CRYSPOM 25

IX International Workshop on Crystallization in Porous Media

Barcelona
17-19 September 2025

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PROGRAM

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Wednesday 17th September	*C1 building, 2nd floor, Zienkiewicz room*	
9:00 – 9:30	Registration	
9:30 – 9:40	Opening CRYSPOM 25	
	Fundamentals of salt crystallization in porous or confined media & imaging tools Chairwoman Hannelore Derluyin	
9:40 – 10:20	**Noushine Shahidzadeh, R.J. Wijnhorst and Marc Prat**	**Keynote lecture - Self similarity in salt creeping efflorescence crystallization**
10:20 – 10:40	Yousra Haddad Belfkih, Stéphane Veesler, Romain Grossier, Miguel Ángel Durán-Olivencia and Alexander Van Diessche	The combined effect of additives and confinement on nucleation kinetics: synergism or antagonism?
	Coffee break	
11:10 – 11:30	Georgiy Baroncha, Rustem Valiullin and Eustathios Kikkinides	Relating phase transitions of confined materials and topology of pore network
11:30 – 11:50	Mykyta V. Chubynsky, Nihal M. Habeeb, Fatima-Zohra Sahraoui, Haida Liang, Lucas Goehring, Pascale Sénéchal, Hannelore Derluyn, David Thickett and Ran Holtzman	Pore-scale modelling and experiments of evaporation-induced salt precipitation
11:50 – 12:10	Maarten W. Saaltink and M. Carme Chaparro	Mineral precipitation and dissolution in concrete. A modelling study of the radioactive waste disposal facility at El Cabril, Spain
	Lunch	
	Crystallization in engineering problems Chairwoman Anja Diekamp	
13:40 – 14:20	**Eduardo Alonso and Anna Ramon**	**Keynote lecture - Tunnel lining design in expansive anhydritic claystone**
14:20 – 14:40	Mohammad Nooraiepour, Mohammad Masoudi, Hannelore Derluyn, Pascale Senechal, Peter Moonen and Helge Hellevang	Role of continuous brine access on salt precipitation dynamics - Implications for injectivity and containment integrity during geological CO_2 storage
14:40 – 15:00	Nicolò Tognon, Giovanna, Xotta, Carlos M. López, Daniel Garolera and Ignacio Carol	Concrete expansions caused by secondary ettringite crystallization during external sulphate attack (ESA)
15:00 – 15:20	Vincenzo S. Vespo, Liliana Gramegna, Adriano Fiorucci, Gabriele Della Vecchia and Guido Musso	Deformation behaviour of a carbonate clay subjected to calcite and dolomite dissolution in acidic environment
15:20 – 15:40	*CRYSPOM Meeting*	
17:30 – 19:30	**Guided visit to the National Museum of Catalunya's Art (MNAC Museum)** How to arrive to MNAC Museum: https://www.museunacional.cat/en/getting-here	

Thursday 18th September *D2 building, 3rd floor, Geology room 304*		
Crystallization in Crystallization in Heritage monuments, buildings and arts Chairwoman Paula Carmona-Quiroga		
9:00 – 9:40	**Pere Rovira and Lucía Fernández**	**Keynote lecture - The problem of the salts in the conservation of the historic and artistic Heritage**
9:40 – 10:00	Sotiria Kogou, Yu Li, C. S. Cheung, X. N. Han, Florence Liggins, Golnaz Shahtahmassebi, Haida Liang and David Thickett	Integrated remote sensing and machine learning for salt detection and analysis on heritage monuments
10:00 – 10:20	V A Anupama, Pascale Sénéchal, Manu Santhanam and Hannelore Derluyn	Understanding salt weathering in khondalite through mineralogy and microstructure
10:20 – 10:40	Érika v. Bedoya; Jose Carlos Morgado and Lluís Aranda	Study of a case of efflorescence in building constructions
Coffee break *D2 building, 2nd floor, Seminars' room 216*		
11:00 – 11:30	Joan Martinez-Bofill, Àngels Canals, Neus Otero and Sandra Amores	Application of isotopic techniques to determine the origin of sulphate neoformation: A case study from Barberà de la Conca, Spain
11:30 – 11:50	Bilal M. Hawchar, Tulio Honorio, Matthieu Vandamme, Florian Osselin, Jean-Michel Pereira, Lionel Mercury, and Laurent Brochard	Fluorescence-based detection of crystallization pressure in microfluidic channels
11:50 – 12:10	Jade Genetelli, Xavier Dollat, Fabien Menilgrente, Antoine Naillon, Marc Prat and Pierre Joseph	Crystallization of sodium chloride in microfluidic pore systems
12:10 – 12:30	M. la Bella, M. Sarkis, C. Noiriel, J. Ball, H. Fang, J. Wright, F. Emeriault, C. Geindreau and A. Naillon	Insights on the textural and crystallographic properties of calcite obtained through MICP using scanning 3D X-ray diffraction
Lunch + PHOTO *D2 building, 2nd floor, Seminars' room 216*		
Crystallization applied to new or advanced materials for construction, bio-engineering and medicine Chairman Vincenzo Sergio Vespo		
14:00 – 14:40	**Rosa María Espinosa Marzal**	**Keynote lecture - Learning from coral biomineralization to engineer (living) materials**
14:40 – 15:00	Jan Grzelak, Ines Bueso-Inchausti, Anna Cloeren and Maria-Pau Ginebra	Engineering antimicrobial calcium phosphate nanocrystals for enhanced bone regeneration
15:00 – 15:20	P.M. Carmona-Quiroga and M.T. Blanco-Varela	On the role of BaCO3 on preventing sulphate attack on Portland cement concrete
15:20 – 15:40	M. la Bella, C. Noiriel, L. Schröer, V. Cnudde, F. Emeriault, C. Geindreau and A. Naillon	Assessment of the durability of bio-cemented sand exposed to acidic conditions by X-Ray µ-tomography
Coffee break *D2 building, 2nd floor, Seminars' room 216*		
16:10 – 16:30	Imren Basar and Lucía Fernández	Crystallization phenomena in the pore network of lime binders incorporating natural additives
16:30 – 16:50	N. Cotón, A.K.M. Morita1, R. Fernández, C. Mota-Heredia, J. Alonso-Azcárate and J.M. Moreno-Maroto	Zeolite crystallization within pores as a disruptive method for developing advanced and sustainable construction materials

