



AI-Enabled Strategies for Reducing CO₂ Emissions in Cement and Concrete: A Comprehensive Study of Materials, Models, and Industry Practices

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Abstract

Modern infrastructure is supported by concrete, which, however, is one of the most significant sources of anthropogenic CO₂ emissions on an industrial scale, mainly due to clinker manufacturing, energy-intensive processing, and the widespread use of virgin aggregates. Following the intensification of climate regulations and net-zero goals, the literature investigating the practical use of low-carbon binders, CO₂-sequestering concrete, circular-material solutions, and sophisticated modelling applications has increased exponentially as a plausible approach to decarbonizing the cement and concrete value chain. This paper synthesizes recent developments in three interconnected domains: (i) material innovations, including CO₂-carbonated concretes, recycled aggregate and recycled cement systems, LC3 and CSA-based binders, alkali-activated and geopolymer materials, and waste-derived supplementary cementitious components; (ii) data-driven and AI-based frameworks for predicting mechanical performance, durability, and embodied emissions, encompassing supervised learning, hybrid optimization (e.g., ANN-GA, PSO-, and gradient-boosted models), generative mix design, and uncertainty-aware forecasting; and (iii) process- and system-level strategies such as plant-scale operational optimization, carbon capture integration, electricity-based emission accounting, and national or regional emission scenario modelling. Throughout these threads, the review demonstrates that multi-objective optimization and machine learning can reduce embodied CO₂ by significant margins while simultaneously achieving or exceeding traditional performance metrics. Alternative binders and circular solutions have the potential to reduce process emissions by 20-80% under the right conditions, and intelligent operational control can provide an immediate and low-capital benefit in additional mitigation. The remaining issues are data standardization, model transferability, interpretability, and the incorporation of technological innovations, along with policy, economic, and implementation limitations. It is based on these insights that the paper proposes a research and implementation agenda: material innovation is coupled with AI-enabled design, monitoring, and decision support to accelerate the shift toward sustainable, intelligent, and climate-resilient concrete infrastructure.

Keywords: Low-Carbon Cementitious Materials; Machine Learning Optimization; CO₂ Emissions Reduction; AI-Driven Concrete Design; Sustainable Construction Materials

1 Introduction

Concrete is the most popular construction material in the globe, which is the skeletal framework of structures, transport networks, energy infrastructure, and literally every aspect of society advancement. The concrete consumption in the world has been in tandem with urbanisation, industrialisation and population growth, and is projected to go on with growth in decades to come as the emerging economies develop their infrastructure bases. However, regardless of its widespread use and engineering flexibility, traditional concrete manufacture also drives up anthropogenic emissions of carbon dioxide (CO₂) through its dependence on energy-intensive clinker manufacturing, high-temperature kiln burning, and extraction and processing of natural aggregates on a massive scale. A high proportion of process emissions in the cement value chain can be explained by the clinkerisation process as such, including the combustion of fuels and the decarbonation of limestone. With the approach of making the global climate policy tougher and more ambitious (with more nations pledging to achieve net-zero or deep-decarbonization), there is an acute necessity to re-invent concrete technologies, optimise production routes, and innovate new materials and modelling ways that can significantly decrease the environmental footprint of the cement and concrete industries. It is under this context that, with recent progress in low-carbon binders, carbonated materials, artificial intelligence (AI), machine learning (ML), generative modelling, and energy-emissions analysis, the traditional carbon-heavy industry has a way to become a more intelligent and sustainable one. Low-clinker cements, alkali-activated binders, recycled aggregate systems, CO₂-sequestering concretes, and hybrid cementitious matrices are currently being tested not only on a laboratory level but also on pilot and industrial basis. Meanwhile, digitalisation and data-driven tools are progressively integrated into production lines, quality control systems, and supply-chain management and allow creating much accurate control over the mix design, energy consumption, and emissions. The literature reviewed in this paper represents this move away of strictly empirical, trial and error practice with a combination, model based framework that explicitly ties mechanical performance, durability, cost and environmental impact. Collectively, these advances offer a wide-ranging and deep base to build superior decision-support systems that are capable of leading decarbonization in both materials, processes, operational tactics and policy processes in a coherent and scalable way. Recent technologies like CO₂ Concrete are an essential change towards incorporating carbon capturing directly into the production of concrete. By carbonating recycled aggregates, decreasing the use of virgin aggregate materials, and reusing masonry waste that has been crushed, CO₂ Concrete helps to incorporate the principles of the circular-economy into structural materials, minimizing the environmental effect caused by the materials used in the construction process. The technique utilises CO₂ as an active reagent instead of a waste gas, which allows permanent mineralisation in hydrated cement phases and recycles aggregates. One of the best contributions of this technology is that even though it has sustainability benefits, the technology does not affect structural performance. Researchers have shown high predictive performance using artificial neural networks (ANNs) in compressive strength with multiple R of 0.98 and an R^2 of 0.95, with validation errors of an average of 3.43 percentage points only [1]. These findings reveal that the complex relationship among the CO₂ curing conditions, mix proportions, and mechanical properties can be reliably predicted with the help of ML-based predictive modelling. More generally, they show that data-driven models can strongly assure quality of the emerging green concretes, that the perceived risk of the technology is minimized by data-driven models to the designers, the contractors and the regulators and hence the mainstream adoption

of carbon-sequestering technologies. In addition to the material-level innovations, the creation of alternative low-carbon binders is also strategically important in the process of decreasing the carbon footprint of the cement industry. Ordinary Portland cement (OPC) continues to be the most common binder in the world, although its manufacture is by nature a carbon-intensive process because of the limestone content and the high temperatures necessary in the kiln. Depending on regional supply and long-term durability, supplementary cementitious materials (SCM) like fly ash, slag, calcined clays, and other pozzolans can be used as a replacement of clinker to some degree. In addition, the current CO₂ accounting frameworks are not sufficient as they rely on the data of plants that are in operation, and thus cannot be used to measure new binders that are yet to be manufactured on a large scale. In order to reduce this gap, theorists have come up with heat-balance-based models of direct CO₂ emission of alternative cements, which determines direct CO₂ emission of alternative cement, and enables prediction of the emissions even prior to the industrial application of the cement sample in question [2]. Through this model, calcium sulfoaluminate (CSA) clinker was demonstrated to produce direct CO₂ emissions that were 34% below those of OPC, at much increased material cost. The high-belite CSA (HB-CSA) became a cheaper substitute, and its emissions were similar, and the costs of raw materials were reduced significantly [2]. The insights offer fundamental advice to future binder design, but they indicate the importance of SCMs and energy-efficient chemical design and show that the benefits of climate must be considered alongside economic viability and resource availability. With the large concentration of the global cement production by China it is critical to learn the pattern of any emission long-term change in the China cement industry to any viable global decarbonization route. An in-depth historical examination (1980-2014) showed that cement-based CO₂ emissions grew 18 folds within the timeframe and peaked at 1270.55 Mt in 2014 [3]. This was a dramatic increase which was facilitated by high rate of urbanization, expansion of infrastructure and mass production of housing. Although there was an increase in energy efficiency, which reduced the emission factors by 852.12 kg/t to 513.15 kg/t, total emissions remained on the increase because of the growing activity, a phenomenon known as the so-called rebound effect in which the gains in efficiency are compensated by higher activity levels. It was projected in scenarios as at 2020 that process will not be sufficient to counteract emissions, whereas energy-efficiency gains will be far more effective, and that alternative fuels and industrial byproducts have to be incorporated to make more profound cuts [3]. The hybrid Random Forest of Multilayer Perceptron of Linear Regression (RF MLP LR) model in complementary research found that the consumption of cement in 31 Chinese provinces can be estimated with great accuracy (MAPE less than 10% in most provinces) which confirms that economic prosperity, urbanization and construction of houses are the main factors that drive cement demand. These type of region-specific knowledge, which is inspired by the ML-based prediction, is necessary to design sustainable, balanced, and specific policy action that can be based on spatial heterogeneity of demand and resource availability and structural characteristics of industries. A reduction of emissions is also a key issue in underground operations with cement, including CO₂ capture and storage (CCS) and CO₂-enhanced oil recovery (EOR). In such applications, cement can be used as a major resistance to fluid migration in wellbores. Long-term well integrity should be maintained thus since the oil-well cement can be compromised by CO₂ exposure, corrosion can occur and leaks can be formed, compromising storage security and environmental safety. An extensive survey of experimental studies has depicted that there is a considerable difference in tests procedures of the world, equipment setups, and modeled underground environments [4]. This variation poses significant difficulties in the production of a uniform evaluation of cement in CO₂ environments and makes it difficult to compare the findings between the laboratory and the project. Research has also indicated that the degradation of cement is highly influenced by the chemical composition, brine chemistry, thermal environment, mechanical stress, and the fracture properties. Simultaneously, another modelling study on cement fracture sealing during exposure to CO₂ showed that diffusion rates, reaction rates, salinity of brine, and geometry of the fracture have a significant impact on self-sealing

