and changing plant conditions.

Integrated LCA, techno-economic analysis, and system dynamics modeling are needed to evaluate decarbonization options consistently across environmental, economic, and infrastructure dimensions. At the deployment level, progress will require coordinated development of alternative binders, CCUS, circular-economy platforms, and shared industrial infrastructure.

To strengthen the practical relevance of these research priorities, future work should translate them into measurable research and implementation milestones. In the near term, priority should be given to harmonized cement and concrete data infrastructure, reproducible AI/ML benchmarking, and independent validation of physics-informed and explainable models [66], [105], [122], [123]. Key indicators should include dataset completeness, standardized metadata reporting, externally validated predictive performance, quantified using root mean square error (RMSE) and coefficient of determination (R^2), uncertainty bounds, and out-of-domain prediction performance [105], [122], [123].

In the medium term, research should prioritize multi-plant field validation of deployable AI systems, integration of prospective LCA with techno-economic analysis and system dynamics, and pilot-scale validation of alternative binders under durability and performance-based standards [66], [124]. Relevant indicators should include the number of industrial pilot trials, measured kiln energy-intensity reduction, verified CO_2-intensity reduction, product-quality stability, downtime reduction, durability performance, and cost-performance indicators [52], [66], [124].

In the long term, research should support regional industrial cluster planning, CCUS integration, hydrogen and electrification readiness, and circular material platforms [52], [79], [125]. Progress in these areas should be evaluated using indicators such as capture efficiency, energy penalty, storage readiness, traceability of Scope 1 and Scope 2 emissions, secondary-material quality assurance, and readiness for standards or policy adoption [52], [79], [125]. By defining these measurable indicators, future studies can move computational sustainability from conceptual frameworks toward validated tools for industrial cement decarbonization.

Table 7. Research priorities for computational sustainability in cement decarbonization.

Strategic Priority	Research need	Expected Outputs	Decarbonization Relevance	Implementation Pathways	References
Open cement and concrete data infrastructure	Limited availability of representative, standardized, and long-term datasets for cement and concrete constrains robust AI/ML development.	Open-access datasets covering mix designs, curing regimes, SCM systems, durability, and long-term performance.	Enables reproducible model development, benchmarking, and generalization across materials and regions.	Establish shared data repositories, reporting templates, metadata standards, and funding-linked data-sharing requirements.	[36], [47]
Physics-informed and hybrid AI models	Purely data-driven models often generalize poorly outside the training domain.	Hybrid models combining ML with thermodynamics, kinetics, hydration chemistry, and process constraints.	Improves extrapolation, interpretability, and reliability under limited data and changing operating conditions.	Develop physics-informed neural networks, surrogate models, and multi-scale modeling frameworks.	[35]
Explainable and deployable industrial AI	Black-box models limit operator trust and safety-critical deployment.	Explainable AI tools with uncertainty quantification, safety constraints, and human-in-the-loop control.	Supports reliable plant-level optimization, predictive maintenance, and process control.	Validate AI systems through long-term industrial trials, operator dashboards, and staged deployment.	[18], [47]
Integrated LCA, techno-economic, and system modeling	Decarbonization options are often assessed in isolation without consistent economic and system-level evaluation.	Integrated prospective LCA, techno-economic analysis, and system dynamics models.	Supports robust comparison of clinker reduction, fuel switching, electrification, CCUS, and alternative binders.	Build decision-support platforms that evaluate carbon, cost, performance, and infrastructure requirements under uncertainty.	[39], [40]
Cross-sector coordination and industrial symbiosis	Cement decarbonization depends on external systems, including steel, energy, waste, hydrogen, and CO_2 infrastructure.	Integrated planning models for material, energy, and infrastructure sharing across industrial clusters.	Improves the feasibility of SCM supply, alternative fuels, hydrogen use, and shared CCUS networks.	Develop industrial-cluster models, shared infrastructure planning, and public-private investment frameworks.	[19], [42], [43], [69], [87]
Alternative binders and novel cement systems	Emerging binders require further validation for durability, standardization, cost, and supply reliability.	Validated performance datasets and design rules for AAMs, CSA cements, calcined clays, and bio-based binders.	Reduces reliance on clinker and expands the portfolio of low-carbon cementitious materials.	Combine AI-assisted formulation screening with pilot-scale testing, standards development, and supply-chain assessment.	[4], [5], [26], [41]
Cement-specific CCUS innovation	CCUS remains essential for residual process emissions but faces energy, cost, and integration barriers.	Lower-energy capture systems, AI-designed sorbents/solvents, and plant-specific integration models.	Enables deep reductions where calcination emissions cannot be avoided through materials substitution alone.	Advance pilot demonstrations, modular capture systems, CO_2 transport/storage planning, and cost-reduction learning.	[20], [39], [78], [79]
Circular Economy and Digital Material Platforms	Circular cement systems require better tracking of waste, secondary materials, and reverse logistics.	Digital platforms for material-flow tracking, waste-to-resource matching, and recycled-material quality assurance.	Reduces virgin material demand, improves resource efficiency, and supports SCM and the use of recycled aggregate.	Deploy digital passports, blockchain-enabled traceability, and optimization tools for reverse logistics.	[36], [60], [61], [62], [76], [77]

9.2. Industry implementation pathways

In the implementation process, focus should be on digital infrastructure and data systems that support real-time monitoring, predictive analytics, and adaptive control, and enable integration of sites and organizations through interoperability and common data standards [18], [34]. AI-based optimization should be piloted in selected plants using high-value, well-scoped applications, e.g., kiln control and predictive maintenance, and then extended across the plant network once performance and return on investment are verified [18]. Cement producers are encouraged to collaborate with research institutions and technology vendors to develop and test models that reflect operational constraints, safety considerations, and compliance requirements [34].

