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Cementitious Materials in the Low Carbon Era
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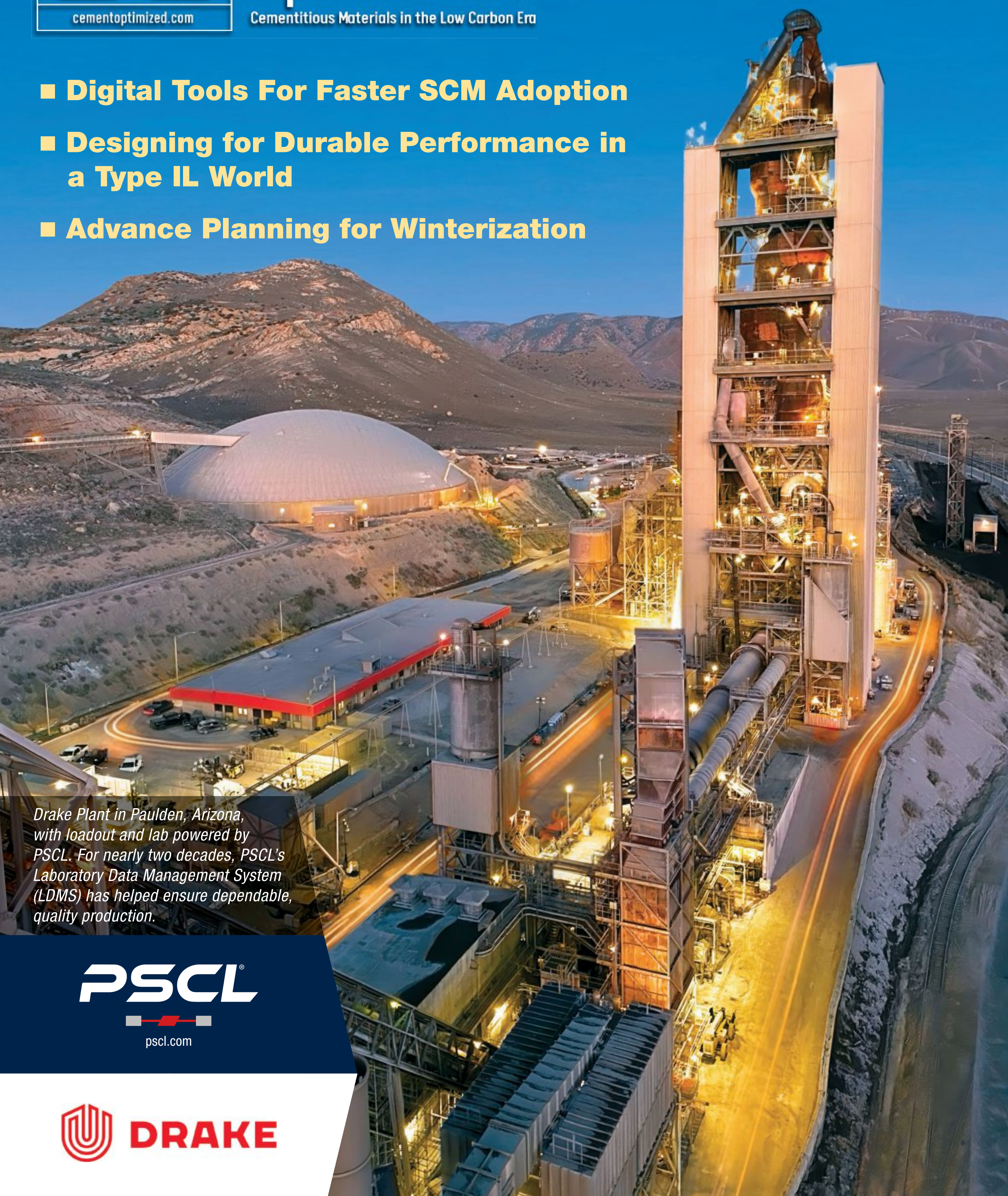


Drake Plant in Paulden, Arizona, with loadout and lab powered by PSCL. For nearly two decades, PSCL's Laboratory Data Management System (LDMS) has helped ensure dependable, quality production.

Digital Tools for Faster SCM Adoption

AI And Predictive Modeling Tools That Compress Cement Blend Validation From Weeks To Hours Have The Potential To Accelerate The Adoption Of Novel Supplementary Cementitious Materials While Maintaining Rigorous Performance Standards.