behavior in cement fractures under the effect of CO₂ exposure [5]. Such results highlight that coupled chemo-hydro-mechanical processes control degradation and self-sealing, and these hold significant consequences to long-term and safe application of geological CO₂ storage methods. They also point out that there is a significant prospect of using physics-oriented models to be combined with ML to create predictive tools on well integrity in hostile field conditions. Even further into the scope of emission forecasting and optimization of operations, the necessity of a high-quality data-driven modelling is not restricted to material science and subsurface engineering. As an example, models based on artificial neural networks (ANNs) have been applied to forecast emissions of carbon dioxide due to the manufacturing of cement in the Beijing-Tianjin-Hebei area with high accuracy ($R^2 = 0.962$) using complex data based on national statistics [6]. Such models are able to be trained on multi-dimensional variables including clinker production, fuel composition, electricity consumption, technology of production and macroeconomic variables and can give real or near real-time predictions. These methods can be generalized to other sectors or regions of industry, providing a versatile means of analyzing the situation in terms of emissions, assessing policies and benchmarking performance. In the day-to-day variation of the performance of the plant level, another important and frequently ignored opportunity to reduce the emissions is the day-to-day one. A study of a cement plant in the UK with a pre-calciner kiln proved that the changes in CO₂ emissions produced by fuel daily can be quite significant, and the ability to operate the plant on the days it performs best could lead to a reduction in the emissions by almost 20% and energy usage by 8.5% without any significant technological improvements to the system and equipment used in the facility [7]. This observation reinforces the concept of operational optimization as a cost-neutral or low-cost mitigation measure, which emphasizes the importance of data analytics, process control, and staff training as a means of generating emission reductions in the near future. Scaling down emissions to a continental level also adds more weight to the need to combine the use of ML and mathematical optimization. A multi-objective model that has been created to predict the emission of the North American cement industries showed significant advances in forecast accuracy, which was decreasing the mean of the error by 48.13% with the Generalized Reduced Gradient (GRG) technique [8]. It was projected that CO₂ emission will slowly rise between the year 2020 and 2050 in the scenario of a baseline, thus, giving the policymakers quantitative evidence regarding the urgency of adopting the net-zero pathway that will integrate efficiency, fuel switch, and innovative binders. Meanwhile, uncertainties-driven modelling models like the interval grey number-based V-GM(1,N) give a more adaptable description of emission uncertainties where simulation accuracy of over 97% is achieved in the cement industry of China [9]. With such explicitly modeling interval uncertainties in important drivers and parameters, these models are more useful in making climate-sensitive decisions where both central estimates and plausible ranges of future emission levels need to be taken into account. These approaches show that an integration of ML, optimization, and grey-system theory could produce effective strategic planning tools in the environment of deep uncertainty. In addition to the emissions forecasting, system dynamics (SD) modelling can also provide a comprehensive view of the effect that mitigation policies, technological advances and resource limitations have on the impact over the period of time. A recent survey of SD applications has discovered that models have been applied to explore the broad range of mitigation strategies, including alternative fuel and low-carbon binders, carbon capture, energy efficiency, and waste heat recovery, among others [10]. SD models have feedback loops, time delays and non-linear interactions across technological change, policy, investment, and market dynamics, which make them especially ideal in the investigation of long-term transition pathways. Nevertheless, the review lists that a significant number of studies fail to cover the aspects of the barriers to implementation, stakeholder involvement, and financial limitations, which opens up considerable possibilities in the future research. The inclusion of behavioural reactions, policy inertia and funding mechanisms with SD structures will be essential in changing the technical feasibility research to realistic transition roadmaps. At the material design level, more recent development has gone beyond the conventional empirical mix design

to the use of computationally guided and AI-read design frameworks. It was shown in detail that low-CO₂ cements can attain high durability, with their microstructural chemistry, especially the availability of alkali-activated system-based on aluminium being well-regulated in this regard [11]. This article highlights that decarbonization should not be sought in terms of a reduction of clinker only, but supplemented with the need of microstructural engineering, which guarantees carbonation resistance, chloride intrusion, and other degradation processes. Developing thermodynamic databases and moving away progressively towards performance-based codes are necessary measures to facilitate the use of these new materials, as they will enable designers to state what performance they want, and not what material should be used. In the meantime, a self-compacting concrete (SCC) and self-compacting steel fiber-reinforced concrete (SCSFRC) represents a new two-stage optimization framework that involves a nonlinear programming strategy to optimize economic and environmental costs by combining mechanical and rheological modelling and self-compacting concrete (SCC) application; Findings indicated a maximum of 4.2% reduction in CO₂ emission without any mechanical performance loss, and that CEM II 32.5 based systems tend to be more sustainable than CEM I. These results demonstrate the strength of multi-objective optimization in disclosing non-obvious mixes that can balance flowability, strength and emissions. Generative AI has created new opportunities in concrete mix design, being a leading edge in the field of data-driven material science. Training CatBoost, XGBoost, LightGBM, and other sophisticated ML models on close to 5,000 data elements of various batching plants, the researchers created a generative framework that could produce new concrete mix designs with a desired strength level and a low cost and embodied CO₂ amount of the concrete scheme [12]. Bayesian optimization was used to make sure that the predictive models selected the best hyperparameters that greatly enhance their reliability and generalisation. The developed mix designs were experimentally verified to be feasible in practice and their measured strengths were seen to be within acceptable error margins to the predicted values. The research finally led to a web-based tool that could help practitioners make decisions in real time, where the engineers could input desired performance and cost constraints and optimize mix recommendations could be provided to them [12]. This paper represents an example of generative modelling and ML to transform a concrete mix design process that relied on rules of thumb and expert judgement into an automated and data-driven decision support system. Lastly, proper carbon accounting is still a part and parcel of emission mitigation, especially since most jurisdictions have implemented carbon-pricing systems, emissions trading, and mandatory reporting controls. The process of traditional carbon accounting in the cement manufacturing industry entails comprehensive and high-resolution data on various stages of production and flow of materials, expensive and time consuming to obtain and maintain. Another innovative methodology came up with electricity-carbon ML models, which do not depend on any carbon data to predict CO₂ emissions, demonstrating a high predictive accuracy of these models, with low-quality error indicators, such as the R² = 0.96) [13]. Comparing the purchased electricity, waste heat recovery, and machine-level electricity consumption, the research obtained essential predictors and proved that electricity-based models are capable of contributing to faster and more effective carbon accounting, which is one of the essential steps to include the cement facilities into the national emission trading system and digital reporting software. This methodology highlights the fact that, with proper training and validation, the ML can play a significant role in the reduction of the data load related to environmental compliance and monitoring.