16:50 – 17:50	**Poster Session**	
	Khadijeh Zare, Lucas Goehring and Ran Holtzman	MRI-based Investigation of Gas Hydrate Crystallization in Porous Media
	Arianna Paschetto, Chiara Caselle and Anna Ramon.	Multiscale investigation of crystallization-induced swelling in anhydrite
	Annika Leonie Franzmann, Sabrina Jungmann, Andreas Schretthauser and Anja Diekamp	Hydration-Driven Transformations of Magnesium Sulfate Salts and Their Role inDolomitic Lime Weathering in Historic Monuments
	Blanca Zarzalejos Vicens, Miguel Gómez Heras and Encarnación Ruiz Agudo	Salt crystallization modifiers in porous media contaminated with salt mixture
20:00 – 23:00	**Workshop dinner**	

Friday 19th September	*C1 building, 2nd floor, Zienkiewicz room*	
	Crystal growth in cementitious materials Chairman Jose Manuel Moreno-Maroto	
9:00 – 9:40	**Michael Steiger**	**Keynote lecture - Deliquescence and hygroscopic properties of salt mixtures**
9:40 – 10:00	Joaquín Liaudat, Carlos M. López and Ignacio Carol	Multi-Scale investigation and modelling of Alkali-Silica Reaction in concrete under confinement
10:00 – 10:20	Marcelo Laviña, Andrés Idiart, Virginia Cabrera, Benoit Cochepin, Nicolas Michau and Jean Talandier	Sulphate attack and chemical damage in concrete structures in deep geological repositories for nuclear waste storage
10:20 – 10:40	Marilda Barra, Susanna Valls and Diego Aponte	Sulphate Attack in cement-stabilized materials: Influence of slate-containing recycled aggregates
	Coffee break	
11:00 – 11:30	Lucía Fernández, Abigail Jimenez and Pouria Nouri	Pore crystallization in carbonated low-clinker cements reinforced with nonwoven textile fibers
11:30 – 11:50	Micha Baur, Nikolaos Prasianakis and Sergey Churakov	High Performance Pore Scale Reactive Transport Model for Cement-Claystone and Cement-Iron Interface Interactions
12:10 – 12:30	**Closure**	

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Self similarity in salt creeping efflorescence crystallization

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Keywords: Crystallization, evaporation , efflorescence, fractal, self-assembly, porous media

Salt creeping is a phenomenon where salt crystals continue to precipitate far from an evaporating salt solution by a self-amplifying mechanism. Due to multiple nucleation sites of crystallization at the evaporation front , the spreading of the salt solution is enhanced well beyond the initial liquid/air front and creates a self-amplifying process[1]. The process results in three-dimensional crystalline networks at macroscopic distances from the salt solution . Such crystallization process can initiate and grow on flat surfaces and on the surface of porous materials such as soil or stones, known as salt efflorescence. The latter poses significant challenges in cultural heritage conservation, materials degradation such as frescoes or wall paintings and soil sodification, due to the ability of salt solutions to infiltrate porous materials through capillary rise from groundwater, followed by evaporation and crystallization as efflorescence at the surface of the porous material. Here we investigate the mechanisms for the formation of NaCl efflorescence focusing on the emergence of self-similar, cauliflower-shaped structures [2-3]. Through controlled evaporation experiments of salt creeping and micro-scale analysis of the resulting salt deposit, our results reveal a hierarchical organization of cubical micro crystals within the efflorescence structure. Scanning electron microscopy images, X-ray microtomography results, and fractal dimension analysis reveal the intricate structure and self-similar patterns of the cauliflower-shaped efflorescence. Our finding reveals that salt creeping crystallization height are primarily governed by the initial salt mass available, rather than by the competition between capillary and viscous effects within the porous efflorescence structure. Our findings shed some light on how mineral precipitation and growth self-organizes into macroscopic hierarchical structures such as salt efflorescence on top of porous materials. The phenomenon can also lead to spectacular macroscopic salt deposit structures, such as desert roses in arid desert regions or salt pillars near saline lakes in nature.e.

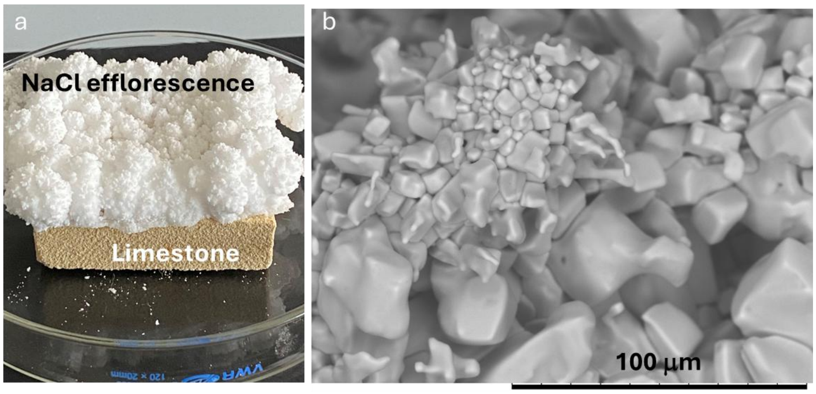

FIG. 1. (a) NaCl Efflorescence on top of a Limestone sample; (b) self-similar salt deposit at the microscale .

References:

1- Qazi, M. J., Salim, H., Doorman, C. A. W., Jambon-Puillet, E., & Shahidzadeh, N. (2019). Salt creeping as a self-amplifying crystallization process. *Science advances*, *5*(12), eaax1853.
2- Wijnhorst, R. J., Prat, M., & Shahidzadeh, N. (2025). Self-similarity in creeping salt crystallization. *arXiv preprint arXiv:2508.18779*.
3- Wijnhorst , R., Salt Crystallization in Cultural Heritage. From Fundamentals to Deterioration, PhD manuscript 2024.

The combined effect of additives and confinement on nucleation kinetics: synergism or antagonism?

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Keywords: Induction time, Nucleation, Crystallization, Microfluidic, Confinement

Mineral precipitation is a multiscale process from geological scales (GL) down to picoliters (pL). In confined environments, the crystallization of soluble salts within porous materials is one of the major causes of rock decay in nature (Charola, 2000); its nucleation kinetics, whether controlled or unwanted, are strongly influenced by chemical additives. While the effect of additives alone is extensively studied, the combined influence of additives and reaction volume (confinement) remains largely unexplored. This study aims to unravel how confinement modulates the effect of additives on the nucleation kinetics of gypsum ($CaSO_4.2H_2O$).

To achieve this, gypsum precipitation induction times were determined across different solution volumes using two complementary high-throughput methodologies at 20 °C. Firstly, nucleation in a bulk environment was assessed using a multicell UV-Vis spectrophotometer setup (Ramírez-García et al., 2022). Equivolume solution of Na_2SO_4 and $CaCl_2$ were mixed in 2 mL cuvettes (continuously stirred at 800 rpm) to achieve final concentrations ranging from 30 mM to 150 mM $CaSO_4.2H_2O$. Induction times were defined as the interval between mixing and the first detectable change in absorbance, automatically identified using a custom Python script.