By Jonathan Rowland

According to the American Cement Association, the average clinker-to-cement ratio in the United States is 0.864. The figure is similar in Canada, where the implied clinker ratio was about 0.83 in 2024, according to the Cement Association of Canada.

Reducing this is a key factor in the industry's decarbonization thinking, but doing so is not as simple as it might seem. Even with a shift from prescriptive to performance-based standards, diversifying cement composition poses operational challenges, as higher volumes of supplementary cementitious materials (SCMs) affect cement reactivity and, in turn, concrete production and durability.

"It is a question of speed," explained Dr. Wilson Ricardo Leal da Silva, head of process and materials R&D at Fuller Technologies. "We have the chemistry knowledge to design low-carbon blends. What we need are the digital tools to validate them quickly and confidently, despite the inherent variability in novel SCMs." The EU-funded DETOCS project is tackling this challenge head-on, bringing together academic and industry partners – including Fuller, with Dr. Leal da Silva serving as project coordinator – to develop digital tools to support greater adoption of SCMs.

Combining Chemistry and Data

Cement plants are already awash in data. DETOCS aims to combine this data with a fundamental understanding of cement chemistry to develop advanced predictive models. "In a nutshell," Dr. Leal da Silva said, "digital tools can be considered as enablers, allowing cement plants to adjust blends in real-time, optimizing the use of low-CO_2 materials while minimizing clinker content."

So far, so promising. However, there is an elephant in the room: the many terabytes of data generated at plants relate to known processes, materials and blends. When considering novel SCMs with no production history, how do you build the data foundations that predictive models require? To answer this question, DETOCS is pursuing a combined modeling approach that bridges data and materials science. According to Dr. Leal da Silva, the key lies in combining:

- Novel data-driven modeling frameworks.
- Soft sensors that can be deployed in any cement plant.
- A fundamental understanding of cement chemistry and raw meal composition.

First principle models based on thermodynamics and hydration kinetics to predict the performance of novel clin-

Digital tools and real-time data are enabling cement producers to optimize SCM blends and compress validation timelines. Photo: Fuller Technologies ker and cement blends with higher SCM content.

Critically, the deployment of such models will feed instructions back into the production process to maintain stability. "This is of utmost importance when handling alternative materials," Dr. Leal da Silva said, "as they are inherently more variable than the ones traditionally used to produce cement."

This hybrid approach addresses another critical requirement: explainability. A plant operator who receives a recommendation from an AI system to adjust, for example, raw meal composition or reduce kiln temperature, needs to understand why. Given human behavior, if the model's logic is opaque, the recommendation is likely to be doubted (or even ignored). But if the system can explain that the suggested change will promote a greater share of alite formation while maintaining free lime within specification, the operator is far more likely to act on it.

Compressing Validation Timelines

Several DETOCS doctoral researchers are demonstrating that these principles work in practice, producing results that compress validation timelines from weeks or months to days or even hours.

For example, Sandra Mujombi, working across Fuller Technologies, the University of Illinois, and RWTH Aachen University in Germany, is developing an integrated test framework that predicts the 28-day compressive strength of Limestone Calcined Clay Cement (LC^3) within 24 hours.

The framework combines three tests that measure the dissolution of alumina and silica over 15 minutes, track 24-hour heat release as a proxy for pozzolanic reactivity, and quantify the kinetics of the aluminate-sulfate reaction. Applied to four natural clays calcined at different temperatures and formulated into LC^3-50 blends1, the integrated model predicted 28-day strength with a coefficient of determination (R^2) of 0.96 for the tested subset of clays. Complementary tests are being conducted across a broader range of clay compositions to validate the proposed concept further.

This compression matters on an industrial scale. Take a flash calciner producing 1,250 tpd of calcined clay. Standard 28-day testing of cement mixes made with this material creates a lag during which tens of thousands more tons are produced before quality feedback arrives. Compressing this feedback to 24 hours or fewer enables near-real-time process adjustments and reduces the risk that off-specification material reaches the market.

Meanwhile, Thorsten Kalb, working between the University of Padua in Italy and Statwolf Data Science, has demonstrated that machine learning models trained on production data can predict 28-day compressive strength with 26% to 31% lower error than baseline predictions. Using 17 months of data from a plant producing LC^3-50, Kalb's model uses measurements already collected daily, including X-ray fluorescence (XRF) for chemical composition, Blaine fineness, sieve analysis, and water demand.

