

Recent Advances in the Chemistry of Sustainable Concrete Materials

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Abstract.

The cement sector is responsible for roughly 8% of global carbon dioxide (CO₂) emissions, and as such, prompts urgent efforts to develop sustainable concrete alternatives (Habert et al., 2020). Recent developments in concrete materials' chemistry seek to decrease their environmental impact while also keeping or enhancing performance. Novel materials, such as Limestone Calcined Clay Cement (LC³), have been reported to reduce CO₂ emissions by up to 40% by replacing clinker with calcined clay and limestone (Scrivener et al., 2018). Moreover, inclusion of nano-silica has also improved the robustness, hydration level, and the longevity of cementitious composites leading to its better performance ability on highly demanding conditions (Nazari & Riahi, 2023). Carbon Capture and Utilization (CCU) breakthroughs include carbon-negative concrete that stores much more CO₂ than it emits during its manufacturing. This is accomplished by incorporating industrial waste as reactive fillers and applying internal & external CO₂ curing for an increase in strength and durability of up to 100% (Chen et al., 2025). Studies conducted at RMIT University also showed that biochar derived from waste coffee grounds can substitute up to 15% of sand in concrete, achieving an enhanced strength of up to 30% while sequestering carbon (Hashash et al., 2024). These improvements are indicative of transitioning towards more sustainable, circular, and resilient construction. Material science and chemistry can help the concrete industry curb its global carbon emissions or reduce them substantially.

Keywords: Sustainable concrete, Low-carbon cement, Limestone Calcined Clay Cement (LC³), Nano-silica, Cement chemistry, Carbon capture and utilization (CCU), Concrete durability, CO₂ curing, Biochar, Industrial waste utilization, Green construction material.

1 Introduction

Concrete is the dominant construction material worldwide—constituting the ground of modern-day city facilities with its ability to be strong and versatile and lower price. The worldwide demand is on the rise, with the production of cement worth around 4.1 billion metric tons in 2023 and increasing by about 15% over the past 10 years (International Energy Agency [IEA], 2024). The production needs change with the demand, and today concrete is one of the most important construction materials as it produces 5% of the energy for urban applications and provides stability to residential properties (IEA, 2024). From buildings to bridges, dams, and transport systems, the long-lasting performance of concrete has become the building industry standard. Concrete, while being widely utilised, brings many environmental challenges. The main binder in concrete is Portland cement, which generates around 8% of worldwide CO₂ emissions due primarily to carbon embodied in the construction material (IEA, 2024; Habert et al., 2020), because of the thermal and emissions-intensive method of calcination and burning. Furthermore, durability problems, such as sulfate attack, chloride ingress, alkali-silica reaction and freeze-thaw damage, also contribute to the environmental burden with an increasing need for regular repairs and replacements which contribute to more lifecycle emissions and more resources.

As such, the chemistry of construction materials as a field in relation to sustainability and durability development is increasingly important. A notable progress includes the production of Limestone Calcined Clay Cement (LC³), which substitutes up to 50% of clinker with a calcined clay and limestone blend resulting in a 30–40% CO₂ reduction without affecting mechanical properties (Scrivener et al., 2018). Likewise, incorporation of nano-silica particles has been found to promote hydration reactions and optimize pore shape yielding high strength and enhanced chemical protection (Nazari & Riahi, 2023).

A related, yet more promising innovation is the incorporation of carbon capture and utilization (CCU) methods in concrete production. For instance, CO₂ curing methodologies and carbon mineralization methods can sequester up to 250 kg of CO₂ per m³ of concrete to prepare products with a net negative carbon footprint (Chen et al., 2025; NRCan, 2024). According to recent RMIT University research, converting 15% fine aggregate to biochar used from former coffee grounds can increase the compressive strength by 25% or more, and keep atmospheric carbon in the matrix (Hashash et al., 2024).

