ISSUE #5

Jun 2026

DETOCS Newsletter

Data **E**nabling **T**ransformation and **O**ptimization towards **C**oncrete **S**ustainability

DETOCS

Here's what has happened in the last quarter and what's to come!

Welcome to the quarterly DETOCS newsletter! We are excited to share the latest project milestones, details of training events, and give our doctoral candidates the opportunity to shed some light on their ongoing research.

A project meeting was held in April to discuss the progression of the individual projects with all of the project partners and collaborators. The last quarter has seen most of the DCs enter the third year of their projects, shifting the focus towards summarizing results, writing papers, and the path towards wrapping up their theses. One of the journal was recently published in Cement and Concrete Research, titled **"Strength performance and environmental assessment of Portland clinker"**, authored by DC15 (Pippa Edwards) and her collaborators.

A CEMulator® course, hosted by Fuller Technologies in Copenhagen, was held for a subset of the DCs in May. A comprehensive summary of the course is included in this edition.

The DCs have also continued attending conferences, including ESCAPE36 in Sheffield, UK and the 53rd International Conference on Computer Coupling of Phase Diagrams and Thermochemistry in Quebec City, Canada. This issue also contains accounts of the DCs' experiences at these conferences, as well as a description of the work that they presented there.

Enjoy this quarter's newsletter!

— Sruthi Sreeram, DC3

In this newsletter you will be briefed on:

Cement Production Seminar with CEMulator®: Pyroprorcess and Grinding

M. Stefan, DC9

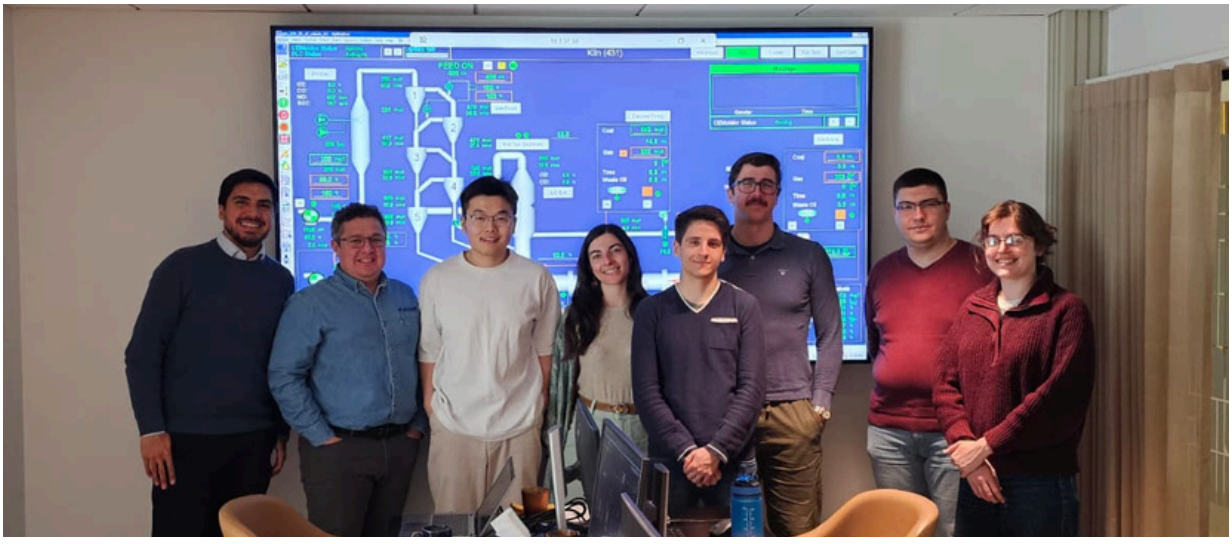
In May 2026, a subset of DETOCS Doctoral Candidates and their supervisors participated in the CEMulator® Cement Production course led by Boris Salazar (Senior Field Service Engineer) at Fuller Technologies in Copenhagen, Denmark. The course provided a valuable lessons on cement plant operation through a combination of theoretical learning and hands-on simulator-based training for both pyro and grinding stages in cement production. The participants were introduced to the role of cement plant operators, where they experienced, in a simulated environment, the operational complexity cement production: helping connect theoretical knowledge with practical industrial reality.