Secondly, nucleation in confined microscale environments was studied using a microfluidic platform (Candoni et al., 2019). Droplets with a volume of 0.77 µL were generated by mixing equivolume solutions of Na_2SO_4 and $CaCl_2$, stored in a spiral tube, and optically monitored. Each droplet acts as an independent batch crystallizer, allowing for statistically significant data collection. Crystallization events within individual droplets were detected using automated image analysis via a Python script. Initial $CaSO_4.2H_2O$ concentrations in the microfluidic setup ranged from 60 mM to 90 mM in additive-free experiments.

Next, the influence of additives was investigated using both platforms under specific conditions: 70 mM gypsum with 50 ppm of tri-sodium citrate dihydrate; 70 mM gypsum with 50 ppm of malic acid; and 70 mM gypsum with 50 ppm of sodium hexametaphosphate.

This presentation will summarize the key findings, comparing nucleation kinetics between bulk and confined volumes, both with and without additives. The results will directly address whether the combination of confinement and additives leads to synergistic or antagonistic effects on gypsum nucleation.

References:

Candoni, N., Grossier, R., Lagaize, M. and Veesler, S., 2019. Advances in the use of microfluidics to study crystallization fundamentals. *Annual Review of Chemical and Biomolecular Engineering*, **10**(1), pp.59–83. https://doi.org/10.1146/annurev-chembioeng-060718-030312

Charola, A. E., 2000. Salts in the Deterioration of Porous Materials: An Overview. *Journal Of The American Institute For Conservation*, **39(3)**, pp. 327-343. https://doi.org/10.1179/019713600806113176

Ramírez-García, P., Durán-Olivencia, M.A., Kellermeier, M. and Van Driessche, A.E.S., 2022. Determining the operational window of green antiscalants: A case study for calcium sulfate. *Desalination*, **544**, pp.116-128. https://doi.org/10.1016/j.desal.2022.116128

Relating phase transitions of confined materials and topology of pore network

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Keywords: Phase transitions; Network models; Pore size distribution; Average connectivity; Pore network topology; Statistically-disordered & correlated structures.

Measuring adsorption/desorption and melting/freezing transitions in porous materials is a common route to obtain information about pore structure. Often it is done by reducing the pore space to a simple collection of individually idealized pores, such as bundles of cylinders with different pore sizes. In this way, the network effects become fully ignored. To describe phase transition behavior in porous solids with complex pore space architectures we exploit statistical network models including cooperative effects emerging due to interpore connectivity. By considering statistically-disordered random-branching Bethe lattices we show that in addition to more accurate pore size distributions also the average pore connectivity can be assessed. Furthermore, we show that beyond average connectivity, phase transitions are largely insensitive to finer topological details of the pore network.

Pore-scale modeling and experiments of evaporation-induced salt precipitation

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Keywords: Salt precipitation, Evaporation, Heritage, Pore-scale, Pore network modeling, X-ray micro-computed tomography

Fluids move in a porous material with an ease that depends on the size and connectivity of its pores [1]. Flow-induced precipitation of solids (e.g. salts, carbonates, gas hydrates) is controlled by the feedback between fluid flow and the alteration of transport properties [2]. While these mechanisms are influenced by microstructural heterogeneity at the pore (micron to cm) scale, their impact is felt at scales of meters and above [1,2]. We develop a modeling platform, based on a computationally-efficient pore-network approach, that aims to perform this upscaling. The model is trained and validated by laboratory mock-ups – glass bead samples soaked in brine and left to dry under controlled environmental conditions. We use both time-lapse photography of quasi-2D bead monolayers as well as micro-CT imaging of 3D samples. Our approach can provide a method to predict salt buildup in cultural heritage applications, as well as advance understanding of other processes such as mineralization in carbon geosequestration.

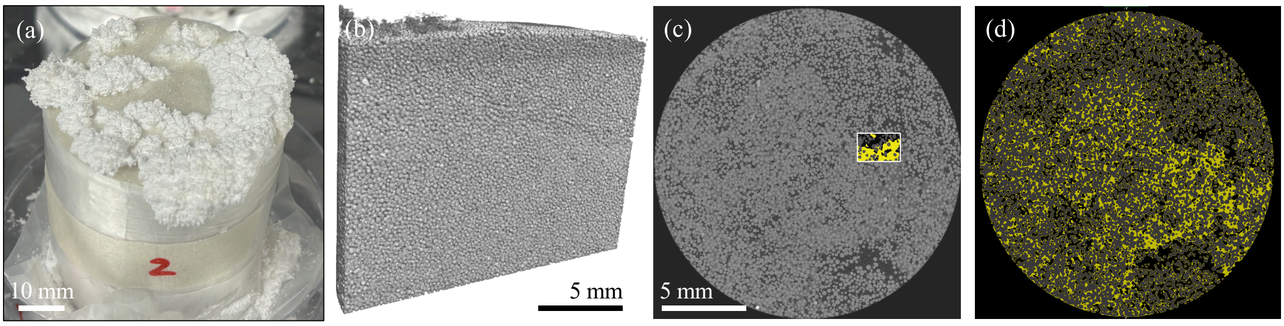

FIG 1: Visualizing salt precipitation in 3D samples. (a) Fully dried specimen, contaminated by sodium sulfate, displaying extensive efflorescence. (b) Transverse section of a 3D micro-CT tomogram (10 μm resolution). (c) Horizontal slice of the same tomogram, after pre-processing (training region highlighted). (d) Fully processed and segmented slice, showing salt (yellow), beads (grey) and air (black).

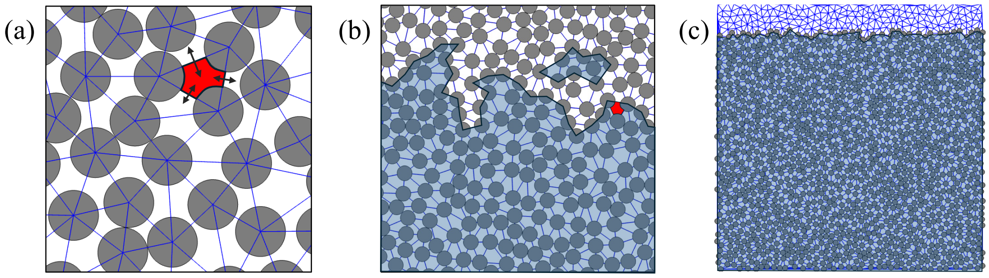

FIG 2: Model setup (in 2D). (a) A porous stone is approximated by a set of grains. A triangulation of their centres yields a network of pores (white areas) connected by throats (blue lines). An exemplar pore (red) can exchange material (arrows) with 3 neighbours. (b) The simulation follows the evolution of the air/water interface. An invaded pore (red) releases water into all wet pores connected to it. (c) Initially, all pores are wet, except for a thin boundary layer of air.