For the evaluated scenario, explainable AI analysis revealed that loss-on-ignition (a limestone proxy) and particle-size/surface-area metrics were the most important predictors of strength variability. In contrast, clinker oxide features were of low importance, largely due to the stable clinker production in this specific case. For operators, this promises actionable insights, as fluctuations in strength stem primarily from milling conditions and limestone dosing. This points to specific process improvements rather than to vague recommendations for optimizing the blend.

Real-Time Quality Control

Even with predictive blend models, cement producers face a final challenge: they cannot wait 28 days – or even 24 hours – to know if today's production met specification. What is needed is real-time inference of product quality from readily measurable process variables.

Mihnea Stefan, also working at the University of Padua and at Fuller Technologies, is developing an adaptive soft-sensor framework to predict the alite fraction in clinker production, among other clinker properties. Traditionally, alite is determined through offline X-ray diffraction (XRD) analysis, which introduces delays and limits sampling frequency. But modern cement plants collect hundreds of online measurements at high frequency, including kiln temperature, torque, gas composition, and material flow rates, that retain the "fingerprint" of clinker quality.

Stefan's soft sensor uses a quasi-ensemble Partial Least Squares modeling framework that self-adapts as plant operational conditions evolve. A key innovation relates to the quasi-ensemble approach: the system creates multiple sub-models with independent hyperparameter settings, then selects a set of predictions using a given set of decision rules to achieve high model accuracy.

Variability among sub-models provides operators with a measure of prediction uncertainty: a critical factor for deciding whether to trust the output. For producers, this means the soft sensor can complement rather than replace laboratory testing, providing real-time estimates between

Deploying AI-based blend optimization will require laboratory infrastructure capable of providing reliable, well-structured sample data. Photo: Fuller Technologies

laboratory samples, enabling faster process adjustments.

Optimizing Raw Material Processing

Machine learning can predict product quality from process data, but it cannot eliminate the fundamental challenge: if input materials are inconsistent, the output will be too. For calcined clays, this problem begins at the thermal activation stage.

Wang Qun, working between Fuller Technologies, the University of Grenoble Alpes in France, and the University of Aberdeen in the UK, is developing a systematic framework for modeling the kinetics of kaolinite dihydroxylation: the process by which clay minerals lose structural water and become pozzolanic. Dihydroxylation behavior varies significantly with clay mineralogy, necessitating models that accommodate this diversity.

Wang's framework evaluates multiple kinetic modeling methods using thermogravimetric data collected at different heating rates, comparing them not only on fitting accuracy but on their ability to generalize beyond the experimental heating profiles.

This is critical for predicting how different clays will behave under industrial flash calciner conditions, where heating rates and temperature profiles differ substantially from those in laboratory furnaces. For producers concerned with high variability in clay composition from their local deposits, a well-validated kinetic model provides a faster answer than trial-and-error experimentation and feeds into the broader DETOCS vision of creating digital twins of SCM production processes.

The Deployment Challenge

These advances compress feedback loops that have historically constrained SCM adoption. But translating research results into industrial deployment requires more than algorithms.

For example, the difference between a machine learning model that works and one that fails often comes down to whether measurement time and sampling time are correctly distinguished: a distinction that matters little in traditional quality control but is critical when training predictive algorithms.

"As producers introduce novel SCMs with variable chemistry and mineralogy, the analytical demand increases," observed Jens Asbjørn Pedersen, global product manager for Fuller's QCX laboratory solutions.

According to Pedersen, prediction models rely on reliable, well-structured sample data – typically achieved with fully automated production laboratories that handle the entire process from sample collection through preparation to analysis. "This complete setup allows for high sample throughput while minimizing the risk of human error," he said. For demanding applications that require frequent sampling and short turnaround times, online analytical equipment (XRF, XRD, or particle-size analyzers) installed near sample points may supplement the central laboratory.

"In short, you need more frequent sampling, tighter control of sample preparation procedures, and rigorous data timestamping so that analytical results can be correctly matched to process conditions. Laboratory automation and data management systems thus play a critical role in making AI-driven quality control viable."