Concrete producers and contractors should support the adoption of low-carbon cement products by educating customers on the performance and advantages of SCM-blended and alternative-binder cements [4], [28]. Industry groups and pre-competitive partnerships can help accelerate the adoption of best practices, the development of standards, and policy advocacy [34], [43]. Lastly, organizations must prepare and regularly update decarbonization roadmaps that are consistent with science-based targets, focusing on intervention portfolios in materials and processes, as well as enabling infrastructure, as these undergo technological and policy change [19], [40].

9.3. Policy and regulatory frameworks

Policymakers and regulators should prioritize and implement durable carbon-pricing instruments, such as carbon taxes or cap-and-trade systems, that better reflect the social cost of carbon and provide credible long-term signals for investment planning [39], [40]. They should also introduce green public procurement policies for low-carbon cement and concrete in infrastructure projects to create demand and support market development [19], [28]. They should also update building codes and material standards to adopt performance-based specifications that explicitly accommodate novel binders and low-carbon materials, thereby reducing regulatory barriers to innovation [5], [26], [41]. Meanwhile, specific assistance is required in R&D and demonstration of high-risk, high-reward choices like alternative binders, carbon capture, and hydrogen, coupled with public investment and planning on how to facilitate the infrastructure networks of CO_2 transport and storage, hydrogen production and distribution, and grid upgrades to support electrification that can be achieved individually [5], [19], [71], [79]. Finally, policy, standards, and technology transfer are necessary at the international level to prevent carbon leakage and remain competitive, as well as programs to build the workforce in computational sustainability, materials science, and industrial decarbonization [5], [33], [44].

10. Conclusion

This review synthesized the role of computational sustainability in accelerating decarbonization of the cement sector across materials design, plant operations, LCA, techno-economic evaluation, and system-level planning. The main finding is that computational sustainability is most valuable when it functions as an integrated decision-support framework rather than as a set of isolated AI or optimization tools. AI/ML models, physics-informed neural networks, digital twins, multi-objective optimization, prospective LCA, techno-economic analysis, and system dynamics can collectively support low-carbon binder screening, kiln and process optimization, environmental-impact evaluation, infrastructure planning, and policy-relevant pathway assessment.

The evidence indicates that SCM-based clinker substitution and energy-efficiency improvement remain the most mature near-term decarbonization options, while alternative binders, electrification, hydrogen use, and cement-specific CCUS require further validation, cost reduction, infrastructure development, and standards alignment before broad deployment. AI-enabled process optimization and digital twins are promising for reducing energy intensity, improving process stability, and supporting predictive maintenance, but their industrial value depends on high-quality data, integration with legacy control systems, operator trust, cybersecurity, and long-duration plant validation. For materials discovery, supervised learning, ensemble models, PINNs, and explainable AI can reduce the experimental burden and improve formulation screening, but model transferability remains limited by dataset representativeness, material variability, and insufficient evidence of field-scale durability.

Three major gaps emerge from the review. First, open, standardized, and long-term datasets remain insufficient for reliable AI/ML generalization across cement chemistries, SCM sources, curing regimes, plant conditions, and regional supply chains. Second, many computational studies report strong predictive or optimization performance but lack independent external validation, uncertainty quantification, and industrial-scale verification. Third, decarbonization options are still frequently evaluated in isolation, whereas net-zero-compatible cement production requires coordinated assessment of carbon, cost, durability, energy demand, infrastructure readiness, and policy feasibility.

Future work should therefore prioritize four actionable directions. (i) The research community should develop harmonized open datasets and benchmark protocols for cementitious materials, plant operations, LCA parameters, and durability performance. (ii) AI and optimization models should be externally validated using independent datasets and long-duration industrial trials, with transparent reporting of RMSE, R^2, uncertainty bounds, model drift, and out-of-domain performance. (iii) Prospective LCA, techno-economic analysis, and system dynamics should be integrated to compare decarbonization portfolios under regional resource, infrastructure, and policy constraints. (iv) Industry and policymakers should support pilot-to-fleet deployment through performance-based standards, green procurement, carbon-pricing mechanisms, shared CO_2 and hydrogen infrastructure, and workforce development in computational sustainability.

In general, computational sustainability can strengthen the transition from laboratory-scale innovation to validated industrial implementation, but its impact will depend on the quality of evidence, model transparency, infrastructure readiness, and coordinated policy support. The most effective pathway is not the deployment of AI alone, but the integration of data-driven models, physical understanding, environmental assessment, techno-economic reasoning, and systems planning into robust decision frameworks for low-carbon and net-zero-compatible cement production.

Competing Interests Statement

The authors declared no potential conflicts of interest regarding the research, authorship, or publication of this article.

Data Availability Statement

No new primary data were generated in this study. The data supporting this review are derived from the cited literature. Additional screening and extraction materials are available from the corresponding author upon reasonable request. For access, please contact the corresponding author via oluwafemii@dut.ac.za or phemmyigoh@yahoo.com

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Musasa Kabeya: Supervision, Validation, Writing – review and editing, Funding acquisition.

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References

[1] J. S. Chatha, "Advances in sustainable technologies for industry and environment for a greener future," *Environmental Science and Pollution Research,* vol. 32, no. 58, pp. 30971-31017, 2025, doi: 10.1007/s11356-025-37299-y.

[2] E. Khalil and M. AbouZeid, "A global assessment tool for cement plants improvement measures for the reduction of CO2 emissions," *Results in Engineering,*

vol. 26, p. 104767, 2025, doi: 10.1016/j.rineng.2025.104767.

[3] G. Habert et al., "Environmental impacts and decarbonization strategies in the cement and concrete industries," *Nature Reviews Earth & Environment,* vol. 1, no. 11, pp. 559-573, 2020, doi: 10.1038/s43017-020-0093-3.

[4] S. Barbhuiya, F. Kanavaris, B. B. Das, and M. Idrees, "Decarbonising cement and concrete production: Strategies, challenges and pathways for sustainable development," *Journal of Building Engineering,* vol. 86, 2024, Art no. 108861, doi: 10.1016/j.jobe.2024.108861.