Taken together, the reviewed literature highlights three overarching themes. First, there is a clear and pressing need for innovative low-carbon binders and carbon-sequestering concretes that directly address the emissions intensity of traditional clinker-based systems [1, 2, 11, 14]. Second, the transformative role of machine learning, generative AI, and uncertainty modelling in predicting performance, emissions, and consumption patterns is increasingly evident, with applications spanning mix design, plant operation, national and regional forecasting, and subsurface integrity assessment [3, 5, 6, 8, 9, 12, 13, 15]. Third, the

importance of operational optimization, system-level modelling, and scalable accounting frameworks in accelerating industry-wide decarbonization is underscored by studies showing substantial mitigation potential without major capital-intensive retrofits [7, 10]. These diverse yet interconnected research streams collectively demonstrate that the transition to low-carbon concrete and cement systems is not only technologically feasible but also economically and operationally advantageous when supported by intelligent modelling and informed policy. Building upon these foundations, the present study aims to advance the integration of data-driven approaches with material innovation, with the broader goal of supporting the global move toward sustainable, intelligent, and climate-resilient concrete infrastructure. The rest of this paper is structured into three broad sections to offer a rigorous and coherent analysis of the current avenues of decarbonizing the cement and concrete industries to cover the three complementary aspects of the problem. In section 2, a comprehensive Literature Review is brought together, summarizing the recent developments in sustainable cementitious materials, low-clinker, waste-based binders, CO₂-sequestering concretes, and circular-economy solutions like recycled aggregates and recycled cement. The section also provides a survey of the fast development of the machine learning and artificial intelligence techniques in mixture proportioning, performance forecasting, emissions modeling, and optimization of industrial processes. The literature review provides a multi-dimensional vision of the changing fundamentals of concrete sustainability by incorporating discoveries in many different areas such as material chemistry, thermodynamic modelling, life cycle assessment, emissions forecasting, and plant-level process optimization. Section 3 contains a critical Discussion that is an integration of cross-cutting knowledge in the literature and the evaluation of newly emerging synergies between material design, computational modelling, and industrial practice. In this section, the authors note the role of AI-based structures in improving exploration of high-volume and complex design spaces, uncovering new mix compositions, performance optimization in the environment, and optimizing operational strategies in cement plants. It also highlights the ways in which the low-carbon binder technologies, carbonation-based materials and other production pathways can be systematically combined with intelligent modelling, which will form robust and scalable solutions to the minimization of the embodied and operational CO₂ emissions. Additionally, the discussion recognizes some of the main challenges such as fragmentation in the data set, geographical dispersions in raw materials, the low interpretability of black-box models, slow adoption of alternative binders through lack of standardization, and policy and economic landscape constraints. These concerns allow the discussion section to create a subtle outlook on the present situation in the field as well as the practical obstacles, which need to be overcome, in order to make industry-wide decarbonization a reality. Lastly, in Section 4, there is the Conclusion and Future Work that summarizes the most important findings and their implications on sustainable construction materials and practices. In this section, there is the need to introduce material innovations with machine learning, generative design and system-level optimization so as to generate meaningful cuts in CO₂ emissions throughout the entire concrete value chain. It also suggests future and prospective direction in research, such as the creation of large, harmonized, open-access datasets; the creation of hybrid physics-AI models; the implementation of real-time digital twins to provide predictive and adaptive control of plants; and the creation of standards of performance-based design to facilitate the adoption of low-carbon binders. Moreover, the work of the future shows the necessity of ensuring technological innovation and supporting policy frameworks, economic incentives, and cross-sectoral collaboration. The combination of these strategic directions will enhance the shift towards low-carbon, intelligent, and resilient global concrete infrastructure system.

2 Literature Review

The integration of machine learning (ML) in the field of cement and concrete has transformed the scientific and industrial arena as it allows complex investigations into the material behavior, modelling of emissions, and optimization of the mixtures. This trend is closely connected to the urgency of minimizing the carbon footprint of the construction sector and enforcing the high levels of safety and performance standards. The conventional mix-design and process-control methods have been based on time-consuming empirical charts, simple equations and human judgement, which is ill-posed to work in high-dimensional parameter spaces. In comparison, the complex, nonlinear associations between varied and huge experiment and operations data can be learned with ML models, permitting the concurrent examination of numerous inputs-e.g., binder composition, aggregate grading, curing conditions, and process parameters, and numerous outputs, e.g., strength, workability, durability, and embodied CO₂. One of the most vibrant fields of research is ultra-high-performance concrete (UHPC), which, in spite of its high mechanical and rheological properties, is severely criticized due to its high embodied carbon. To overcome these issues, a recent study produced a hybrid, ML-based framework, which is initially trained to estimate compressive strength and slump flow to eliminate the necessity of expensive full-scale experimental campaigns and to do so at a fraction of the cost of this type of campaign [16]. The model has a prediction error of below 10%, which implies a high robustness and generalization in the design space under study. The genetic algorithm (GA) is then applied to these ANN predictions as inputs and it is then used to search through the high-dimensional space of UHPC constituents in terms of strength, workability, component proportions, and volumetric consistency constraints [16]. The result is a UHPC mix that has been optimized and a substantially smaller carbon footprint of 688 kg/m³, which evidences the practical potential of the ML-based multi-objective optimization in the creation of more sustainable high-performance concretes. Notably, this methodology shows how performance can be maximized, and environmental impact reduced, through data-driven tools, which can be seen as the opposition of the two goals. Another complement to the above-mentioned study is a literature on ML applications in the optimization of high-strength concrete (HSC) and ultra-high-strength concrete (UHSC) that hold a vital niche in high-rise buildings, long-span bridges, and heavy-loaded infrastructure. These are materials that have found a large market in the market because of their outstanding structural qualities but because of the high content of cement they emit a lot of carbon. In one of them, a large experimental dataset was compiled using the literature to build ML models, which can predict compressive strength using constituent materials, such as cement, water, aggregates, SCMs, and admixtures [17]. The embodied carbon was calculated with respect to each mix using these predictions which related mix composition to standardized factors of emission. Significantly, the analysis found that the same compressive strength could be obtained using several mix designs but with significant variation on the embodied carbon variance in the mix designs [17]. This many-one mapping of mixture composition to performance accentuates that conventional design practices, in which practically all attention is on meeting the target strength, can unintentionally miss low-carbon alternatives. By analyzing the statistical data and using this technique of trend mapping relying on the ML, the authors suggested the use of benchmark intervals to set the allowable embodied-carbon levels in each of the strength grades, in effect establishing a performance-emission design envelope. These understanding are essential to tangible practitioners who aim to formulate low-carbon blends without compromising mechanical performance and it offers viable benchmark of codes, certification organizations and green procurement policies. The focus has also been made on calcification process of producing clinker which is also a significant source of process related CO₂ emission. Breakdown of calcium carbonate and other carbonates, and high-temperature combustion of fuels cause large direct and indirect emissions. Since the emission in the process of calcinations is a function of chemical composition, particle size distribution, residence time, and thermal exposure, simpler models of the processes that assume simplified kinetics find it challenging