The theoretical part of the course introduced the fundamentals of pyro and grinding processes from a first-principles perspective, explaining how the main process elements function and key process variables influences during material processing. Next, the practical part of the course took place using Fuller Technologies' advanced process simulator (i.e. CEMulator®), the same type of tool used for operator training. Through this simulator, the participants gained experience in steady-state operation, production ramp-up, process start-up, anomaly detection, and corrective actions to control the process. These exercises made the training particularly engaging and allowed the DCs to apply the concepts learned during the theoretical sessions in a realistic operational setting.

The experience was especially relevant for the projects of DC9, M. Stefan, and DC11, T. Kalb. Both projects are closely connected to process operation, control, and modelling, with a focus on machine learning for control, explainability, optimisation, and quality monitoring in cement production. Besides, DCs 1, 2, and 15 also joined the course since their industrial research on clinker phase formation, thermodynamics, pyroprocessing, and life cycle assessment are closely connected to cement production and quality control.

For DC9's industrial research project - focuses on soft-sensor development for quality monitoring and prediction - the course offered important practical insight. By interacting directly with the pyro process during various production scenarios, I gained a more functional understanding of how different process variables affect clinker quality. This perspective is valuable for feature selection, signal time alignment, and the interpretation of process dynamics. The hands-on experience also helped clarify how changes introduced in one part of the plant, e.g. the preheater tower, propagate through the kiln and flame and ultimately influence the quality of the final product.

The participants would like to thank the DETOCS project and Fuller Technologies for making this valuable training opportunity possible. A special thanks for Boris Salazar for his patience and enthusiasm through the whole course. The course not only broadened academic and professional perspectives, but also created a positive environment for interaction between DCs and instructors, encouraging discussion, exchange of ideas, and the development of meaningful professional connections.



53rd International Conference on Computer Coupling of Phase Diagrams and Thermochemistry: A Summary

Ramon Bandak, DC1

I attended a Calculation of Phase Diagrams (CALPHAD) conference for the first time, the 53rd International Conference on Computer Coupling of Phase Diagrams and Thermochemistry, held in Québec city, Canada. This experience was valuable for my research because the methodology of CALPHAD is the way to predict clinker mineralogy, which forms the basis of my project. I had the opportunity to present part of the coupled experimental and modelling work in the ternary system CaO-MgO-SiO_2.

The chemical base of any OPC cement is the CaO-SiO_2 binary system. Specifically, the two key compounds tricalcium silicate (Ca_3SiO_5) and dicalcium silicate (Ca_2SiO_4). In cement, they are called alite and belite respectively, due to minor elements presence in the crystal structure. The motivation of this work is that the availability of high-purity natural limestone ($CaCO_3$), the main raw material for cement production, is decreasing while higher dolomite ($CaMg(CO_3)_2$) quantities are present, leading to higher MgO in the future cement. From a chemical perspective, this leads to MgO insertion in alite and belite with a considerable impact on their reactivity behavior in the final cement product.

This underscores the importance of CALPHAD, which has the ability to handle multicomponent systems better than the current industrial standard to predict mineralogy - Bogue's equations - when the databases are available. The work presented used the latest thermodynamic datasets in literature as a starting point and added to it by modelling the solid solubilities of MgO in the CaO-rich area, specifically, in Ca_3SiO_5 and the high temperature a' and a-Ca_2SiO_4 polymorphs. Our new modeling was compared to the available ones in literature and commercial databases (FToxid, GTOX for FactSage). Finally, an interesting result to note was that the datasets in the commercial databases give different results in the CaO-rich region. FToxid v8.4 is not in agreement with the fact that Ca_3SiO_5, Ca_2SiO_4 and MgO are simultaneously observed in true cement clinker samples, and GTOX v8.4 does not include solid solubility into alite.