1.1 Aim and Scope : This article reports the recent development in the chemistry of environmentally sustainable concrete materials, including binder inventions, nanomaterials, carbon-negative systems, and the reutilization of waste-processed additives. It seeks to offer a scientific basis for shaping next-generation concrete in the decarbonization and climate-resilient infrastructure through performance, environmental contribution and life service performance of said systems.

2. Background / Fundamentals

2.1 Chemistry of Portland Cement Hydration. When the cement phases of Portland cement meet water, the resulting enamel forms a solid matrix that interacts with aggregate particles to form hydration. The main clinker phases—tricalcium silicate (C₃S), dicalcium silicate (C₂S), tricalcium aluminate (C₃A), and tetracalcium aluminoferrite (C₄AF)—react with water to form calcium silicate hydrate (C–S–H), calcium hydroxide (CH), and ettringite. The leading phase of strength building is C–S–H which accounts for approximately 50–60% of hardened cement paste (Taylor, 1997; Scrivener & Nonat, 2011). A good hydration of C₃S leads to early strength, and hydration of C₂S results in long-term strength. At the same time, C₃A reacts with gypsum very quickly to generate ettringite, controlling the time required for setting and diminishing flash setting (Ramachandran et al., 2002).

2.2 Commonly Used Chemical Admixtures and Their Functions: During mixing, setting and hardening, chemical admixtures are added to concrete to adjust it. Such admixtures play an important role in current concrete technologies with the objective of increasing performance and environmental sustainability (Mindess et al., 2003). Superplasticizers (typically polycarboxylate ethers) reduce water demand and enhance flowability while retaining strength (Collepari, 2001). Accelerators, such as calcium nitrate and calcium chloride, are utilised to hasten early hydration, particularly in colder environments. Retarders — like lignosulfonates and citric acid — slow down fixing time (set-time), which can be deployed in warm climates or with complex placements.

Air-entraining agents induce stable microbubbles, improving freeze-thaw durability (Neville, 2011).

Corrosion inhibitors: calcium nitrite reduces the corrosion of the reinforcement in the presence of chloride (ACI Committee 222, 2010). These admixtures interact with the hydration chemistry and the microstructure. to obtain higher workability, greater tensile strength control, and better durability.

2.3 The Microstructure and Its Relationship to Performance: The microstructure of the hydrated cement paste determines the performance of concrete. Calcium Silicate Hydrate (C–S–H): Strength is also granted by an extremely disordered and cohesive gel phase.

Capillary Pores: Control permeability and are characteristic of the water-to-cement ratio. • Calcium Hydroxide (CH): which is found to have advantages for maintaining high pH, but it also can potentially make the system prone to leaching and more susceptible to chemical attack.

Interfacial Transition Zone (ITZ): A weak porous area surrounding coarse aggregates that during stresses may become a microcracking area (Mehta & Monteiro, 2014). Novel products like nanoscale silica have shown promise in the densification of ITZ and in the refinement of pore structure and have been reported to possess improved compressive strength and reduced susceptibility to aggressive environments (Nazari & Riahi, 2023; Singh et al., 2021).

3.Recent Advances in Materials Chemistry

3.1 Nanotechnology in Concrete. Nano-silica (nS) and carbon nanotubes (CNTs) in concrete are nano-scale materials found in the context of nanotechnology. Nano-silica acts as a pozzolan which reacts with the calcium hydroxide to yield extra calcium silicate hydrate (C–S–H), which in this way increases microstructure volume. CNTs add mass to the whole mass, so that it is able to retain its strength and take on more resistance and strength in its final shape. At the same time their exceptional tensile strength and high aspect ratio contribute to mechanical reinforcement. Recent Breakthroughs: According to Nazari and Riahi (2023) the incorporation of 2% nano-silica caused more than a 20% increase in compressive strength and had better chloride resistance. Sharma and Kaushik (2021) reported a 150% enhancement for flexural strength and large decrease of microcracking when using CNT-reinforced concrete. Effects:

- 1) Mechanical: improved compressive and flexural strength.
- 2) Durability: Lower permeability, increased resistance to chemicals.
- 3) Sustainability: Minimized cement content and lifecycle pollution.