[5] S. Griffiths et al., "Decarbonizing the cement and concrete industry: A systematic review of socio-technical systems, technological innovations, and policy options," *Renewable and Sustainable Energy Reviews,* vol. 180, p. 113291, 2023, doi: 10.1016/j.rser.2023.113291.

[6] Andrew, "Global CO2 emissions from cement production, 1928–2018," *Earth Syst. Sci. Data,* vol. 11, no. 4, pp. 1675-1710, 2019, doi: 10.5194/essd-11-1675-2019.

[7] M. Guo, G. Gong, Y. Yue, F. Xing, Y. Zhou, and B. Hu, "Performance evaluation of recycled aggregate concrete incorporating limestone calcined clay cement (LC3)," *Journal of Cleaner Production,* vol. 366, 2022, Art no. 132820, doi: 10.1016/j.jclepro.2022.132820.

[8] M. Zhang, X. Zhu, S. Pyo, Y. Yang, B. Liu, and J. Shi, "Feasibility of using high-volume pozzolanic fillers to develop sustainable engineered cementitious composites (ECC)," *Powder Technology,* vol. 428, 2023, Art no. 118853, doi: 10.1016/j.powtec.2023.118853.

[9] H. Du and K. H. Tan, "Properties of high volume glass powder concrete," *Cement and Concrete Composites,* vol. 75, pp. 22-29, 2017, doi: 10.1016/j.cemconcomp.2016.10.010.

[10] A. Al-Fakih, M. A. Al-Shugaa, M. A. Al-Osta, and B. S. Thomas, "Mechanical, environmental, and economic performance of engineered cementitious composite incorporated limestone calcined clay cement: A review," *Journal of Building Engineering,* vol. 79, 2023, Art no. 107901, doi: 10.1016/j.jobe.2023.107901.

[11] J. A. Olsson, S. A. Miller, and M. G. Alexander, "Near-term pathways for decarbonizing global concrete production," *Nature Communications,* vol. 14, no. 1, p. 4574, 2023, doi: 10.1038/s41467-023-40302-0.

[12] R. M. Andrew, "Global CO2 emissions from cement production," *Earth Syst. Sci. Data,* vol. 10, no. 1, pp. 195-217, 2018, doi: 10.5194/essd-10-195-2018.

[13] A. I. B. Farouk, S. Abdulrahman, M. A. Al-Osta, S. I. Malami, and S. I. Abba, "Optimizing ultra-high-performance concrete with recycled fine and CO_2 reduction strategies: a machine learning and swarm intelligence approach," *Innovative Infrastructure Solutions,* vol. 10, no. 7, p. 309, 2025, doi: 10.1007/s41062-025-02083-x.

[14] O. E. Ige and M. Kabeya, "Decarbonizing the Cement Industry: Technological, Economic, and Policy Barriers to CO2 Mitigation Adoption," *Clean Technologies,* vol. 7, no. 4, p. 0085, 2025, doi: 10.3390/cleantechnol7040085.

[15] D. Cheng et al., "Projecting future carbon emissions from cement production in developing countries," *Nature Communications,* vol. 14, no. 1, 2023, Art no. 8213, doi: 10.1038/s41467-023-43660-x.

[16] K. M. Ripley, F. H. Saadi, and Z. L. H. Burke, "Cost-motivated pathways towards near-term decarbonization of the cement industry," *RSC Sustainability,* vol. 3, no. 1, pp. 255-263, 2025, doi: 10.1039/d4su00590b.

[17] D. Baskaran and H.-S. Byun, "Future-proofing CO2 mitigation towards a circular economy: A systematic review on process integration and advanced tools," *Environmental Science and Ecotechnology,* vol. 26, p. 100587, 2025, doi: 10.1016/j.ese.2025.100587.

[18] D. A. K. Singh, "Smart Cement Plants: Enhancing Productivity and Sustainability with AI," *International Journal for Research in Applied Science and Engineering Technology,* vol. 13, no. 7, pp. 2801-2807, 2025, doi: 10.22214/ijraset.2025.73457.

[19] S. Barbhuiya, B. Bhusan Das, and D. Adak, "Roadmap to a net-zero carbon cement sector: Strategies, innovations and policy imperatives," *Journal of Environmental Management,* vol. 359, p. 121052, 2024, doi: 10.1016/j.jenvman.2024.121052.

[20] S. Paltsev, J. Morris, H. Kheshgi, and H. Herzog, "Hard-to-Abate Sectors: The role of industrial carbon capture and storage (CCS) in emission mitigation," *Applied Energy,* vol. 300, p. 117322, 2021, doi: 10.1016/j.apenergy.2021.117322.

[21] S. S. Volaity et al., "Towards decarbonization of cement industry: a critical review of electrification technologies for sustainable cement production," *npj Materials Sustainability,* vol. 3, no. 1, p. 23, 2025, doi: 10.1038/s44296-025-00068-6.

[22] Y. Yuan, L. Zhang, J. Sun, S. Yan, T. Du, and H. Na, "Decarbonizing hard-to-abate sectors: CO_2 emission characteristics and mitigation pathways for steel, aluminum, and cement in China," *Resources, Conservation and Recycling,* vol. 224, p. 108568, 2026, doi: 10.1016/j.resconrec.2025.108568.

[23] I. Tiseo, "Global carbon dioxide emissions from cement manufacturing 1990–2024, by country," Statista, Hamburg, 2024. Accessed: April 15 2026. [Online]. Available: https://www.statista.com/statistics/1091672/carbon-dioxide-emissions-global-cement-manufacturing/

[24] M. U. Siddiq, M. K. Anwar, F. H. Almansour, M. A. Qurashi, and M. Adeel, "AI-Driven Optimization of Fly Ash-Based Geopolymer Concrete for Sustainable High Strength and CO2 Reduction: An Application of Hybrid Taguchi–Grey–ANN Approach," *Buildings,* vol. 15, no. 12, p. 2081, 2025, doi: 10.3390/buildings15122081.