This new modeling work will be the base of a database to include alternative fuel induced minor elements into the major OPC clinker mineralogical phases, reducing variability and directly lower energy consumption and emissions in clinker production.

ESCAPE36: European Symposium on Computer Aided Process Engineering

Mihnea Stefan, DC9

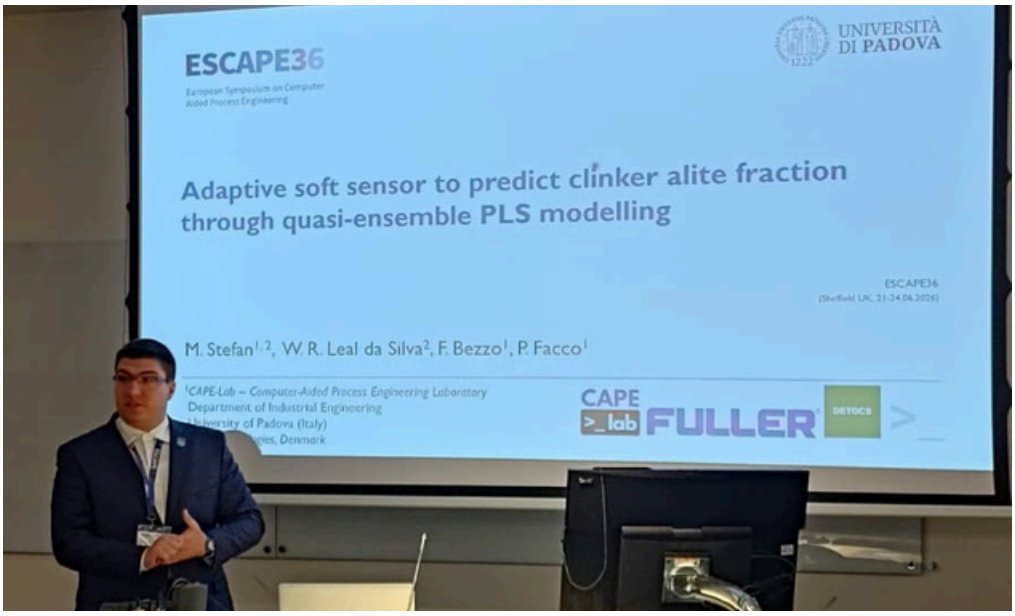
Between 21 and 24 June 2026, I participated in ESCAPE36 in Sheffield, UK. ESCAPE36, the 36th European Symposium on Computer Aided Process Engineering, is one of the main European conferences in the CAPE field, and attending it was a valuable opportunity to present and discuss my research.

The programme combined oral presentations, poster sessions, plenary lectures, and workshops. The topics covered a broad range of areas, including modelling and simulation, concepts, methods and tools, and CAPE applications in clean energy systems.

During the “Concepts, Methods and Tools” session, I presented my work titled Adaptive soft sensor to estimate alite fraction in clinker production through quasi-ensemble PLS modelling. The work addresses the challenge of monitoring quality indices in drifting, highly dynamic industrial processes, using clinker production as a case study. Many conventional soft sensors are static: they are trained once, deployed, and gradually lose accuracy as process conditions change. Also modern soft sensors are based on neural networks that not only are static but also black box in nature and cannot be interpreted from a process points of view In contrast, the proposed approach combines the interpretability of PLS modelling with the adaptability of Just-in-Time learning to give birth to a recursive-adaptive sensor, ALD-PLS. The performance of this novel modelling approach is dependent on a relatively large number of interconnected hyperparameters. The choice of their value is critical for the proper operation of the sensor; hence a key part of the proposed methodology is Quasi-Ensemble PLS, which builds multiple ALD-PLS sub-models across physically meaningful hyperparameter combinations. Their predictions are averaged into a final ensemble estimate, while the variability between sub-models provides a measure of prediction uncertainty. The method showed strong performance on real alite fraction data collected from a cement production plant.