to predict the nonlinear relationships between decarbonisation reactions. To eliminate these shortcomings, scientists evaluated diverse advanced AI-based models, such as deep neural networks (DNN), ant colony optimization-enhanced ANN (ACO-ANN), and genetic algorithm-enhanced ANN (GA-ANN), to estimate CO₂ emissions of raw materials during the calcination process [18]. These models train on experimental or plant-based data, thereby implicitly learning complicated kinetic and heat-transfer effects without being explicit about the mechanism. Having R² values above 0.99 and average relative errors of less than 1.04%, particularly the DNN, these methods show remarkable modelling precision, confirming ML as an effective method to determine complex thermochemical relations in clinker production [18]. In addition, convergence and overfitting minimisation by using meta-heuristic algorithms to optimise neural network hyperparameters (ACO, GA) further enhances the convergence, as well as, the advantages of jointly applying global search strategies to process modelling functions that are approximately represented by a flexible functional framework. On a macrolevel, the ML has been applied to predict the national-level emission of CO₂ in the cement industry, thus connecting the phenomena occurring on the plant- and material-level to the long-term policy and planning. An exhaustive paper implemented an Improved Particle Swarm Optimization- Backpropagation (IPSO-BP) predictive model to 44 cases using second generation dry cement production technologies [19]. In this model, a BP neural network is tuned with PSO and this minimizes the chances of local minima and enhances the long-term predictability. According to the findings, with the capacity reduction measures and the use of the advanced dry-process technologies, the cement-related CO₂ emissions of China might reach the peak way before 2030; in some scenarios, the peak could be pushed forward by approximately 20 years, compared to the business-as-usual scenario, the peak emissions of cement-related activities would be only 742 Mt [19]. These findings indicate that national emission pathways can be transformed radically with the choice of strategic mixes of structural policies (e.g., disbanding old-fashioned kilns), technological modernization, and emission quotas. These long-term forecasting systems are essential in the planning and implementation of policies that aim to balance industrialization and the national carbon-neutrality objectives and in the assessment of the duration and intensity of the interventions that will be necessary to fulfill the climate commitments. At the mix-design and structural level, ML has facilitated the innovations in cement-use optimization of those elements that are favourable to deferred loading. Conventionally mix proportioning relies upon the attainment of a strength in the form of 28-day compressive strength a practice which is historically derived based on testing tradition and not on realistic loading conditions. Service loads on foundations, pavements and mass concrete are usually imposed months or even years after casting in the real world. This time dimension can greatly be exploited to help minimize cement consumption. In one of the studies, ANN and regression were used to forecast the cement content necessary to obtain the 28-day and 90-day strengths of a mix on the basis of mix parameters and curing regimes [20]. The comparison of various regressions, such as Elastic Net, Ridge and ordinary least squares revealed Elastic Net regression as the most dependable, with a prediction accuracy of up to 94% accuracy of predictions being accurate up to 94% [20]. The capability of the model to deal with multicollinearity and the variable selection is especially useful in the mix-design scenarios where the inputs are correlated. Using these ML-based predictions with a real reinforced concrete project, the authors projected that cement reduction by 10% and carbon emissions reduction by 10% would be achieved, which is indeed practical evidence of environmental benefits of ML-based design optimization. This example also shows that even minor modifications in the design philosophy like the ability to design to be stronger in later age can contribute to significant improvements in emissions as long as strong predictive tools are in place. A second significant input to national-scale modelling was based on extensive carbon-emissions inventory of Chinese cement industry to evaluate predictive power of six ML models ridge regression, polynomial regression, Random Forest, support vector regression, gradient-boosted regression trees and feed-forward neural networks [21]. Through a system of comparative analysis of these models with a common data paradigm, the research was a very useful reference point in the

choice of method to use in future studies. The highest predictive performance ($R^2 \approx 0.99$) was achieved with the use of both nonlinear parametric and nonparametric models: polynomial regression and neural network models, indicating that both can be used to effectively describe the relationships between the cement output, energy consumption, fuel mix and CO₂ emissions. Analysis of feature-importance showed that clinker production and coal consumption contributed almost 95% of the national cement-associated emissions, which quantitatively supported their prevailing proportions of the impact on climate of the sector. Spatial emission tendencies were also given in the study indicating that the emissions of the cement sector in China are controlled by North, South and Southwest. These results demonstrate the importance of model interpretability in supporting regional decarbonization policies to show where alternative fuels, efficiency/efforts, or structural capacity changes can be leveraged most. Further extending ML to detailed process modelling, another study applied six ML techniques to over 6000 historical manufacturing data points to analyze oxidation and calcination degrees in cement calcination [22]. By focusing on CO₂ molecular composition and conducting sensitivity analyses, the study identified the process parameters—such as tertiary air flow, fuel flow, and feed rate—with the most significant impacts on CO₂ release. These insights enrich process engineers' understanding of thermal dynamics and provide targeted pathways for improving kiln and calciner efficiency, for example, by adjusting combustion stoichiometry or residence times to reduce incomplete combustion and excessive over-firing. The use of a large, plant-derived dataset also demonstrates that ML can be directly embedded in industrial environments, functioning as a virtual sensor or soft-sensor that infers unmeasured states (e.g., oxidation degree) from easily measured operational variables.

A growing body of work also focuses on modelling CO₂ sequestration within cement-based materials, aligning concrete technology with long-term carbon storage objectives. A study integrating extensive experimental datasets with literature data applied Decision Trees, Random Forests, and XGBoost to predict carbonation depth, a critical indicator of CO₂ uptake and durability, under varying mix compositions and exposure conditions [23]. XGBoost significantly outperformed linear regression, demonstrating its ability to capture nonlinear and interaction-dominated relationships among input variables such as water-to-binder ratio, curing regime, cement type, and exposure environment [23]. With aid from SHAP interpretability tools, the study also revealed the previously underappreciated role of cement type—especially CEM II/B-LL and CEM II/B-M—in influencing carbonation behavior. This suggests that nuanced changes in clinker-SCM combinations can materially affect both CO₂ uptake and reinforcement corrosion risk. These findings foster a deeper understanding of the chemical drivers of carbon sequestration and provide a basis for designing concretes that both store CO₂ and maintain long-term durability.

Kiln-stack CO₂ emissions have also been modelled using ML with a focus on operational control and compliance. Drawing on 22 operational variables from a clinker production line in the UAE, researchers evaluated models including k-nearest neighbors (KNN), linear regression, decision trees, Random Forest, Gradient Boosting, and ANN [24]. Random Forest and Gradient Boosting proved most reliable, achieving R^2 values of 0.984 and low RMSE/MAE values, indicating strong agreement between predicted and measured emissions [24]. Kiln feed rate emerged as the dominant factor affecting stack emissions, suggesting that targeted operational adjustments—such as smoothing feed-rate fluctuations and avoiding overload conditions—could directly improve emission outcomes. The use of ensemble methods in this context demonstrates their robustness to noise and their capacity to handle heterogeneous operational datasets. Recently, more attention is being paid to the possibility of replacing biochar (BC) with cement mortar as the way to valorise biomass residues and enhance concrete sustainability. A comprehensive experimental study indicated that BC increases compressive and tensile strength, decreases water absorption, and increases durability because it is pozzolanic and has a porous microstructure, which can fine-tune pore structure and alter hydration