3.2 Geopolymers and Alkali-Activated Materials. Chemical Principles: Geopolymers are inorganic polymers generated from alkali activation of aluminosilicate material (such as fly ash, metakaolin). The reaction forms a three-dimensional Si–O–Al bond framework, which obviates the requirement of previous clinker-related cement (Provis & van Deventer, 2014). Recent Breakthroughs: Recent work by Zhang et al. (2022) showed a 35% increase in compressive strength of fly ash-based geopolymer concrete with nano-silica. With alkali-activated slag, it has long-term ability against sulfate attack and high temperatures. Effects:

- 1) Mechanical: Equal to OPC or stronger than OPC.
- 2) Durability: Strong resistance to chemical and heat breakdown.
- 3) Sustainability: Up to 80% less CO₂ emissions (Davidovits, 2020).

3.3 Chemical & Biological self-healing mechanisms. Chemical principles: It is possible to use encapsulated agents such as sodium silicate in chemical self-healing which polymerize upon water exposure. Biological self-healing employs bacteria (e.g., *Bacillus subtilis*) that precipitate calcium carbonate (CaCO₃) when activated by water and nutrients in cracks (Wiktor & Jonkers, 2011). Recent breakthroughs: Van Tittelboom et al. (2021) indicated bacteria-based techniques recovered up to 60% flexural strength after cracking. Long-term hydration leads to internal closing of microcracks, improving self-healing in CNTs (Singh et al., 2023).

- 1) Mechanical: Strength recovery up to partial or complete.
- 2) Durability: To prevent crack propagation.
- 3) Sustainability: Lesser strain maintenance and repairs.

3.4 SCM. Chemical Principles. For instance, SCMs such as fly ash, ground granulated blast-furnace slag (GGBFS), and silica fume react with OPC hydration Ca(OH)₂, producing more C–S–H by-products, thereby strengthening and reducing porosity (Mehta & Monteiro, 2014). Recent innovations: Ternary blends (e.g., OPC + fly ash + slag) have been developed to perform effectively under adverse conditions (Juenger & Siddique, 2015). By introducing silica fume, compressive strength increases of over 25% and permeability of materials is effectively reduced. Effects:

- 1) Mechanical: Delayed but greater final strength.
- 2) Durability: More resistant to chloride and sulfate attacks.
- 3) Sustainability: Less clinker factor and lower power consumption.

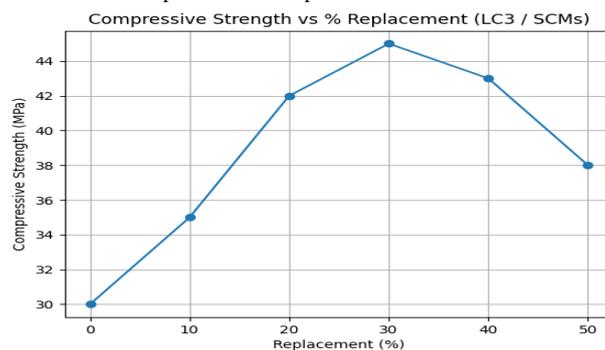


Figure 1: Variation of compressive strength with percentage replacement of cement using sustainable materials.

Description to include: The compressive strength initially increases with replacement percentage due to pozzolanic reactions and improved microstructure, reaching an optimum around 25–30%. Beyond this level, strength decreases due to dilution of cementitious compounds.