References:
[1] Pore Scale Geochemical Processes (eds Steefel, C. et al.), De Gruyter, 2015.
[2] Seigneur, N. et al. Rev. Mineral. Geochem. 85, 197, 2019.

MRI-based Investigation of Gas Hydrate Crystallization in Porous Media

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Keywords: Crystallization, Gas hydrates, Imaging, Porous media

The formation of gas hydrates, where gases (e.g. CO_2 or CH_4) mix with water to form crystalline ice-like solids, can clog the pore space in sediments, inhibiting further flow, mixing and reactions. CO_2 hydrates can form during carbon geosequestration, as CO_2 rapidly expands, impeding the efficiency of the sequestration operations. Despite its crucial importance, the two-way coupling between (i) flow, mixing and (ii) transport property alteration due to the hydrate formation remains poorly understood.

We present Magnetic Resonance Imaging (MRI) experiments of tetrahydrofuran (THF) hydrate formation in model porous media. Analysis of flow-through experiments within an MRI chamber are used to correlate spatial hydrate distribution with transport properties, as they evolve dynamically in time. Our methodology produces unique 4D data from which we quantify hydrate saturation and structure. These findings will support pore-network simulations, which will provide a quantitative link between the dynamics of hydrate formation and sample permeability, as they are affected by the evolving microstructure.

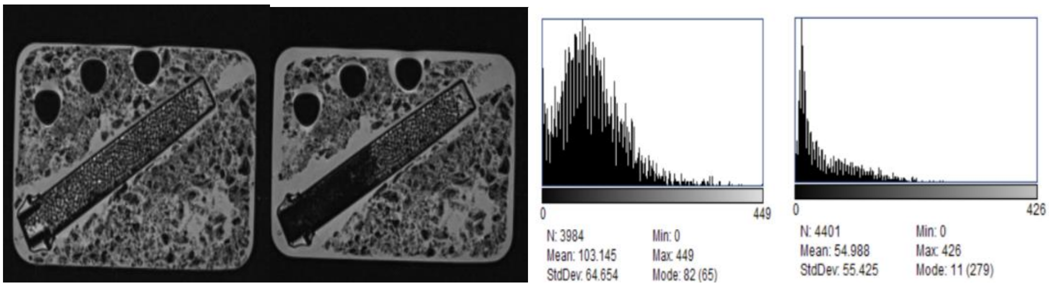

FIG. 1. MRI images (a-b) and signal intensity histograms (c-d) from a hydrate formation experiment in which we inject THF into water-saturated glass bead pack (a,c before and b,d after injection). Hydrate formation, shown as dark material in the lower half of the tube (b) is evident as signal loss in the histograms (d).

References:

Mahabadi, N., Dai, S., Seol, Y., Jang, J., 2018, Impact of hydrate saturation on water permeability in hydrate-bearing sediments, Journal of Natural Gas Science and Engineering, 58, 244–250.

Taylor, C. J., Miller, K. T., Koh, C. A., Sloan, E. D. Jr., 2007, Macroscopic investigation of hydrate film growth at the hydrocarbon/water interface, Chemical Engineering Science, 62, (23), 6524–6533.

Xue, K., Zhao, J., Song, Y., Liu, W., Lam, W., Zhu, Y., Liu, Y., Cheng, C., Liu, D., 2012, Direct observation of THF hydrate formation in porous microstructure using magnetic resonance imaging, Entropy, 14, (4), 698–707.

Zhao, Y., Lei, X., Zheng, J., Li, M., Johns, M. L., Huang, M., Song, Y., 2021, High-resolution MRI studies of CO_2 hydrate formation and dissociation near the gas–water interface, Journal of Natural Gas Science and Engineering, 91, 103950.

Mineral precipitation and dissolution in concrete. A modelling study of the radioactive waste disposal facility at El Cabril, Spain

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Keywords: Reactive transport, Multiphase flow, Concrete, Numerical model.

Two-dimensional numerical models, together with temperature and humidity measurements, suggested flow of water within the concrete of the radioactive waste disposal facility at El Cabril, Spain. The models suggested that this flow is caused by a combination of thermohydraulic processes occurring in the unsaturated concrete, such as capillary rise from the groundwater, evaporation, and condensation due to temperature gradients caused by seasonal temperature fluctuations outside. As these processes may affect the mineralogy of the concrete, 1D reactive transport models have been developed following the 2D thermo-hydraulic model. When minerals are controlled by fast kinetics, the model results show that the cement phases precipitate and dissolve, clearly following the yearly fluctuations of condensation and evaporation. However, when minerals are controlled by slow kinetics, the reactions are less affected by the hydraulic processes. The models suggest that precipitation-dissolution could be particularly important near an air gap in the concrete, where water condenses and evaporates more easily. More details of the models are given by Chaparro and Saaltink (2025)

References:

Chaparro, M. C., Saaltink, M. W., 2025, Modelling reactive transport in unsaturated concrete under evaporation and condensation processes, *Frontiers in Built Environment*, 11, 1601568, https://doi.org/10.3389/fbuil.2025.1601568.

Tunnel lining design in expansive anhydritic claystone

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Keywords: Back analysis, gypsum crystals, heterogeneity, rock expansion, structural model, tunnels

High swelling pressures (4 to 5 MPa) against a experimental curved invert of a tunnel under excavation in anhydritic claystone, were measured at an early stage of construction (Alonso et al., 2013). This information led to a heavily reinforced circular lining that was monitored for several years once the tunnel went into service. However, the measured lining stresses were not consistent with design expectations.

The presentation provides an explanation for the observed results. They could be explained by the spatial heterogeneity of swelling forces against the tunnel lining. The guiding idea to determine the intensity and spatial distribution of swelling forces was to perform a "back analysis" of the intensity and distribution of field forces so that they were capable of reproducing the internal lining stresses of reinforcement steel bars. The necessary model for this back analysis was a three-dimensional tunnel lining structure embedded in the swelling rock. The procedure provided useful information to estimate the field heterogeneity of swelling pressures, a necessary information for the design of tunnels and other structures in contact with the expansive anhydrite claystone (Alonso et al., 2023).