products [25]. Corroborating results of AdaBoost and linear regression which utilized complimentary ML data confirmed that the mechanical and durability characteristics of BC-modified mortars can be predicted with a high degree of certainty, with AdaBoost offering significantly higher accuracy since it has the capability to concentrate on hard-to-predict samples as well as minimizing biasness in the results of the prediction process [25]. This underscores the combination between experimental and computational methods in the development of sustainable cement mortars and justifies the increased application of ML as an adjunct to the screening of the preferred replacement levels and curing conditions without labor intensive laboratory investigations. The lack of certainty in the combustion systems is also a problem in terms of emission control and process stability. This problem has been solved by a study based on ANN surrogate models trained with 700 dynamic simulations of kiln and calciner processes including 10% uncertainty in major input flows including coal, air and raw meal [26]. A space of operation was then searched using these surrogates with GA, PSO, and hybrid GA -PSO optimizers under uncertainty conditions. The hybrid solution offered the best stable and correct solutions, balancing between exploration and exploitation in search process [26]. Further sensitivity analysis revealed that total coal and tertiary air flow were the most significant factors that affected CO₂ and CO production, which gave solid recommendations on how to control the process. The paper shows the possibility of real-time intelligent optimization of industrial cement processes and how a high fidelity simulation combined with ML surrogates can significantly reduce computational cost whilst maintaining predictive fidelity. ML is also useful in the use of calcined sludge as a partial cement replacement, which helps to achieve the circular-economy goals, diverting waste streams on landfills towards value-added construction materials. Six variable experiments (with sludge content, water-to-binder ratio, curing age, etc. as parameters of the mixtures) were fed with six ML regressors, such as convolutional neural networks (CNN), ensemble regression, MLP-ANN, support vector regression (SVR), and Random Forest, to predict compressive strength [27]. CNN and ensemble regression were the most successful models, which demonstrates that even models that were developed to work with images can be used to process tabular material-property data when correctly configured [27]. The use of ML-based robustness assessment confirmed that curing age was the most influential factor in strength, which relates to the central importance of hydration development in blended systems. The results of this study can assist in creating sustainable waste-based binders with more predictable behavior and show that ML can be used to determine the safe replacement thresholds and curing regimes. Another area where ML has surpassed the drawbacks of semi-empirical kinetic models is in hydration kinetics in OPC containing mineral additives, where in most cases one has to calibrate the model on a case-by-case basis. Using Random Forests, a single study showed reliable forecasting of time dependent hydration behavior where physiochemical properties, including composition, fineness, and temperature, were applied as inputs to the hydration behavior prediction tool [28]. The model was also able to generate mix designs that meet user-specified kinetic constraints (e.g. desired heat-release shapes or setting times), allowing targeted performance requirements without necessarily having specific mechanistic kinetic models. It is especially applicable to mass concrete, precast elements, and 3D printing, where it is important to control the early-age heat evolution and setting behavior as a means of controlling cracks and making production schedules. The sustainability benefits of geopolymer mortars incorporating eggshell powder (ESP) and rice husk ash (RHA) were explored using both Response Surface Methodology (RSM) and ML-based prediction [29]. A dataset of 606 compressive strength results was used to train Gaussian Process Regression (GPR), ANN, and Gradient Boosting models, with GPR achieving the highest accuracy and providing probabilistic uncertainty bounds [29]. Experimental results showed improved strength and reduced CO₂ emissions relative to conventional binders, indicating that agricultural wastes can serve as effective aluminosilicate sources in geopolymer systems. The combined use of RSM and ML enabled both global trend identification and local fine-tuning of mix parameters, demonstrating the practical value of ML-enhanced mix optimization for alternative binders and highlighting the role of uncertainty-aware models in guiding

experimental campaigns. Further advances in the modelling of cement-based materials were demonstrated in a study assessing five ML techniques—SVM, Random Forest, decision tree, AdaBoost, and KNN—to predict compressive strength using a large experimental database [30]. AdaBoost and Random Forest models achieved the strongest performance, reflecting the effectiveness of ensemble learning in capturing complex structure–property relationships with limited overfitting [30]. The analysis of variable influence provided valuable insights into how cement grade, curing age, water-to-binder ratio, and sand characteristics affect strength development, confirming and extending traditional empirical knowledge with quantitative importance rankings. Such models can serve as generic predictive engines embedded in design tools, educational platforms, or quality-control systems. Finally, ML has been widely applied to optimize flexural strength (FS) in cementitious composites containing waste glass powder (WGP). Experimental testing showed that WGP enhances FS at replacement levels up to 15%, depending on whether cement or fine aggregate is replaced, largely due to its pozzolanic reactivity and micro-filler effects [30]. ML models—including SVM and a bagging regressor—were trained on six input parameters, with the bagging regressor achieving the best predictive performance by aggregating multiple base learners to reduce variance [30]. This study highlights the ability of ML to accelerate evaluation of waste-derived cementitious composites and supports the broader goal of sustainable materials development by enabling rapid screening of replacement strategies, curing conditions, and performance targets. Collectively, the body of work reviewed in this section shows that ML is not only a predictive tool but also a transformative design and optimization paradigm for decarbonizing cementitious materials across scales—from microstructural engineering and mix design to process control and national emissions modelling. To provide a clear and systematic overview of the diverse machine learning approaches applied to cementitious materials and decarbonization strategies, Tables 1 and 2 summarize the key characteristics of the studies reviewed. Table 1 focuses primarily on material-scale investigations, including mix-design optimization, strength prediction, carbonation modelling, and the development of low-carbon binders. In contrast, Table 2 concentrates on process-level and system-scale studies—such as kiln-emission modelling, surrogate-based optimization of industrial operations, national emissions forecasting, and the assessment of circular-material strategies. Together, the two tables categorize each contribution according to its objective, methodological approach, and major findings, thereby offering a structured and comparative understanding of how computational intelligence is being integrated into different stages of the cement and concrete value chain. The combined insights presented in Tables 1 and 2 highlight the accelerating convergence of material science, machine learning, and sustainability analytics. They illustrate how advanced models—including neural networks, ensemble methods, hybrid meta-heuristic optimizers, convolutional architectures, and grey forecasting techniques—are being deployed to improve predictive accuracy, reveal nonlinear dependencies, and optimize performance–emissions trade-offs. By organizing the literature in this dual-table format, the review makes it possible to identify methodological trends, knowledge gaps, and emerging research directions. This structured synthesis not only clarifies the current state of the field but also supports the development of future AI-driven frameworks for low-carbon, high-performance concrete technologies.

3 Discussion

The literature review shows that the situation has changed rapidly with low-carbon binders, CO₂-sequestering concretes, and AI-driven modelling colliding to transform the cementitious materials design, production, and management. In both the material-scale and the system-scale research, the same trend can be observed: the most effective decarbonization strategies are those based on simultaneously considering chemistry, mix

Table 1: Summary of Reviewed Studies on ML Applications in Cement and Concrete (Part 1)

Reference	Objective	Methodology	Key Findings
[16]	Develop a low-carbon UHPC mix with reduced embodied CO ₂ .	Hybrid ANN-GA framework predicting strength and slump; GA optimizes mix proportions.	ANN achieved < 10% error; optimized UHPC reduced carbon footprint to 688 kg/m ³ .
[17]	Identify low-carbon alternatives for high-strength concrete.	Large experimental dataset; ML prediction of compressive strength; embodied CO ₂ calculated from emission factors.	Different mixes reach same strength but vary greatly in CO ₂ . Proposed benchmark embodied-carbon ranges.
[18]	Predict CO ₂ emissions during clinker calcination.	DNN, ACO-ANN, GA-ANN trained on calcination data; meta-heuristic hyperparameter tuning.	Models achieved R ² > 0.99; DNN highest accuracy. ML captured non-linear thermochemical behavior.
[19]	Forecast national cement-sector CO ₂ emissions for 44 scenarios.	Improved PSO-BP neural network for long-term modelling of dry-process technologies.	Peak emissions could occur before 2030 with structural and technological changes; minimum peak = 742 Mt.
[20]	Reduce cement usage by designing for later-age strength.	ANN and regression models (Elastic Net, Ridge, OLS) predicting 28- and 90-day strength requirements.	Elastic Net achieved 94% accuracy; real project saw 10% cement and CO ₂ reduction.
[21]	Benchmark ML models for national CO ₂ emissions prediction.	Six ML models (RR, PR, RF, SVR, GBDT, FNN) trained on China's emissions data.	Polynomial regression and FNN achieved R ² ≈ 0.99. Clinker + coal = 95% of emissions.
[22]	Model oxidation and calcination degrees for process optimization.	Six ML methods applied to 6000+ manufacturing points; sensitivity analysis.	Key drivers: tertiary air, fuel flow, feed rate. ML accurately predicted calcination-related CO ₂ .
[23]	Predict carbonation depth and CO ₂ uptake in concretes.	Decision Trees, RF, XGBoost with SHAP interpretability.	XGBoost best performer; cement type strongly influences carbonation.