3.5 Carbon-Cured Concrete (CO₂-Reactive Binders). Chemical Principles:

Carbonation curing is an early phase application of CO₂ to hydration phase in reaction with the calcium phases to create a phase of calcium carbonates (CaCO₃) as well as the stronger matrix where more CO₂ is sequestered (Monkman & Shao, 2006). Recent Breakthroughs: Chen et al. (2025) CO₂-cured concretes sequester as much as 250 kg CO₂/m³ and enhance early-age compressive strength by 25% in their research. And companies like CarbonCure and Fortera are currently scaling those technologies even more up for commercial use. Effects:

- 1) Mechanical: Very early mechanical strength was a notable advantage.
- 2) Durability: Increased resistance to carbonation and sulfate attack.
- 3) Sustainability: Net carbon-negative performance.

3.6 Molecular Modeling and Simulation of Hydration. Chemical Principles - Molecular, mesoscale and kinetic simulations (e.g., molecular dynamics, DFT) model the behaviour of hydration products and the effects of additives that change nucleation, ion diffusion patterns, and pore structure evolution. (Pellenq et al., 2009)

Recent Breakthroughs - recent models by Masoero et al. (2021) and Pellenq et al. have accounted for nano-silica's effects on densification of C-S-H and a slowdown in chloride diffusion, and also have accorded with the experimental result. Effects:

- 1) Mechanical: Customized mix designs with engineered strength.
- 2) Durability: Long-term effectiveness benefits from predictive models.
- 3) Sustainability: Less trial and error for mix design.

3.7 Quantitative Assessment of CO₂ Reduction: Recent advancements in sustainable concrete materials demonstrate significant reductions in carbon emissions compared to conventional Portland cement systems. Figure X illustrates the comparative CO₂ reduction potential of various innovative concrete technologies. Geopolymer concrete exhibits the highest reduction (up to 80%) due to the elimination of clinker, whereas LC³ achieves around 30–40% reduction through partial clinker substitution. CO₂ curing technologies contribute to both emission reduction and carbon sequestration, achieving up to 50% reduction. Similarly, biochar-based concrete and nano-modified systems provide moderate reductions while improving material performance.

Table 1: CO₂ Emission Reduction of Sustainable Concrete Materials

Concrete Type	CO ₂ Reduction (%)	Key Mechanism
Ordinary Portland Cement (OPC)	0%	High clinker content
LC ³	30–40%	Clinker replacement with calcined clay & limestone
Geopolymer Concrete	70–80%	Alkali activation (no clinker)
Nano-silica Modified	15–25%	Improved hydration efficiency
CO ₂ -Cured Concrete	40–60%	Carbon sequestration during curing
Biochar Concrete	20–30%	Carbon storage + aggregate replacement

3.7.1 Durability Performance Comparison

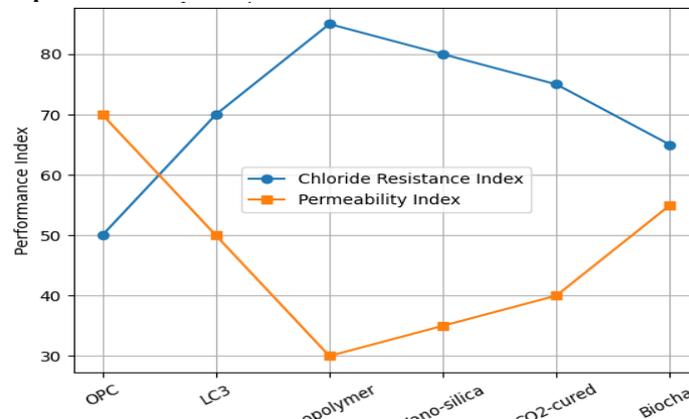


Figure 2: Comparative durability performance of sustainable concrete materials in terms of chloride resistance and permeability.

Description to include: Geopolymer and nano-silica modified concretes exhibit superior durability due to refined pore structure and reduced ion diffusion. CO₂-cured and LC³ concretes also show improved resistance compared to OPC, while biochar-based concrete demonstrates moderate performance due to increased porosity.