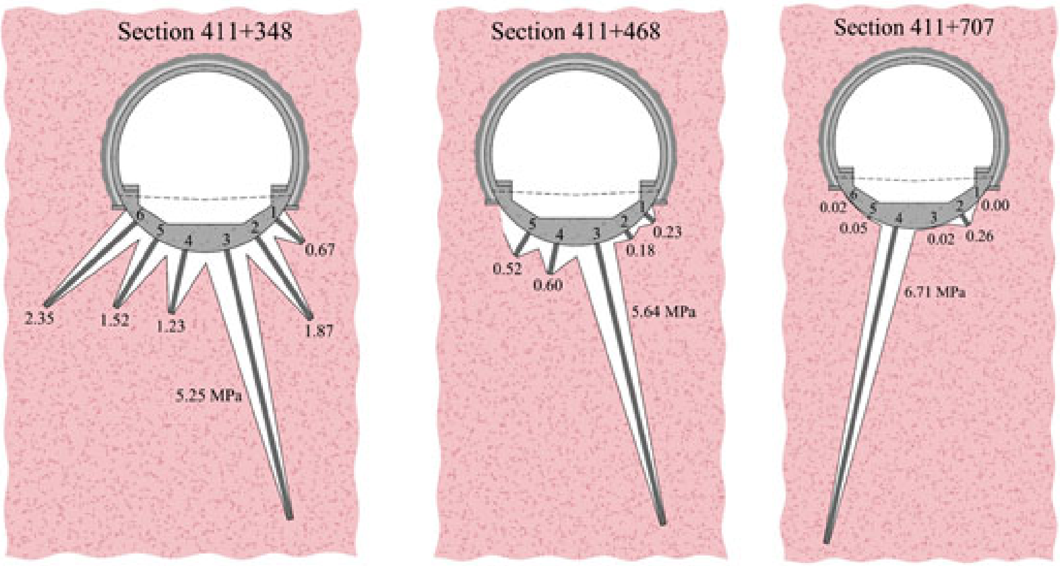

Figure 1. Recorded swelling pressures at three different cross sections at Lilla tunnel.

References:

Alonso, E.E., Berdugo, I.R. and Ramon, A. (2013). Extreme expansive phenomena in anhydritic-gypsiferous claystone: the case of Lilla tunnel. *Géotechnique* 63 No. 7, 584 – 612

Alonso E, Ramon-Tarragona, A. & Verda, L. 2023.Designing Tunnel Lining in Anhydritic Claystones. Intensity and Distribution of Swelling Forces. *Rock Mechanics and Rock Engineering* 56, 1467–1487.

Role of Continuous Brine Access on Salt Precipitation Dynamics ─ Implications for Injectivity and Containment Integrity during Geological CO_2 Storage

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Keywords: Mineral growth; Porous media; Probabilistic nucleation; Salt precipitation; Saline aquifer.

Geological carbon storage emerges as a critical strategy for mitigating climate change via capturing and storing human-made CO_2 emissions. Salt precipitation during CO_2 injection in saline aquifers can cause pore clogging near the wellbore, reducing permeability and increasing pressure buildup, which may find significant consequences for injectivity, containment integrity, and the overall safety and efficiency of CO_2 storage operations. While increasingly more literature focuses on CO_2-induced salt precipitation, the underlying physics, growth dynamics, and fluid-solid interface behavior remain elusive. This study investigates the role of continuous brine access on pore-scale salt precipitation dynamics, significance for self-enhancing growth nature, and its broader implications for injectivity and containment criteria. Using laboratory techniques, including microfluidics, a Hele-Shaw cell, a flow-through system, a large-scale sandbox setup, and a triaxial geomechanical cell we explore the mechanisms governing brine evaporation and salt crystal growth, their pore occupancy and chemo-mechanical couplings. A key finding is the critical role of continuous brine sources, which significantly alter salt nucleation and growth dynamics by controlling solute availability and continuity through water film movement. Laboratory results reveal substantial salt accumulation near the injection port, emphasizing the importance of solute availability in exacerbating salt accumulation severity. Two mechanisms accelerate growth dynamics. First, evaporation shifts the gas-liquid interface from larger to finer pores, expanding the surface area for brine evaporation and salt formation. Second, hydrophilic, hygroscopic halite crystals, nucleating on existing precipitates as secondary substrates via probabilistic nucleation, amplify reactive surface area and create a feedback loop. Salt crystallization can weaken reservoir rock, reducing mechanical strength and increasing susceptibility to shear failure. This weakening, evidenced by reduced Young's and shear moduli, may lower the fracture gradient, posing a risk of unintentional fracturing during injection. By elucidating the role of continuous brine access on precipitation dynamics and the interplay of hydro-mechanical-chemical processes, the research offers insights for optimizing injection strategies and enhancing containment integrity. The findings underscore the need to incorporate these mechanistic aspects into reservoir-scale models to predict better and manage the impacts of salt precipitation on subsurface injection operations.

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Concrete Expansions Caused by Secondary Ettringite Crystalization during External Sulfate Attack (ESA)

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Keywords: External sufate attack, meso-mechanics, coupled finite element analysis

External sulfate attack (ESA) is a chemical degradation process in concrete that may take place when concrete is in contact with water rich in sulfate ions with cement expansions and general degradation of the concrete. Sulfate ions diffuse into the concrete material through the cement pores, reacting with the aluminate products present in the hardened cement paste, and leading ultimately to the formation of ettringite crystals and overall volumetric expansion, which may lead to crack formation and spalling. In the numerical study presented in this work, concrete is represented at the meso-scale, as composed of aggregate particles numerically generated, embedded in a mortar matrix. The possibility of fracture is introduced in the analysis by inserting zero-thickness interface elements in between continuum elements along pre-selected paths representing main potential crack paths [1-3]. The chemical attack is simulated by solving the diffusion/reaction process over the same FE mesh, and considering the opened interface elements as preferential diffusion paths. In this way, as the sulfate attack takes place and expansion starts in the outer layers of the mortar phase, cracks start developing and diffusion increases, accelerating the process, which constitutes a coupled C-M phenomenon [4]. However, in this approach as the number of aggregate particles grows, meshes become very large and computations very costly, which is tackled via MPI parallelization using the PETSC libraries [5]. In this context, the work describes the coupled C-M model, presents the latest results obtained with various meshes of progressively larger sizes (Fig. 1), and shows the scalability of the parallel implementation developed.