Regulatory approval presents another barrier. Even if a producer can demonstrate through predictive modeling that a novel blend will meet performance specifications, cement standards in most markets remain prescriptive rather than performance-based. A blend that falls outside the compositional limits defined in standards may require formal testing, documentation and approval processes that extend over months or years, regardless of how accurately AI models predict its behavior.

“AI should not be seen as a panacea,” Dr. Leal da Silva emphasized. “It is a powerful tool, but it requires a strong foundation: good data, sound chemistry knowledge, and operators who understand both the process and the models. When those elements are in place, the potential is enormous. But the technology alone is not sufficient.”

The Road Ahead

One of the DETOCS research programs is examining these non-technical and regulatory barriers hindering sustainable solutions in cement and concrete. The program promotes performance-based design standards, citing Latin American markets such as Colombia and Mexico, where general-purpose cement with high SCM fractions is already commercially available.

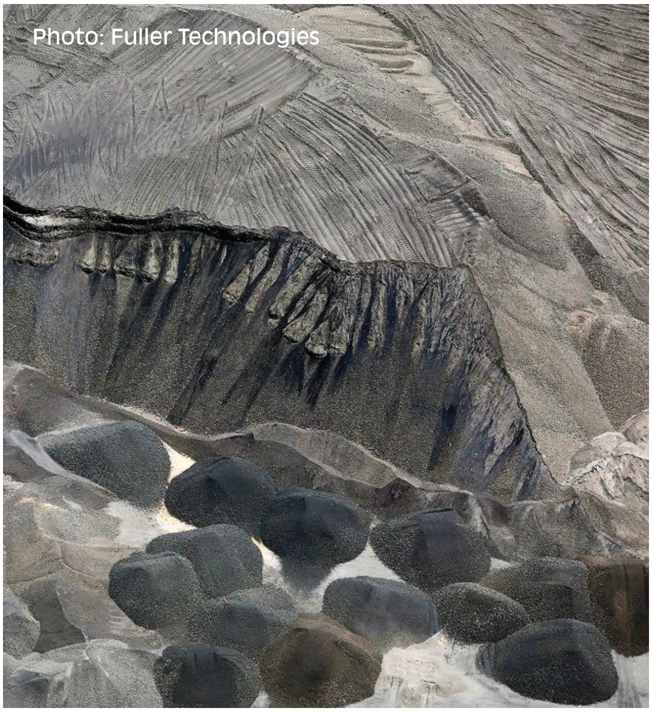
“We are studying these markets to understand how non-technical challenges can be overcome to generate new workflows, business models, and marketing tools that promote the deployment of novel SCMs and low-clinker cement blends,” Dr. Leal da Silva explained.

Will AI-accelerated validation change the relationship between research organizations, standards bodies, and the market – and thus facilitate faster SCM adoption? This is a “tough question,” Dr. Leal da Silva acknowledged. While he is confident that AI-accelerated validation will make cement plants more adaptable to new raw materials and reduce the need for extensive experimental campaigns, structural challenges are likely to hamper an immediate transformative shift.

In the short term, AI-informed models will “become an essential – and probably unavoidable – part of the production process,” with focus on reducing operating costs and emissions while extending the service life of existing equipment. Standards bodies and market adoption will adapt “more slowly, say, beyond five years, given the responsibility that comes with the use of cement.”

What seems clear is that the status quo is increasingly misaligned with the pace of decarbonization required. If the industry is to reduce its clinker factor and emissions within this decade, it will need tools that can compress validation timelines while maintaining rigorous performance standards.

The early DETOCS results suggest that such tools are within reach. Whether they can be scaled from research datasets to global industrial deployment remains to be demonstrated. But for an industry that has historically relied on rather conservative blend designs (with some exceptions) and remains bound by technical standards, even the possibility of data-driven, AI-accelerated material qualification represents a significant shift.



Novel SCMs such as calcined clays are more variable than traditional fly ash and slag, posing new challenges for blend optimization and quality control.

As Dr. Leal da Silva puts it: “We are trying to equip the cement industry with better tools: tools that let cement plants move faster, test more formulations, and make data-driven decisions. If we can do that, we can accelerate the transition to low-carbon cement without compromising quality or safety. That is the ambition.”

Note

An LC3-50 blend typically comprises 50% clinker, 30% calcined clay, 15% limestone, and 5% gypsum.

Acknowledgement

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