[25] K. Hasan, M. T. Islam, R. Ferdaus, and F. M. Yahaya, "Experimental study on environment-friendly concrete production incorporating palm oil clinker and cockle shell powder as cement partial replacement," *Materials*

Today: Proceedings, vol. 107, pp. 254-262, 2024, doi: 10.1016/j.matpr.2023.11.150.

[26] M. L. Nehdi, A. Marani, and L. Zhang, "Is net-zero feasible: Systematic review of cement and concrete decarbonization technologies," *Renewable and Sustainable Energy Reviews,* vol. 191, p. 114169, 2024, doi: 10.1016/j.rser.2023.114169.

[27] K. Boakye, D. Winters, O. Oguntola, K. Fenton, and S. J. Simske, "A Review of Strategies to Achieve Net Zero Targets in the Cement and Concrete Sectors," *Reducing Carbon Footprint in Different Sectors for Sustainability,* p. 184, 2024, doi: 10.5772/intechopen.1005051.

[28] S. Stephen, C. Aigbavboa, and A. Oke, "Revolutionising Green Construction: Harnessing Zeolite and AI-Driven Initiatives for Net-Zero and Climate-Adaptive Buildings," *Buildings*, vol. 15, no. 6, p. 885, 2025, doi: 10.3390/buildings15060885.

[29] A. Raghav, B. Singh, K. Wongmahesak, R. Raghav, and U. Yadav, "Artificial intelligence in environmental and climate changes: A sustainable future," *Maintaining a Sustainable World in the Nexus of Environmental Science and AI,* pp. 485-506, 2024, doi: 10.4018/979-8-3693-6336-2.ch019.

[30] K. Devesh, "Harnessing Artificial Intelligence for Global Sustainability: A Systematic Review of Applications, Challenges, and Future Directions," in *Eurasia Conferences*, 2025, Vienna, Austria, 2025, doi: 10.62422/978-81-981590-7-6-001.

[31] V. Alevizos, I. Georgousis, and A. Kapodistria, "Toward Climate Neutrality: A Comprehensive Overview of Sustainable Operations Management, Optimization, and Wastewater Treatment Methods," *Pollutants*, vol. 3, no. 4, pp. 521-543, 2023, doi: 10.3390/pollutants3040036.

[32] F. Bauer, T. Hansen, and L. J. Nilsson, "Assessing the feasibility of archetypal transition pathways towards carbon neutrality – A comparative analysis of European industries," *Resources, Conservation and Recycling,* vol. 177, p. 106015, 2022, doi: 10.1016/j.resconrec.2021.106015.

[33] C. Arthur et al., "Decarbonizing Concrete: Ultra-Low-Carbon Pathways and Policy Integration," *Scientific Journal of Engineering, and Technology,* vol. 2, no. 1, pp. 134-142, 2025, doi: 10.69739/sjet.v2i1.669.

[34] X. Binggang, W. Jingbo, J. Wanshun, Z. Yuwei, and C. Yuan, "A Global Study of Green Cement Intelligent Manufacturing Based on Artificial Intelligence," *Science and Engineering,* vol. 2, no. 6, p. 160, 2023, doi: 10.57237/j.se.2023.06.003.

[35] M. A. Rahman and Y. Lu, "EcoBlendNet: A physics-informed neural network for optimizing supplementary material replacement to reduce the carbon footprint during cement hydration," *Journal of Cleaner Production,* vol. 464, 2024, Art no. 142777, doi: 10.1016/j.jclepro.2024.142777.

[36] A. Arvizu-Montes, O. Guerrero-Bustamante, R. Polo-Mendoza, and M. J. Martinez-Echevarria, "Integrating Life-Cycle Assessment (LCA) and Artificial Neural Networks (ANNs) for Optimizing the Inclusion of Supplementary Cementitious Materials (SCMs) in Eco-Friendly Cementitious Composites: A Literature Review," *Materials*, vol. 18, no. 18, p. 4307, 2025, doi: 10.3390/ma18184307.

[37] M. Toum Benchekroun, S. Zaki, and M. Aboussaleh, "Kiln predictive modelization for performance optimization," *The International Journal of Advanced Manufacturing Technology,* vol. 127, no. 3, pp. 1333-1339, 2023, doi: 10.1007/s00170-023-11563-2.

[38] V. Colla, C. Pietrosanti, E. Malfa, and K. Peters, "Environment 4.0: How digitalization and machine learning can improve the environmental footprint of the steel production processes," *Matériaux & Techniques,* vol. 108, no. 5-6, p. 507, 2020, doi: 10.1051/mattech/2021007.

[39] A. Müller et al., "Decarbonizing the cement industry: Findings from coupling prospective life cycle assessment of clinker with integrated assessment model scenarios," *Journal of Cleaner Production,* vol. 450, 2024, Art no. 141884, doi: 10.1016/j.jclepro.2024.141884.

[40] V. Mittal and L. Dosan, "System Dynamics Modeling of Cement Industry Decarbonization Pathways: An Analysis of Carbon Reduction Strategies," *Sustainability*, vol. 17, no. 15, p. 7128, 2025, doi: 10.3390/su17157128.

[41] M. L. Nehdi and A. Yassine, "Mitigating Portland Cement CO2 Emissions Using Alkali-Activated Materials: System Dynamics Model," *Materials,* vol. 13, no. 20, p. 4685, 2020, doi: 10.3390/ma13204685.

[42] Y. He, Z. Li, and P. Liu, "A Co-production system of cement and methanol: Unveiling its advancements and potential," *Journal of Cleaner Production,* vol. 473, 2024, Art no. 143523, doi: 10.1016/j.jclepro.2024.143523.

[43] E. A. Moore et al., "How can the Cement Industry Enable Industrial Decarbonization at Scale?," *Environmental Science & Technology,* vol. 59, no. 36, pp. 19233-19243, 2025, doi: 10.1021/acs.est.5c02831.