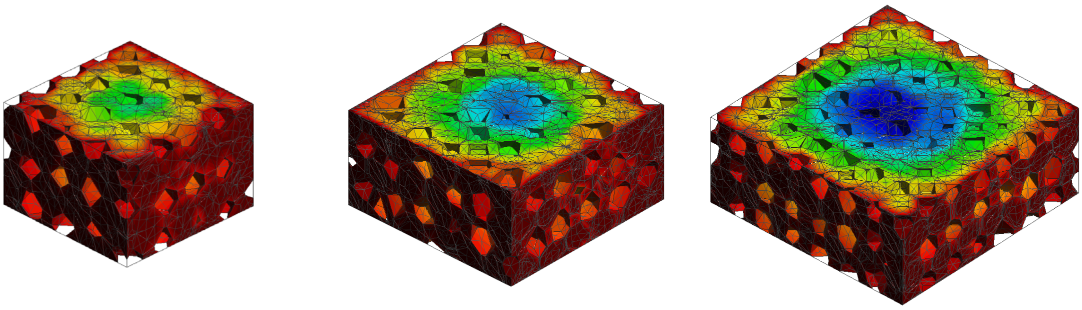

FIG. 1. Sulfate ingress at 4000 days for the 6x6x4, 8x8x4 and 10x10x4 cm^3 meshes

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Deformation behaviour of a Carbonate Clay subjected to calcite and dolomite dissolution in acidic environment

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Keywords: acidic exposure tests, caprock, chemo-hydro-mechanical processes, CO_2 storage, dissolution of carbonates.

In CO_2 storage operations the containment of the stored fluid is ensured by caprocks, typically evaporites or clayey rocks. A comprehensive study of the sealing capacity of caprocks requires evaluating their threshold capillary pressure (*e.g.* Vespo et al., 2024), their mechanical strength (*e.g.* Rutqvist 2012) and the impact of the geochemical interactions on their mechanical behaviour (*e.g.* Ciancimino et al., 2025). Chemical interactions between the injected CO_2 and the caprock can modify the sealing rock's internal structure and mineral content. Consequently, these changes may lead to alterations in its fabric and hydro-mechanical properties.

The goal of this study was to investigate the effects of the geochemical and geomechanical processes on a Carbonate Clay, traced back to a typical carbonate-clay caprock, due to the exposure to acidic solution. This material is noteworthy for comprising over 50 % carbonates, a factor that becomes critical when considering the potential acidification of the pore fluid by CO_2.

Titration tests allowed to analyse the geochemical equilibria between the solid phase and increasing quantities of H^+, as well as the role played by each carbonate species on the overall buffer capacity of the material. It was deduced how the material was able to buffer the pH as long as carbonates remained in the solid phase, which were subject to dissolution according to their binding energy (details reported in Vespo 2024). The tests' results were used to validate a reactive transport geomechanical model, through which it was possible to determine the reactive surface area and the equilibrium constant characteristic of the calcite and dolomite constituting the material.

Long-term exposure experiments with a 10^{-3} M HCl solution, pH equal to the one following the dissolution of CO_2 in the pore fluid, were conducted to assess the geomechanical impact of prolonged exposure on reconstituted Carbonate Clay specimens (details reported in Vespo 2024). These tests were performed under oedometer constant stress conditions. To investigate the influence of transport mechanisms, two distinct exposure methodologies were implemented: one based on H^+ diffusion from the oedometer basin into the specimen (exposure time: 329 days), the other on the advective flow of the solution through the specimen (exposure time. 184 days).

The results highlighted the important role that the transport mechanism, exposure times and concentrations have on the geochemical interactions with the solid phase, and in particular the increased dissolution of carbonates and related microstructural variation in presence of advective flow. Furthermore, the correlation between the amount of dissolved carbonates and deformations due to chemical reactions was determined using a reactive transport geomechanical model.

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Multiscale investigation of crystallization-induced swelling in anhydrite

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Keywords: Anhydrite Swelling, Digital Volume Correlation, Geotechnical Applications, Gypsum Crystallization, Hydration, X-ray Computed Tomography.

This study investigates the mechanisms of crystallization-induced swelling in anhydrite, a process that poses serious risks to the stability of underground infrastructures such as tunnels, caverns, and deep storage facilities (e.g., Steiner, 1993; Alonso et al., 2023; Kovári et al., 1987). The primary focus is on understanding microscale structural evolution through advanced X-ray Computed Tomography (CT) analysis, complemented by chemical and morphological characterization.

Six cylindrical specimens (Ø10 mm × 20 mm) of Triassic anhydrite from the Western Alps (Signols, Susa Valley, Italy) were partially immersed in calcium-sulphate saturated water and monitored over one year using the CoreTOM scanner (TESCAN XRE) at the Ghent University Centre for X-ray Tomography (UGCT), with a resolution of 10 µm, as part of an EXCITE TNA project. The CT data were processed using Digital Volume Correlation to localize internal strain and visualize expansion zones. To complement the CT-based investigation, additional samples were immersed in $CaSO_4$ aqueous solution and subjected to varying temperatures (15°C, 40°C, 60°C). Macro-scale measurements (mass, volume, visual inspection) and micro-scale analyses (SEM-EDS) were performed to identify mineralogical transformations, especially the hydration of anhydrite into gypsum and the precipitation of secondary crystals.

The results revealed consistent volumetric expansions of 2-3% and identified distinct zones of crystal growth and transformation. The influence of chemical composition and temperature of the infiltrating fluid on swelling behavior and mineralogical evolution was also characterized.

These multiscale experimental results confirm that swelling is driven by a combination of dissolution-precipitation reactions and crystallization in confined pore spaces. The findings improve our mechanistic understanding of swelling behavior, highlighting the importance of temperature, fluid composition, and structural constraints. This knowledge could support the refinement of predictive models and constitutive laws used in geotechnical design, enabling more accurate forecasts of swelling magnitude and timing in real-world engineering applications such as civil tunnelling, mining, slope stability, and underground energy storage.

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The problem of the salts in the conservation of the historic and artistic Heritage

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Keywords: Alteration, conservation, efflorescence, heritage, mural painting, restoration, salts.

Abstract:

Most of the historical and artistic heritage preserved in situ, both in buildings and in archaeological sites, have intrinsic conservation problems derived from poor maintenance and the environment that surrounds them. The alterations are basically caused by water and humidity, temperature and relative humidity, as well as biological colonization, among other agents of deterioration such as light, pollutants, fire, and above all the human factor.

If we focus on the conservation problems derived from water, these are always caused by the state of the roofs of the buildings, direct rain and poor evacuation of water (rain or canalized). These waters, in their journey and evaporation, drag their own or incorporated components (such as cements), and which affect the surfaces of walls, stone sculptures and ornaments, mortars, mural paintings, mosaics and ceramic and metal objects, what they call efflorescence, sub-efflorescence or deposits, and which are usually composed of soluble salts.