Beyond my own presentation, the conference offered many stimulating sessions. One particularly memorable plenary lecture was delivered by Dr. Jan Rittig from RWTH Aachen University on graph machine learning for molecular property prediction and design. The talk presented how molecular structures can be encoded using graph neural networks and how thermodynamic consistency can be embedded directly into model training.

Overall, ESCAPE36 was an inspiring and intellectually enriching experience. It offered exposure to new research directions, valuable scientific discussions, and opportunities to expand my academic network.



The work presented at this conference, titled “Adaptive soft sensor to estimate alite fraction in clinker production through quasi-ensemble PLS modelling” can be accessed here.

Interview: Cement Optimized

With Dr. W. R. Leal da Silva

The research project coordinator for the DETOCS project, Dr. Wilson Ricardo Leal da Silva, was one of two experts interviewed recently by Jonathan Rowland for an issue of Cement Optimized, speaking about the use of digital tools and AI for faster SCM adoption.

The interview discussed the motivations behind the project, the different bridges being constructed to enable the effective usage of plant data in predictions centered around low-carbon cement blends and concrete mixes through the different DC projects, challenges faced, and the road ahead. An excerpt from the interview can be found below:

"

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.*

"

The full interview can be found here.

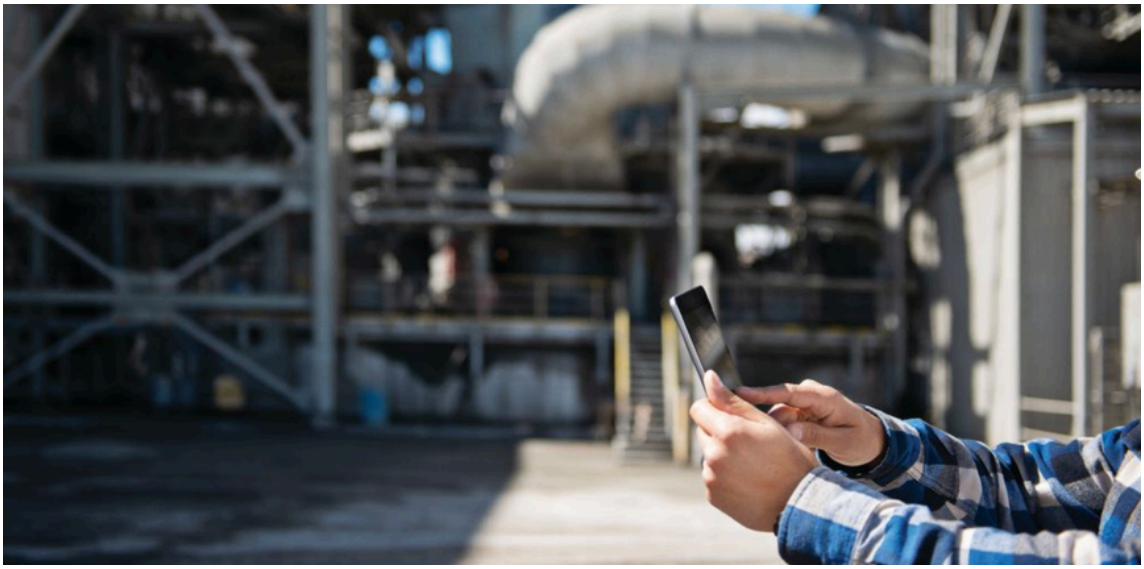


Photo: Fuller Technologies

This project is supported by multiple academic institutions and industrial partners, who are all working together to ensure a more sustainable future for the cement and concrete industry.

Funded by the European Union

This project has received funding from the European Union's Horizon Europe research and innovation programme under the Marie Skłodowska-Curie grant agreement No 101119929. Funded by the European Union. Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union or European Research Executive Agency (REA). Neither the European Union nor the REA can be held responsible for them.

Thank you for reading!

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