[44] M. O. Oyenuga, R. Singh, S. B. Apata, S. Khan, and V. Kumar, *Smart technologies for climate change and net zero policies: Practical approaches towards sustainability*, 1 ed. Cham, Switzerland: Springer 2025.

[45] M. H. Riaz, Y. Zhou, M. Guo, B. Xi, and S. Xiang, "Development of LC3-ECC incorporating recycled fine aggregate: a novel sustainable and ductile material," *Case Studies in Construction Materials,* vol. 22, p. e04547, 2025, doi: 10.1016/j.cscm.2025.e04547.

[46] C. R. Price, S. U. Nimbalkar, K. Thirumaran, and J. Cresko, "Smart Manufacturing Pathways for Industrial Decarbonization and Thermal Process Intensification," *Smart and Sustainable Manufacturing Systems,* vol. 7, no. 1, pp. 41-53, 2023, doi: 10.1520/SSMS20220027.

[47] M. T. Kashifi, B. A. Salami, S. M. Rahman, and W. Alimi, "Using explainable machine learning to predict compressive strength of blended concrete: a data-driven metaheuristic approach," *Asian Journal of Civil*

Engineering, vol. 25, no. 1, pp. 219-236, 2024, doi: 10.1007/s42107-023-00769-0.

[48] H. Arksey and L. O'Malley, "Scoping studies: towards a methodological framework," *International Journal of Social Research Methodology,* vol. 8, no. 1, pp. 19-32, 2005, doi: 10.1080/1364557032000119616.

[49] A. C. Tricco et al., "PRISMA Extension for Scoping Reviews (PRISMA-ScR): Checklist and Explanation," *Ann Intern Med,* vol. 169, no. 7, pp. 467-473, 2018, doi: 10.7326/m18-0850.

[50] T. Umar, "Making future floating cities sustainable: a way forward," *Proceedings of the Institution of Civil Engineers - Urban Design and Planning,* vol. 173, no. 6, pp. 214-237, 2020, doi: 10.1680/jurdp.19.00015.

[51] T. Umar, "Harnessing AI for sustainable engineering: innovations and challenges," *Proceedings of the Institution of Civil Engineers - Engineering Sustainability,* pp. 1-7, 2026, doi: 10.1680/jensu.25.00054.

[52] T. Hills, D. Leeson, N. Florin, and P. Fennell, "Carbon Capture in the Cement Industry: Technologies, Progress, and Retrofitting," *Environ Sci Technol,* vol. 50, no. 1, pp. 368-377, 2016, doi: 10.1021/acs.est.5b03508.

[53] B. He and K.-J. Bai, "Digital twin-based sustainable intelligent manufacturing: a review," *Advances in Manufacturing,* vol. 9, no. 1, pp. 1-21, 2021, doi: 10.1007/s40436-020-00302-5.

[54] O. E. Ige and M. Kabeya, "Multi-Objective Optimization of Raw Mix Design and Alternative Fuel Blending for Sustainable Cement Production," *Sustainability,* vol. 17, no. 16, p. 7438, 2025, doi: 10.3390/su17167438.

[55] O. P. Pfeiffer et al., "Bayesian design of concrete with amortized Gaussian processes and multi-objective optimization," *Cement and Concrete Research,* vol. 177, p. 107406, 2024, doi: 10.1016/j.cemconres.2023.107406.

[56] K. Scrivener, F. Martirena, S. Bishnoi, and S. Maity, "Calcined clay limestone cements (LC3)," *Cement and Concrete Research,* vol. 114, pp. 49-56, 2018, doi: 10.1016/j.cemconres.2017.08.017.

[57] J. Thomas and A. Harden, "Methods for the thematic synthesis of qualitative research in systematic reviews," *BMC Medical Research Methodology,* vol. 8, no. 1, p. 45, 2008, doi: 10.1186/1471-2288-8-45.

[58] T. Umar, "The Planning and Infrastructure Act 2025: challenges and opportunities for the built environment sector," *Proceedings of the Institution of Civil Engineers - Municipal Engineer,* pp. 1-16, 2026, doi: 10.1680/jmuen.26.00001.

[59] D. Zhang, B. Jaworska, H. Zhu, K. Dahlquist, and V. C. Li, "Engineered Cementitious Composites (ECC) with limestone calcined clay cement (LC3)," *Cement and Concrete Composites,* vol. 114, 2020, Art no. 103766, doi: 10.1016/j.cemconcomp.2020.103766.

[60] H. Shoukry, "Development of Nano Modified Eco-Friendly Green Binders for Sustainable Construction Applications," *Nano Hybrids and Composites,* vol. 24, pp. 25-36, 2019, doi: 10.4028/www.scientific.net/NHC.24.25.

[61] Y. Zhu, Z. Zhang, Y. Yang, and Y. Yao, "Measurement and correlation of ductility and compressive strength for engineered cementitious composites (ECC) produced by binary and ternary systems of binder materials: Fly ash, slag, silica fume and cement," *Construction and Building Materials,* vol. 68, pp. 192-198, 2014, doi: 10.1016/j.conbuildmat.2014.06.080.

[62] M. Baawain, H. Shoukry, and K. Al-Jabri, "An Investigation into the Thermo-Physical, Mechanical, and Microstructural Properties of Cement Mortar Incorporating Hybrid Waste Slags," *International Journal of Civil Engineering,* vol. 19, no. 1, pp. 17-26, 2021, doi: 10.1007/s40999-020-00554-z.

[63] O. Oguntola, K. Boakye, and S. Simske, "Towards Leveraging Artificial Intelligence for Sustainable Cement Manufacturing: A Systematic Review of AI Applications in Electrical Energy Consumption Optimization," *Sustainability*, vol. 16, no. 11, p. 4798, 2024, doi: 10.3390/su16114798.

[64] R. Fernández Gassó, L. Sevilla Hurtado, and J. M. Cañero-Nieto, "Optimizing cement kiln operation with expert systems," *The International Journal of Advanced Manufacturing Technology,* 2025, doi: 10.1007/s00170-025-16489-5.