Table 2: Summary of Reviewed Studies on ML Applications in Cement and Concrete (Part 2)

Reference	Objective	Methodology	Key Findings
[24]	Model kiln-stack CO ₂ emissions for operational optimization.	KNN, LR, DT, RF, GB, ANN models trained on 22 kiln variables.	RF and GB achieved $R^2 = 0.984$. Kiln feed rate was the dominant emission driver.
[25]	Evaluate biochar as sustainable cement replacement.	Experimental testing + ML (AdaBoost, LR).	Biochar improved strength and durability; AdaBoost provided best predictions.
[26]	Optimize kiln–calciner operation under uncertainty.	ANN surrogates + GA, PSO, hybrid GA–PSO; 700 simulations.	Hybrid GA–PSO most stable; coal and tertiary air strongly influence CO ₂ /CO.
[27]	Model performance of calcined-sludge blended binders.	CNN, ensemble regression, MLP-ANN, SVR, RF trained on six variables.	CNN performed best; curing age dominant factor. Supports use of calcined sludge.
[28]	Predict hydration kinetics of blended cements.	Random Forest model using physico-chemical descriptors; inverse design capability.	Accurate prediction of hydration evolution; generated mixes matching target kinetics.
[29]	Optimize geopolymer mortars with ESP and RHA.	606-sample dataset; GPR, ANN, GB combined with RSM.	ESP/RHA reduced CO ₂ ; GPR highest accuracy with uncertainty quantification.
[30]	Predict strength of conventional and WGP-modified concretes.	Models: SVM, RF, DT, AdaBoost, KNN; bagging regressor for flexural strength.	RF & AdaBoost best for compressive strength; WGP improved flexural strength up to 15%.

design, process performance, and operational practice and being guided by data-driven forecasting and optimization [1, 2, 3, 16, 18, 19]. These works do not see emissions reduction as some isolated constraint that must be met by the end of the design process, but rather the environmental performance is a co-equal design objective with the strength, durability, rheology, cost, and constructability. This re-framing is the major redefinition of the role of modelling in concrete technology. ML and advanced optimization are not mere reproducers of experimental data; they are decision-support engines that search high-dimensional design spaces and discover trade-offs that are not visible to more traditional empirical methods. This way, they allow transitioning to a change of incremental improvements to truly carbon optimized, system-level decarbonization pathways. One of the main themes of the studies is that ML is used to maximise mixture proportions and estimate performance properties, including compressive strength and slump flow and carbonation depth, hydration kinetics and embodied emissions. The ANN-GA models of UHPC and BSC/UHSC demonstrate the ability of multi-objective optimization to find mix compositions that meet stringent mechanical and rheological criteria and also reduce considerably the cement content and related CO₂ intensity [16, 17]. Those methods always tend to see the invisible mixtures that would not be known through the customary design charts, especially in areas of the design space where multiple variations of SCMs, aggregates, and water-to-binder ratios produce a similar strength but vastly diverse carbon footprints. The same conclusions can be made regarding the CO₂ Concrete, RAC, GPC and binders using recycled or waste material, where models like ANN, Random Forest, Gradient Boosting, XGBoost and CatBoost have high predictive accuracy in strength and environmental indicators [1, 12, 18, 19, 25, 27, 29]. These models also accommodate sensitivity and feature-importance analysis, which are uniformly chosen to determine the cement content, water to binder ratio, curing conditions and aggregate related parameters as the main drivers of the performance and emission. Collectively, these results indicate that data-driven mix design can substantially change the customary trial-and-error practices into statistically directed study of the design space. Nevertheless, the identical research highlights the restrictions and obligations that come with the implementation of ML. The quality, quantity and diversity of underlying data is very critical to the reliability of these models. A large number of training datasets are created over a geographic area or isolated research groups, and there is little diversity in the sources of raw-materials and curing conditions. Consequently, models that work excellently in the training sphere might underscore their performance when extrapolated in: other cements, SCMs, or environmental exposures. The black-box architectures are especially vulnerable to this risk, e.g., deep neural networks. Therefore, multiple studies highlight the necessity of strong training datasets, interpretability of the model (e.g., through SHAP analysis and permutation importance), and cross-validation on independent datasets to prevent overfitting and guarantee generalizability [16, 18, 23, 25, 27, 29]. A new consensus seems to be that ML cannot and should not replace physical understanding with physics-informed features and constraints as protection against unphysical predictions. Regarding the emissions-forecasting and policy-modelling side, the reviewed literature emphasizes the fact that the national and sectoral decarbonization paths cannot be uncoupled with the processes of cement-demand and urbanization, as well as with the processes of economic development. Historical studies of the cement sector in China reveal that the CO₂ emission has soared dramatically even after decreased energy efficiency, indicating that the growth in the number of activities can counter the advances in technology as long as the level of production remains increased [3]. This phenomenon highlights the need to include demand-side factors, including material efficiency, optimization of structural, and alternative practices in construction, in decarbonization efforts, instead of adopting cleaner production technologies. Further results of scenario-based forecasting of the IPSO -BP models, grey-system models, and multi-objective optimization frameworks of the regional and continental sector show that the time and scale of the emission peaks are highly dependent on the concerted application of advanced dry-process technologies, capacity optimization, alternative fuels, and low-clinker binders [3, 8, 9, 15, 19, 21]. The models are always pointing to the fact that efficiency gains are not enough,

deep reductions imply structural adjustments in the intensity of clinker, in fuel mix, and material substitution, and might also involve demand-side measures. Notably, they also have some of the quantitative policy intervention advice, on where regional differences in emission drivers need differentiated policy as opposed to egalitarian rules. Areas containing a lot of coal in the energy mix, high ratios of clinker to cement, or areas with fast-growing construction industries will need more aggressive and more focused action as compared to areas containing already established infrastructure and cleaner power. At the process and plant scale, a number of studies underline that an opportunity that is largely untapped as far as emissions reduction is concerned is operational variability. Daily kiln analyses indicate that adjusting daily operation to schedule and match best-performing days of the plant may decrease both CO₂ emission and specific energy consumption by significant percentages, without significant capital investments [7]. The result contradicts the conventional focus on hardware upgrades as the only path to decarbonization and instead supports the importance of the so-called software advancements: enhanced control of the process, quality training of operators, and data-based optimization of the operating conditions. ML-based models, which are trained on a data set of thousands of process data points, i. e. comprising the degree of calcination, oxidation state, fuel flows, air flows, feed rates, and the properties of the raw materials, have been able to recognize the process parameters that can most strongly affect the release of CO₂ into the environment [22, 24, 26]. In most instances, fewer variables (say total coal flow, tertiary air flow and kiln feed rate) represent most of the variance in emissions, which can give an unequivocal improvement candidates. The combination of surrogate models with GA, PSO, and hybrid optimizers demonstrates that real-time or near-real-time optimization is technically viable, which creates the opportunity of intelligent control systems and digital twins of cement plants [22, 26]. In principle, these systems have the capability to continuously change operating conditions due to changing characteristics of raw-materials, fuel properties, and ambient conditions so as to maximize the intensity of CO₂ but within limits on the quality of clinker and production rate. In complementary studies of electricity-based carbon accounting, based on ML models that only use electrical consumption data, it is argued that strong but inexpensive monitoring systems can be used to integrate with emission trading arrangements, as well as regulatory reporting [13]. Plants can predict emissions using fewer electrical and process indicators than have to be monitored comprehensively with sensor-dense monitoring at every process stage, but the models must be well trained, and updated frequently. Together, these contributions emphasize that operational excellence, which is facilitated by intelligent analytics, is an important pillar together with material innovation as part of the decarbonization agenda. In storage use in subsurface and CO₂ storage Applications In storage applications, we are now talking about the integrity and durability of cement in a harsh geochemical and thermo-mechanical environment. According to reviews of experimental studies of CO₂ degradation of oil-well cement considerable heterogeneity exists in testing procedures, simulated downhole environments, and performance indices such that inter-study comparison is difficult and derivation of universally applicable durability models is complicated [4]. Various experiments use different CO₂ pressures, temperatures, chemistries of the brine, and mechanical boundary conditions, which lead to a continuum of different degradation processes, including the simple decalcification through to complex multi-phase change. Model experiments of fracture self-sealing during CO₂ exposure indicate the critical roles played by the diffusion kinetics, reaction rates, fracture geometry, and brine composition in the control of the permeability and sealing capacity development in fractures and their brine because of CO₂ exposure [5]. These mechanistic observations are supported by ML-based predictive models of carbonation depth and corrosion in oil-well cements and structural concretes, where exposure time, CO₂ partial pressure, humidity, binder type, and water-binder ratio were the dominant predictors that influenced degradation and CO₂ uptake [16, 23]. Collectively, this literature indicates that safe long-term CO₂ storage must not only be chemically resilient binders but also forecasting tools to consider both coupled chemo-hydro-mechanical processes and site-specific conditions. The production of such works identifies a pressing necessity in stan-