4. Challenges and Future Directions: Despite significant scientific progress in the chemistry of sustainable concrete materials and their use in green building materials, several challenges still limit their large-scale application and long-term reliability. Such challenges may be addressed by new developments in manufacturing and logistics, while the integration of materials continues to pose major challenges to performance and efficiency in future applications.

4.1 Durability and Long-Term Performance: Although many nano-modified concretes and geopolymers have shown excellent short-term benefits, their long-term behavior under coupled mechanical and environmental loading remains unclear. The interaction of novel additives with hydration products and reinforcement over decades is still largely unexplored (Scrivener et al., 2018; Van Deventer et al., 2020). Real-world conditions, such as repeated wet-dry and freeze-thaw cycles, require further field validation of the durability of bacteria-based self-healing concrete (Wiktor & Jonkers, 2011).

4.2 Cost and Scalability: Currently, the economics of high-tech materials—e.g., carbon nanotubes (CNTs), nano-silica, and engineered healing agents—are a barrier to universal deployment. The high cost of synthesis, absence of supply chains, and fluctuating performances prevent them from being incorporated into traditional building (Singh et al., 2023). In the same way, alkali-activated and CO₂-reactive binders must possess stringent curing regimes and extra equipment, which is not feasible in all building environments (Bernal & Provis, 2014).

4.3 A Requirement for Mechanistic Insight. More clarification on the basic reaction mechanisms of alternative cement systems is required for some time. As an example, we identify: such kinetics of geopolymer gel formation as well as the contribution of nanoparticle surface chemistry to hydration remain active areas of research (Provis & van Deventer, 2014). Recent efforts to model this knowledge gap with multiple scales have showcased the promise of multiscale simulations (Masoero et al., 2021; Pellenq et al., 2009).

4.4 Future Directions for Research.

To facilitate the successful adaptation of the laboratory findings into applications to the field, these are the following issues that should be focused on:

- Uniform tests of durability of new materials (e.g., chloride ingress, carbonation under real exposure);
- Integrating life-cycle assessment (LCA) into performance-based design (Habert et al., 2020);
- Low-cost production of nanomaterials based on green chemistry;
- The study of high-resolution models, for early stage hydration and microstructure formation;
- Long-term field tests under diverse conditions.

Interdisciplinary research will be necessary to address these challenges and develop resilient low-carbon infrastructure, consistent with international climate and sustainability goals.

5 Conclusion

The evolution in the chemistry of materials is also increasingly promoting sustainable concrete materials, which provide novel approaches to sustainable infrastructure in that they directly address such environmental and durability challenges of traditional Portland cement systems. The current review emphasizes the development opportunities of new approaches including nanotechnology, geopolymers, supplementary cementitious materials, self-healing systems, CO₂-reactive binders, and molecular-level studies and their applications. Nano-silica, carbon nanotubes, and other nanomaterials with integrated materials have been reported as emerging technologies for a better treatment of microstructure, mechanical properties, and resistance to environmental risk. Low carbon alternatives to Portland cement with superior chemical stability and strong durability are available in geopolymer and alkali-activated material. At the same time, self-healing technology—chemical and biological—enables the possibility for longer service lives and less wear and tear. SCMs (like fly ash, slag, and silica fume) are currently, and for the most part, part of eco-friendly concrete design and they enhance performance without appreciably adding to clinker content. CO₂-curing technologies and carbon-mineralizing binders are increasingly emerging to meet the challenge of delivering carbon-neutral (or even carbon-negative) concrete solutions. Still, there are long-term durability validation, cost-effectiveness, and the standardization and scaling up problems that prevent widespread adoption. Addressing these gaps will involve ongoing interdisciplinary examination of material research, in situ demonstrations, and lifecycle performance testing. Concrete is not only a building material but rather a future solution, in the sense that structural needs will depend not only on construction but also on the energy management, climatic stability, and environmental quality characteristics of a building. The realization of the knowledge and engineering of cementitious systems on molecular and microstructural bases can be applied to transform the construction sector to a more sustainable and innovative concept.

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