[65] A. M. Ali, J. D. Tabares, and M. W. McGinley, "A machine learning approach for clinker quality prediction and nonlinear model predictive control design for a rotary cement kiln," *Journal of Advanced Manufacturing and Processing,* vol. 4, no. 4, p. e10137, 2022, doi: 10.1002/amp2.10137.

[66] R. Fatahi, H. Nasiri, A. Homafar, R. Khosravi, H. Siavoshi, and S. Chehreh Chelgani, "Modeling operational cement rotary kiln variables with explainable artificial intelligence methods – a “conscious lab” development," *Particulate Science and Technology,* vol. 41, no. 5, pp. 715-724, 2023, doi: 10.1080/02726351.2022.2135470.

[67] O. Manis et al., "Data-Driven AI Models within a User-Defined Optimization Objective Function in Cement Production," *Sensors*, vol. 24, no. 4, p. 1225, 2024, doi: 10.3390/s24041225.

[68] S. Sundaramoorthy, D. Kamath, S. Nimbalkar, C. Price, T. Wenning, and J. Cresko, "Energy Efficiency as a Foundational Technology Pillar for Industrial Decarbonization," *Sustainability*, vol. 15, no. 12, p. 9487, 2023, doi: 10.3390/su15129487.

[69] J. B. Asere, K. N. Akinsanya, E. E. Smart, F. O. Nasir, I. B. Owunna, and M. N. Dillum, "Hybrid renewable-hydrogen systems for industrial decarbonization," *World Journal of Advanced Engineering Technology and Sciences,* vol. 16, no. 02, pp. 93-111, 2025, doi: 10.30574/wjaets.2025.16.2.1265.

[70] S. Quevedo Parra and M. C. Romano, "Decarbonization of cement production by electrification," *Journal of*

Cleaner Production, vol. 425, 2023, Art no. 138913, doi: 10.1016/j.jclepro.2023.138913.

[71] F. Williams, A. Yang, and D. R. Nhuchhen, "Decarbonisation pathways of the cement production process via hydrogen and oxy-combustion," *Energy Conversion and Management,* vol. 300, p. 117931, 2024, doi: 10.1016/j.enconman.2023.117931.

[72] E. Ali, A. Mansour, E. Mohammed Abdelkader, N. Elshaboury, and T. Zayed, "Digital Twin for Climate Resilience: Transforming Smart Cities for a Sustainable Future," *Int. Arch. Photogramm. Remote Sens. Spatial Inf. Sci.,* vol. XLVIII-G-2025, pp. 139-145, 2025, doi: 10.5194/isprs-archives-XLVIII-G-2025-139-2025.

[73] N. Martínez-Ramón, F. Calvo-Rodríguez, D. Iribarren, and J. Dufour, "Frameworks for the application of machine learning in life cycle assessment for process modeling," *Cleaner Environmental Systems,* vol. 14, p. 100221, 2024, doi: 10.1016/j.cesys.2024.100221.

[74] S. S. A. B. Padavala, S. Avudaiappan, S. R. R. T. Prathipati, Y. Paluri, V. Sainath, and A. M. Kumara, "Integrated experimental, machine learning, and life-cycle assessment of fly ash–silica fume based self-compacting geopolymer concrete," *Scientific Reports,* vol. 16, no. 1, p. 12845, 2026, doi: 10.1038/s41598-026-43052-3.

[75] C. Zhou, D. Xuan, Y. Miao, X. Luo, W. Liu, and Y. Zhang, "Accounting CO2 Emissions of the Cement Industry: Based on an Electricity–Carbon Coupling Analysis," *Energies*, vol. 16, no. 11*,* p. 4453, 2023, doi: 10.3390/en16114453.

[76] A. Oğuz and O. Hansu, "Circular Economy for Climate-Resilient and Sustainable Construction," *Harran Üniversitesi Mühendislik Dergisi,* vol. 10, no. 3, pp. 138-171, 2025, doi: 10.46578/humder.1673599.

[77] S. Pauliuk et al., "Global scenarios of resource and emission savings from material efficiency in residential buildings and cars," *Nature Communications,* vol. 12, no. 1, p. 5097, 2021, doi: 10.1038/s41467-021-25300-4.

[78] C. Carbone, D. Ferrario, A. Lanzini, S. Stendardo, and A. Agostini, "Evaluating the carbon footprint of cement plants integrated with the calcium looping CO2 capture process," *Frontiers in Sustainability,* vol. 3, 2022, Art no. 809231, doi: 10.3389/frsus.2022.809231.

[79] M. G. Plaza, S. Martínez, and F. Rubiera, "CO_2 capture, use, and storage in the cement industry: State of the art and expectations," *Energies,* vol. 13, no. 21, p. 5692, 2020, doi: 10.3390/en13215692.

[80] Z. Qiu, "Applications of Carbon Capture Technologies in Steel and Cement Industries," *Advances in Economics, Management and Political Sciences,* vol. 123, pp. 36-41, 2024, doi: 10.54254/2754-1169/123/2024MUR0109.

[81] W. M. Ashraf and V. Dua, "Machine learning based modelling and optimization of post-combustion carbon capture process using MEA supporting carbon neutrality," *Digital Chemical Engineering,* vol. 8, p. 100115, 2023, doi: 10.1016/j.dche.2023.100115.

[82] F. Hussin, S. A. N. Md Rahim, N. S. M. Hatta, M. K. Aroua, and S. A. Mazari, "A systematic review of machine learning approaches in carbon capture applications," *Journal of CO2 Utilization,* vol. 71, 2023, Art no. 102474, doi: 10.1016/j.jcou.2023.102474.

[83] M. Tawalbeh, M. Sabri, H. Kazim, A. Al-Othman, and F. Almomani, "Artificial intelligence and material design in carbon capture and utilization: A review of emerging synergies," *Carbon Capture Science & Technology,* vol. 16, p. 100470, 2025, doi: 10.1016/j.ccst.2025.100470.