On his way, water can generate many alterations depending on the route and the materials found along the way, which may contain salts. The evaporation of this water with salts will form efflorescences, which will gradually destroy the surfaces and interior layers, causing irreparable damage that will affect the integrity and legibility of the heritage objects. In any case, and especially in old buildings and archaeological sites, quantitative and qualitative studies of the content of soluble salts are very complex and absolutely necessary to make a good diagnosis and a good subsequent conservation.

Once the type of salts is known, and the relationship between the state of conservation and the greater or lesser concentration of salts, preventive conservation and conservation-restoration treatments can be carried out to stabilize the objects and their altered materials, as long as the origin of the cause of deterioration has been located and eliminated, an aspect that is not always easy to carry out. Although we incorporate protective measures, after a short period of time, the materials show significant signs of deterioration associated with the presence of soluble salts.

This presentation will mainly take a tour of monuments, sites and various historical objects that have suffered deterioration caused by salt efflorescence, many of which are not yet stabilized.

FIG. 1. Removal of salts in a mural painting

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Integrated Remote Sensing and Machine Learning for Salt Detection and Analysis on Heritage Monuments

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Keywords: salts, Raman, SWIR imaging, machine learning, salt hydration

Soluble salts activity is one of the main factors contributing to the deterioration of heritage buildings [1]. Salt crystallisation, and the consequent damage, have been thoroughly investigated over the years in several laboratory-based studies. This study introduces a new methodology for the in situ and non-invasive monitoring and identification of salts, combining the complementary use of remote sensing techniques with machine learning [2]. The ground-based remote sensing suite of this study consists of short-wave infrared (SWIR) imaging and Raman spectroscopy. Both techniques operated from standoff distances of 3 to 15 m. The remote SWIR spectral imaging system covers the spectral range between 1 and 2.5 µm, with a spectral resolution of 5.5 nm and spatial resolution of 125 µm at 4 m. The in-house developed remote standoff Raman system [3] uses a 780 nm continuous wave (CW) laser, whose beam is focused to a spot size of ~1 mm on the target at all distances.

In this approach, SWIR imaging is employed to scan large wall surfaces. The resulting spectral imaging data are processed using a machine learning-based clustering method, which groups regions with similar spectra [4]. This analysis produces a material variation map of the wall surface. A detailed examination of the mean SWIR spectra for each cluster allows for a preliminary identification of salts, indicating variations in their volume concentrations. For the precise identification of the salts and their hydration states, remote Raman analysis is subsequently conducted on representative areas within each cluster.

Our method offers a novel, non-invasive, and non-contact tool for gaining deeper insights into salt formation across wall surfaces. It enables the investigation of salt formation processes, including variations in hydration states, over large areas. This analytical approach allows for repeated site visits, facilitating systematic monitoring of salt hydration states under changing environmental conditions.

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Understanding Salt Weathering in Khondalite through Mineralogy and Microstructure

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Keywords: Imaging, Khondalite stone, salt crystallization, weathering, X-Ray tomography

Salt weathering is one of the crucial agents of deterioration in porous building materials, especially in masonry systems along the coast. The cyclic environmental conditions involving changes in temperature, relative humidity and exposure to salt dissolved in moisture synergistically damage the materials. Driven by evaporation and moisture transport, salts like sodium sulphate and sodium chloride migrate through the pore network, undergo phase transitions depending on the salt type, and crystallize, often exerting significant crystallization pressures. These pressures can lead to the development of micro fissures, granular disintegration, scaling and surface blistering. The extent of damage depends on the type of salt, nature of the substrate, exposure conditions etc. [1,2,3]. The role of complex salt-pore interactions in aggravating the damage remains an active area of investigation. These interactions are driven by the mineralogy and microstructure of the substrate as well as the salt composition. To get insights into their complex coupling, studies encompassing the bulk scale and the pore scale are vital.

Our study focuses on the salt weathering of Khondalites, metasedimentary rocks, primarily composed of quartz, feldspar and garnet. They are visually appealing and are extensively used in historic structures along the eastern coast of India, notably in the Konark Sun Temple and Puri Jagannath Temple. The heterogenous mineralogy and microstructure, with regions of varying porosity and pore size distribution, results in preferential crystallization sites during salt weathering. The non-uniform pore structure makes it vulnerable to salt-induced decay under conducive environmental conditions. Characterizing salt weathering at the microscale remains challenging due to the difficulty of capturing in situ crystal formation without disturbing the microstructure, quantifying crystal growth and pore occupancy, and tracking crystallization dynamics.

The current study focuses on tracking the progression of salt weathering of cylindrical Khondalite specimens of diameter 9 mm and height around 2 mm using X-ray computed tomography (X-ray µCT). The development and propagation of sodium sulphate and sodium chloride precipitation, introduced in isolation, as well as crack formation, is tracked across weathering cycles mimicking the coastal climate of Eastern India. Complementary time-lapse µCT imaging allows for quantitative assessment of pore-filling and pore-emptying events during wetting and drying. The integration of imaging data provides critical insights into how crystal growth initiates, propagates, and ultimately contributes to stone failure, underscoring the value of pore-scale observation in understanding salt damage in heritage stones. These findings have broader implications for predictive modelling of salt decay.

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Study of a case of efflorescence in building construction

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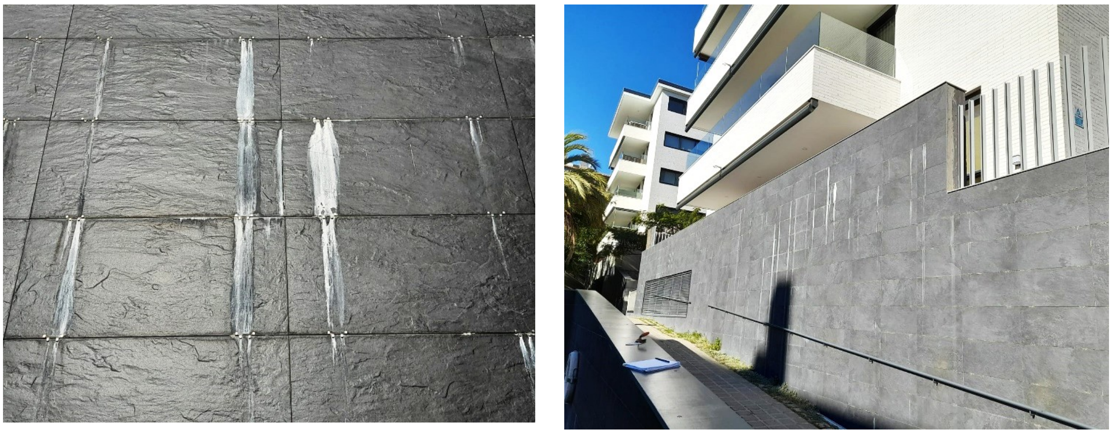
Keywords: crystallization, efflorescence, facades, porosity, portlandite, stains.