standardized experimental systems, large harmonized data sets and hybrid physics machine learning models capable of representing the complex, multiscale processes that underlie safe CO₂ storage and CCS/EOR operations. Another key trend in the literature is the development and testing of low-carbon binders CSA, HB-CSA, LC3, high-belite systems, alkali-activated binders, and other numerous waste-based cements. The theoretically feasible heat-balance-based models of alternative clinkers show that significant CO₂ reductions (up to about a third) can be realized even pre-industrial scale, thus overcoming an important shortcoming of plant-data-sensitive accounting [2]. Genetically algorithmized LC3 systems operating under regional climatic conditions show that the bi-composition of binder should be adapted to local humidity and CO₂ level to achieve a carbonation stability and low emissions simultaneously [23]. This is particularly critical in the changing climate of CO₂ levels in the atmosphere and the local climate transformation. Research on belite-based LC3, recycled cement and recycled aggregate systems goes further to suggest that the strategy that combines clinker reduction with circular-material strategies can save a significant amount of carbon, typically in the range of 5-80%, based on the process route, substitution level and considering the boundary conditions taken into account [18, 22, 24]. Such broad scopes reveal the possibilities as well as the randomness of the benefits, and thus the necessity of life-cycle evaluation and design specific to the context. Other opportunities of CO₂ reduction are provided by alkali-activated binders and systems based on geopolymer using industrial and agricultural wastes (e.g., fly ash, eggshell powder, rice husk ash, calcined sludge), where the mix optimization of MLs, and thermodynamic information are both vital in assuring performance and practicality of the systems [11, 14, 19, 27, 28, 29]. Although such systems may show significantly reduced embodied CO₂ compared to OPC, they also raise new concerns about stability, efflorescence, alkali leaching and supply-chain stability (e.g. long-term access to fly ash). The literature examined shows that, in the right proportions and cured, such binders may possess the same mechanical properties as OPC systems, and reduce emissions greatly. Altogether, these contributions substantiate the idea that the chemistry of low-carbon binders has reached a sufficiently high level to be implemented on a large scale, should the problems of standardization, long-term durability and supply-chain robustness be preemptively overcome by codes, certification and demonstration projects. One approach that is common to these works is that environmental indicators (embodied CO₂, energy consumption, solid-waste generation etc) should be included as direct components in optimization and decision-making models and not as a posteriori evaluation metrics. Multi-objective structures of UHPC, SCC/SCSFRC, RAC, GPC, and other new materials explicitly optimize the mechanical performance as well as environmental metrics, frequently indicating non-intuitive trade-offs and structure zones that would be hard to reach through the conventional linear design processes [14, 16, 18, 19, 26]. As an example, slight strength or stiffness cuts within code limits can in combination with smart material replacement or structural dematerialization produce disproportional cuts in CO₂ emissions. Such models are becoming more and more integrated with economic aspects, such as material cost and the implicit or explicit price of carbon, which reveals possible scenarios where a technically low-carbon solution is not yet economically advantageous at existing carbon prices as in silica fume concrete and some CSA-based binders [2, 29]. These results suggest that technology, standards, and policy tools like carbon pricing, subsidies, public procurement guidelines, and lifecycle-based design guidelines must all develop together to make sure that those technology solutions that are better to the environment are also affordable and appealing to industry. Although there is an impressive developmental improvement, a number of gaps and challenges arise. To begin with, most ML models are trained on geographically, chemically or operationally localized datasets, and their global applicability is questionable. Variations in rare material qualities (e.g. limestone purity, SCM make up), production methods (e.g. grinding fineness, curing processes), and exposure conditions (e.g. temperature, humidity, amounts of pollutants) may restrict the usability of models created in one region or with one family of binders when applied elsewhere [3, 21, 22, 24]. Second, the high application of black-box models though beneficial in terms of accuracy is questionable in terms of in-

interpretability and reliability, especially in structural design and well integrity, which are safety-critical. Even though interpretability tools such as SHAP, partial dependence plots, and sensitivity analyses have started to solve this problem, they are not adopted everywhere yet and tend to be limited in a fraction of academic case studies only as of now [20, 23]. Third, most system-level constructs and SD models propose technically viable pathways of mitigation but place minimal emphasis on barriers to implementation, institutional limits, financing systems and stakeholder behaviour, which may overestimate the speed of the adoption of low-carbon technologies in actual markets [10]. Lastly, interactions between various decarbonization levers, including the combination of low-clinker binders and carbon capture, the incorporation of recycled cement and generative AI mix design, or the connection between plant-level optimization and national-level emission policies, are also not as thoroughly addressed, and integrated evaluation of the interaction between them is relatively uncommon. In prospect, these studies synthesized indicate a number of promising future research and implementation directions. Large, open, and standardized datasets which are applicable across regions, binder chemistries, exposure conditions and structural typologies are clearly needed to allow the creation of more generalizable and transferable ML models. These datasets would also be useful in meta-analyses and cross-study benchmarking and would help minimize redundancy of effort and hasten convergence of methods. Hybrid approaches that integrate physics-based models (e.g., thermodynamic, kinetic, transport, and fracture mechanics models) with data-driven learners can be more accurate and interpretable, especially complex processes like hydration, carbonation, microcracking, high-temperature degradation, etc. [5, 11, 23, 28]. On the plant and system level, the combination of the ML-based optimization and real-time monitoring and digital twins can be used to unlock operational improvement that is continuous and assisting the adaptive control strategies based on emissions and energy key performance indicators (KPIs) [7, 13, 22, 26]. Genetic and Bayesian optimization strategies that have already been applied to mix design can be applied to the entire supply-chain and lifecycle optimization, where the selection of materials relates to quarrying, transportation, energy, and regulatory decisions and constraints [12, 18, 19]. Finally, with the integration of material creativity, high-level modelling, and planning at the system level in a consistent, data-oriented structure, the cement and concrete sectors would be able to take a decisive turn towards climate-resistant, low-carbon directions, realizing the technical, environmental, and economic possibility discussed in the context of this literature.