[84] D. R. Nhuchhen, S. P. Sit, and D. B. Layzell, "Decarbonization of cement production in a hydrogen economy," *Applied Energy,* vol. 317, p. 119180, 2022, doi: 10.1016/j.apenergy.2022.119180.

[85] R. S. El-Emam and K. S. Gabriel, "Synergizing hydrogen and cement industries for Canada's climate plan – case study," *Energy Sources, Part A: Recovery, Utilization, and Environmental Effects,* vol. 43, no. 23, pp. 3151-3165, 2021, doi: 10.1080/15567036.2021.1936699.

[86] B. C. Domingues, D. M. F. Santos, M. Mateus, and D. Cecílio, "Techno-Economic Analysis of Cement Decarbonization Techniques: Oxygen Enrichment vs. Hydrogen Fuel," *Hydrogen*, vol. 5, no. 1*,* pp. 59-69, 2024, doi: 10.3390/hydrogen5010005.

[87] P. Patel, "Could cement and steel team up to cut emissions?," *C&EN Global Enterprise,* vol. 102, no. 17, pp. 3-3, 2024, doi: 10.1021/cen-10217-leadcon.

[88] M. Casazza and F. Barone, "Relevance of Environmental Factors in the Steel Life Cycle for a Transition toward Circular Sustainable Production and Consumption Systems: A Joint Bibliometric and Bibliographic Analysis," *Metals*, vol. 13, no. 3*,* p. 592, 2023, doi: 10.3390/met13030592.

[89] P. Kairouz and H. B. McMahan, "Advances and Open Problems in Federated Learning," *Foundations and Trends in Machine Learning,* vol. 14, no. 1-2, pp. 1-210, 2021, doi: 10.1561/2200000083.

[90] T. Li, A. K. Sahu, A. Talwalkar, and V. Smith, "Federated Learning: Challenges, Methods, and Future Directions," *IEEE Signal Processing Magazine,* vol. 37, no. 3, pp. 50-60, 2020, doi: 10.1109/MSP.2020.2975749.

[91] A. Merchant, S. Batzner, S. S. Schoenholz, M. Aykol, G. Cheon, and E. D. Cubuk, "Scaling deep learning for materials discovery," *Nature,* vol. 624, no. 7990, pp. 80-85, 2023, doi: 10.1038/s41586-023-06735-9.

[92] B. Sanchez-Lengeling and A. Aspuru-Guzik, "Inverse molecular design using machine learning: Generative models for matter engineering," *Science,* vol. 361, no. 6400, pp. 360-365, 2018, doi: 10.1126/science.aat2663.

[93] S. Bishnoi and K. L. Scrivener, "µic: A new platform for modelling the hydration of cements," *Cement and Concrete Research,* vol. 39, no. 4, pp. 266-274, 2009, doi: 10.1016/j.cemconres.2008.12.002.

[94] A. Jain et al., "Commentary: The Materials Project: A materials genome approach to accelerating materials

innovation," *APL Materials,* vol. 1, no. 1, p. 011002, 2013, doi: 10.1063/1.4812323.

[95] M. Honic, I. Kovacic, and H. Rechberger, "Improving the recycling potential of buildings through Material Passports (MP): An Austrian case study," *Journal of Cleaner Production,* vol. 217, pp. 787-797, 2019, doi: 10.1016/j.jclepro.2019.01.212.

[96] T. Adisorn, L. Tholen, and T. Götz, "Towards a Digital Product Passport Fit for Contributing to a Circular Economy," *Energies*, vol. 14, no. 8, p. 2289, 2021, doi: 10.3390/en14082289.

[97] A. Barredo Arrieta et al., "Explainable Artificial Intelligence (XAI): Concepts, taxonomies, opportunities and challenges toward responsible AI," *Information Fusion,* vol. 58, pp. 82-115, 2020, doi: 10.1016/j.inffus.2019.12.012.

[98] D. Gibassier, "Private Standards in the Climate Regime: The Greenhouse Gas Protocol," *Social and Environmental Accountability Journal,* vol. 33, no. 3, pp. 181-182, 2013, doi: 10.1080/0969160X.2013.845037.

[99] B. Downar, J. Ernstberger, S. Reichelstein, S. Schwenen, and A. Zaklan, "The impact of carbon disclosure mandates on emissions and financial operating performance," *Review of Accounting Studies,* vol. 26, no. 3, pp. 1137-1175, 2021, doi: 10.1007/s11142-021-09611-x.

[100] F. S. Islam, "Trustworthy Artificial Intelligence in the Climate Transition: Mandating Life Cycle Accountability for Net-Zero Systems and Infrastructure Resilience," *International Journal of Research (IJR),* vol. 12, no. 12, pp. 32–54, 2025, doi: 10.5281/zenodo.17817875.

[101] I. C. Yeh, "Modeling of strength of high-performance concrete using artificial neural networks," *Cement and Concrete Research,* vol. 28, no. 12, pp. 1797-1808, 1998, doi: 10.1016/S0008-8846(98)00165-3.

[102] B. Ouyang et al., "Learning from Sparse Datasets: Predicting Concrete's Strength by Machine Learning," *Machine Learning Materials Science,* 2020, doi: 10.48550/arXiv.2004.14407.

[103] M. Raissi, P. Perdikaris, and G. E. Karniadakis, "Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations," *Journal of Computational Physics,* vol. 378, pp. 686-707, 2019, doi: 10.1016/j.jcp.2018.10.045.

[104] T. Wuest, D. Weimer, C. Irgens, and K.-D. Thoben, "Machine learning in manufacturing: advantages, challenges, and applications," *Production & Manufacturing Research,* vol. 4, no. 1, pp. 23-45, 2016, doi: 10.1080/21693277.2016.1192517.

[105] J. C. Forsdyke, B. Zviazhynski, J. M. Lees, and G. J. Conduit, "Probabilistic selection and design of concrete using machine learning," *Data-Centric Engineering,* vol. 4, 2023, Art no. e9, doi: 10.1017/dce.2023.5.

[106] J. L. Provis, "Alkali-activated materials," *Cement and Concrete Research,* vol. 114, pp. 40-48, 2018, doi: 10.1016/j.cemconres.2017.02.009.

[107] L. K. Turner and F. G. Collins, "Carbon dioxide equivalent (CO2-e) emissions: A comparison between geopolymer and OPC cement concrete," *Construction and Building Materials,* vol. 43, pp. 125-130, 2013, doi: 10.1016/j.conbuildmat.2013.01.023.

[108] F. Tao, H. Zhang, A. Liu, and A. Y. C. Nee, "Digital Twin in Industry: State-of-the-Art," *IEEE Transactions on Industrial Informatics,* vol. 15, no. 4, pp. 2405-2415, 2019, doi: 10.1109/TII.2018.2873186.

[109] D. Leeson, N. Mac Dowell, N. Shah, C. Petit, and P. S. Fennell, "A Techno-economic analysis and systematic review of carbon capture and storage (CCS) applied to the iron and steel, cement, oil refining and pulp and paper industries, as well as other high purity sources," *International Journal of Greenhouse Gas Control,* vol. 61, pp. 71-84, 2017, doi: 10.1016/j.ijggc.2017.03.020.

[110] A. Sharma, E. Kosasih, J. Zhang, A. Brintrup, and A. Calinescu, "Digital Twins: State of the art theory and practice, challenges, and open research questions," *Journal of Industrial Information Integration,* vol. 30, 2022, Art no. 100383, doi: 10.1016/j.jii.2022.100383.

[111] V. Khatri and C. V. Brown, "Designing data governance," *Commun. ACM,* vol. 53, no. 1, pp. 148–152, 2010, doi: 10.1145/1629175.1629210.

[112] J. Lee, H. Davari, J. Singh, and V. Pandhare, "Industrial Artificial Intelligence for industry 4.0-based manufacturing systems," *Manufacturing Letters,* vol. 18, pp. 20-23, 2018, doi: 10.1016/j.mfglet.2018.09.002.

[113] U. P. D. Ani, H. He, and A. Tiwari, "Review of cybersecurity issues in industrial critical infrastructure: manufacturing in perspective," *Journal of Cyber Security Technology,* vol. 1, no. 1, pp. 32-74, 2017, doi: 10.1080/23742917.2016.1252211.

[114] H. Kayan, M. Nunes, O. Rana, P. Burnap, and C. Perera, "Cybersecurity of Industrial Cyber-Physical Systems: A Review," *ACM Comput. Surv.,* vol. 54, no. 11s, pp. 1-35, 2022, doi: 10.1145/3510410.

[115] S. S. Kamble, A. Gunasekaran, and R. Sharma, "Analysis of the driving and dependence power of barriers to adopt industry 4.0 in Indian manufacturing industry," *Computers in Industry,* vol. 101, pp. 107-119, 2018, doi: 10.1016/j.compind.2018.06.004.

[116] M. Ghobakhloo, "Industry 4.0, digitization, and opportunities for sustainability," *Journal of Cleaner Production,* vol. 252, 2020, Art no. 119869, doi: 10.1016/j.jclepro.2019.119869.

[117] P. S. Fennell, S. J. Davis, and A. Mohammed, "Decarbonizing cement production," *Joule,* vol. 5, no. 6, pp. 1305-1311, 2021, doi: 10.1016/j.joule.2021.04.011.

[118] F. Song et al., "Dissemination and publication of research findings: an updated review of related biases,"

Health Technology Assessment, vol. 14, no. 8, pp. 1-236, 2010, doi: 10.3310/hta14080.

[119] A. Martín-Martín, M. Thelwall, E. Orduna-Malea, and E. Delgado López-Cózar, "Google Scholar, Microsoft Academic, Scopus, Dimensions, Web of Science, and OpenCitations' COCI: a multidisciplinary comparison of coverage via citations," *Scientometrics,* vol. 126, no. 1, pp. 871-906, 2021, doi: 10.1007/s11192-020-03690-4.

[120] P. Jüni, A. Witschi, R. Bloch, and M. Egger, "The Hazards of Scoring the Quality of Clinical Trials for Meta-analysis," *JAMA,* vol. 282, no. 11, pp. 1054-1060, 1999, doi: 10.1001/jama.282.11.1054.

[121] K. G. Shojania, M. Sampson, M. T. Ansari, J. Ji, S. Doucette, and D. Moher, "How Quickly Do Systematic Reviews Go Out of Date? A Survival Analysis," *Annals of Internal Medicine,* vol. 147, no. 4, pp. 224-233, 2007, doi: 10.7326/0003-4819-147-4-200708210-00179.

[122] A. Lavercombe, X. Huang, and S. Kaewunruen, "Machine Learning Application to Eco-Friendly Concrete Design for Decarbonisation," *Sustainability*, vol. 13, no. 24, p. 13663, 2021, doi: 10.3390/su132413663.

[123] M. A. Rahman, T. Zhang, and Y. Lu, "PINN-CHK: physics-informed neural network for high-fidelity prediction of early-age cement hydration kinetics," *Neural Computing and Applications,* vol. 36, no. 22, pp. 13665-13687, 2024, doi: 10.1007/s00521-024-09791-y.

[124] P. Wang, A. J. Robinson, and S. Papadokonstantakis, "Prospective techno-economic and life cycle assessment: a review across established and emerging carbon capture, storage and utilization (CCS/CCU) technologies," *Frontiers in Energy Research,* vol. 12 Art. no. 1412770, 2024, doi: 10.3389/fenrg.2024.1412770.

[125] S. Çetin, D. Raghu, M. Honic, A. Straub, and V. Gruis, "Data requirements and availabilities for material passports: A digitally enabled framework for improving the circularity of existing buildings," *Sustainable Production and Consumption,* vol. 40, pp. 422-437, 2023, doi: 10.1016/j.spc.2023.07.011.