4 Conclusion and Future Work

The production of modern studies on low-carbon cementitious materials, AI-based modelling, and decarbonization strategies at the system level demonstrates that the concrete industry is undergoing a revolutionary change driven by critical climate needs, technological advancement, and the development of new policy frameworks. In materials science, computational modelling, and industrial operations, the papers reviewed repeatedly indicate that significant CO₂ reductions can be achieved without impairing structural performance, operational soundness, or, in most instances, economic viability. LC3 and CSA, belite-rich and various alkali-activated materials, and waste-derived materials are among the low-carbon binders that have demonstrated promising potential to reduce the significance of clinker while simultaneously improving or preserving mechanical performance, especially when their microstructure-chemistry is well crafted. At the same time, recycled-aggregate concrete (RAC), recycled cement (RC), and CO₂-carbonated aggregates, as part of circular-material strategies, demonstrate the possibility of completing material loops in cement production, thereby decreasing the extraction of raw materials and waste production. Added together with optimized mix designs, these innovations have the potential to lower embodied carbon by 20-80% based on

material and process conditions, with a significant impact on the global mitigation effort. Another equally transformative change is the incorporation of machine learning (ML), artificial intelligence (AI), and large-scale optimization algorithms. Since AI-based frameworks can be used in mixture proportioning and performance prediction, as well as in emissions forecasting and operational control, they offer the highest accuracy, flexibility, and responsiveness ever. ANN-GA hybrids, PSO- and CSO-enhanced models, gradient-boosted trees, XGBoost, CatBoost, generative algorithms, and grey-system models have all been shown to be predictive, with accuracy significantly higher than more traditional empirical methods, and many can achieve R² values over 0.95 in complex, nonlinear environments. Their ability to capture nonlinear interactions, determine which variables are predominant, and optimise conflicting goals is beneficial in cementitious systems, where the balance of strength, durability, workability, cost, and environmental performance needs to be optimised concurrently. Significantly, these tools are not limited to mix design, but rather to thorough modelling of calcination, carbonation processes, kiln-stack emissions, plant-level performance variability, and long-term emissions profiles, revealing optimization opportunities that would otherwise be invisible. One significant lesson from the reviewed literature is that process-level and operational enhancements can yield substantial emission reductions, without requiring major technological retrofits or drastic modifications to binder chemistry. Digital monitoring, real-time operational optimization, and intelligent control systems can minimize energy use and fuel emissions by optimizing plant operations on the most effective days and preventing unprofitable transient states. In the same light, carbon accounting models that use electricity facilitate the monitoring of emissions and provide viable opportunities to incorporate facilities into national emission trading schemes by minimizing the data volume required in traditional mass-balance systems. Research has repeatedly demonstrated that significant reductions in emissions can be achieved by optimizing calcination levels and feed rates, fine-tuning combustion variables, and using data-driven decision-making frameworks. These no-regret actions will deliver direct benefits of decarbonization as longer-term investments in low-carbon binders, carbon capture and infrastructure upgrades are developed and implemented. Nevertheless, several obstacles remain and must be overcome to realize the full potential of AI-based decarbonization of the cement and concrete industries. The lack of transferability and the resilience of ML models are constrained by the fragmentation and inconsistency of datasets in studies. Heterogeneous raw materials, variable testing protocols, and regional practices pose obstacles to generalization, particularly for AI-based mix design, durability prediction, and carbonation modelling. Most high-performing models rely on black-box architectures, raising valid concerns about transparency, interpretability, and safety, especially when implications involve structural design, long-term longevity, or CO₂ storage in the subsurface and a conservative, reliable decision is needed. The pace of adoption of such material innovations as alkali-activated binders, CSA clinkers, and recycled cement has been slow due to concerns about long-term performance, scaling characteristics, supply-chain limitations, and the absence of performance-based standards and design tools. At the system scale, predictive models are frequently used to identify viable decarbonization options without fully accounting for practical implementation constraints, economic viability, or policy inertia, leading to overestimates of the rate of low-carbon technology deployment and adoption. In the future, sustainable cement and concrete research will increasingly require greater involvement from materials science, computational modelling, environmental engineering, and policy design. Diversifying and increasing the availability of high-quality open-access data is the key to enhancing the external validity of subsequent ML models, particularly those intended for global use, such as those used for safety-critical decision-making. Standardisation of experimental protocols, data formats, and metadata, which may be globally coordinated (perhaps by international consortia), would significantly improve interoperability and the reuse of research outputs. Physics-informed AI- binding the fusion of thermodynamic simulations, hydration models, transport theory, and fracture mechanics with the information provided by the data, with the model-driven parametric learning process, is a promising direction to better interpretability, extrapolation ability, and reduction of model

uncertainty. These hybrid designs may incorporate existing physical constraints into ML models, including implicit sanity checks, allowing models to remain plausible even in sparse data regions. Cement plants' digital twins, which combine real-time sensor data with predictive analytics and optimization algorithms, may enable continuous reductions in emissions with operational interference. The virtual model that reflects the plant in this vision continuously estimates states and predicts future behavior, and recommends or automatically takes control measures to reduce emissions, energy consumption, and costs whilst maintaining quality constraints. Already in the development of generative AI, which is becoming an effective tool in mix design, it can be applied to lifecycle and supply-chain optimization to identify binder replacements, manufacturing paths, logistical plans, and circular-material plans, achieving the desired sustainability and cost goals. These systems help engineers develop not only individual concrete mixtures but also project-scale material plans that reduce the carbon intensity of a whole building, a system of structures, or an infrastructure system. It is also vital that performance-based standards and revised design codes be required to enable the newly developed low-carbon binders and artificial intelligence-based optimization of concretes to compete on the same level as OPC-based systems. Without this regulatory development, even the most technically well-founded innovations can stall in adoption due to conservative design methods, certification hurdles, or non-codified guidance. Codes and guidelines that directly include performance values, e.g., durability indicators, carbonation resistance, and lifecycle emission limits, would be more flexible and innovation-friendly in structure than prescriptive composition-based rules. Simultaneously, engineers, regulators, and practitioners have a strong impetus to educate and build capacity to ensure that AI tools and low-carbon materials are used appropriately and in a transparent manner, not in a black-box fashion. The policy interventions will have a definitive contribution to future paths. Employing carbon pricing, low-carbon procurement, a green certification scheme, and incentives to promote industrial symbiosis (e.g., cement-steel-waste management integration) can help scale low-carbon technologies faster by internalizing environmental externalities and rewarding low-emission options. Simultaneously, socio-economic studies are required to understand the barriers to adoption in developing areas, where resource limitations, institutional capacity, and market uncertainty remain significant, and cement demand is estimated to increase the fastest. It will also require international cooperation because the global cement industry is highly intertwined through supply chains, international technology transfer, and MNC corporate structures. A combination of technical standards, emissions reporting procedures, and digital monitoring in similar regions can enhance transparency, lower transaction costs, and facilitate cross-border innovation and technology dissemination. To sum up, the path to a low-carbon, innovative concrete ecosystem is becoming increasingly apparent. Material breakthroughs, AI-driven modelling, circular resource approaches, and optimisation at the system level are all needed to deliver significant, sustainable CO₂ reductions. The literature reviewed indicates that this kind of integration is not merely feasible; it is also desirable. Still, it is already being implemented in various areas, including binder chemistry and mix design, plant operation, emission prediction, and CO₂ storage. Further interdisciplinary work, including civil engineering, materials science, computer science, industrial ecology, and policy, will be the key to increasing the transition. With a strong scientific understanding and the latest digital solutions and enabling regulations, the cement and concrete sectors can transform into climate-neutral, resource-efficient, and technologically advanced sectors, without affecting their performance or economic sustainability.

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