It is relatively common to encounter facades affected by the appearance of stains, typically white, on their surface. These are typically efflorescence; namely soluble salts present in some element of the facade that can dissolve in the event of excess moisture and migrate to the surface in solution. The subsequent evaporation of water causes the crystallization of the salts and, consequently, the appearance of stains.

Normally the problem generated by the appearance of efflorescence is purely aesthetic, although sometimes, depending on the nature of the salts and the porosity of the facade coating, the tensions created by the crystals inside the pores can lead to the disintegration of the material.

When studying this type of pathology, it is important, above all, to investigate the following: 1) the way in which the efflorescence is deposited on the surface and 2) the composition of the efflorescence. In the latest investigation carried out by SOCOTEC-Barcelona, we encountered this pathology:



General appearance of a stone cladding and detail of the affected plates

In this case, the efflorescence does not appear in a generalized way. It seems to originate from the joints of the plates, at the height of the clips that hold them. The appearance is of dripping, that is, the water that carries the salts tends to fall by gravity down the cladding.

The X-ray Diffraction analysis of a sample of the deposited salt indicated that it is mainly composed of calcium carbonate $CaCO_3$. Other data collected during the inspection visit that we consider relevant for understanding the problem are as follows:

The wall is made of brick masonry and is plastered with mortar. The union of the plates to the wall is by means of steel clips and cement-rich adhesive.

The crowning pieces of the wall did not fit perfectly, allowing rainwater to enter, which circulated easily through the gaps between the back of the plates and the wall.

With this data, it is easy to explain what happened: Rainwater penetrates through the crown of the wall and circulates through the back of the plates, dissolving the portlandite ($Ca(OH)_2$) from the mortar and cement adhesive. The clips inserted into the wall are a small obstacle for this falling water, and cause part of it to come out to the exterior through the joint. The evaporation of water causes the crystallization of portlandite on the surface, which subsequently reacts with environmental CO_2 forming calcium carbonate.

Hydration-Driven Transformations of Magnesium Sulfate Salts and Their Role in Dolomitic Lime Weathering in Historic Monuments

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Keywords: conservation science, dolomitic lime, magnesium sulfate hydrate, salt weathering

The preservation of historical architectural surfaces in Tyrol and Central Europe, such as those of the Helblinghaus in Innsbruck, is increasingly challenged by salt weathering phenomena linked to environmental sulfate pollution. Many of these surfaces were constructed using dolomitic lime mortars and plasters, produced from dolomite ($CaMg(CO_3)_2$) and dolomite-containing limestone. Following firing and setting, dolomitic lime primarily consists of calcite ($CaCO_3$) and various magnesium phases (e.g. brucite, hydromagnesite), which serve as key reaction partners in weathering processes. The interaction of these materials with sulfate sources - atmospheric SO_2 pollution (already present in medieval Tyrol due to mining activities) or the use of sulfate-containing binders such as gypsum in stucco - introduces sulfate ions that react with the $CaCO_3$ and Mg phases in the set lime. This can lead to the in-situ formation of magnesium sulfate salts, particularly epsomite ($MgSO_4 \cdot 7H_2O$) and its lower hydrates (e.g. hexahydrite $MgSO_4 \cdot 6H_2O$, kieserite $MgSO_4 \cdot 1H_2O$), which are known to be highly damaging due to their crystallization and hydration–dehydration cycles.

This study investigates the crystallization behavior and phase transitions of magnesium sulfate hydrates under microclimatic conditions relevant to Central European heritage sites. We focus on the reversible hydration and dehydration of epsomite crystals within the pore structure of dolomitic lime, examining the associated volume changes hypothesized to drive salt-induced weathering. Our multi-analytical approach combines in situ X-ray diffraction (XRD) to monitor phase transitions, thermogravimetric analysis (TGA) and dynamic vapor sorption (DVS) to quantify water loss and uptake, and optical microscopy to observe morphological changes during hydration cycles.

Our experiments simulate environmental fluctuations in relative humidity (20% to 85%) and temperature (10°C to 60°C), replicating the diurnal and seasonal conditions experienced by historic sites. Preliminary results reveal that neither the transition from epsomite to hexahydrite nor the rehydration process involves significant volume contraction or expansion, suggesting that volume changes are primarily associated with phase transitions to lower hydrates, such as kieserite or starkeyite ($MgSO_4 \cdot 4H_2O$). Furthermore, repeated temperature cycles show that, even without changes in relative humidity, dehydration upon heating and hydration upon cooling occurs. Rapid temperature fluctuations lead to blistering of the crystal surfaces, and eventually result in cracking and deterioration of the crystals, revealing the formation of lower hydrate phases, such as starkeyite. Our findings confirm that repeated hydration and dehydration can accelerate the decay of dolomitic lime at historic surfaces. This research provides a foundation for better understanding the mechanisms by which magnesium sulfate salts contribute to the weathering of dolomitic lime materials. The insights have implications for conservation science, especially in the development of protocols and selection of restoration materials.

In conclusion, this study advances the fundamental knowledge of salt crystallization dynamics and their practical consequences for the conservation of dolomitic lime-based architectural surfaces, offering a valuable contribution to the interdisciplinary field of material technology in conservation science.

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Application of Isotopic Techniques to Determine the Origin of Sulphate Formation: A Case Study from Barberà de la Conca, Spain

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Keywords: Anhydrite, gypsum, mineralogy, petrography, stable isotopes, sulphate.

Since 2010, the village of Barberà de la Conca (Tarragona, Spain) has been affected by the development of cracks, causing significant damage to buildings. Previous studies link this ground movement to volumetric changes associated with deep anhydrite–gypsum transformations (ICGC, 2011). A deep borehole of 232.5 m was drilled in 2017 and the cores were characterized using petrographic analysis and X-ray diffraction. Additionally, the waters from the local aquifers were analyzed, along with the isotopic compositions of both the dissolved sulphates in the waters and the sulphate phases present in the borehole.

The borehole sequence consists mainly of phyllosilicates (illite, muscovite, palygorskite, kaolinite), sulphates (gypsum and anhydrite), carbonates (calcite, dolomite), quartz, and rare pyrite. Gypsum dominates the shallow levels, while anhydrite appears below 75 m and becomes the main sulphate phase at depth. The isotopic compositions of the gypsum samples show little variability in $\delta^{34}S$ along the borehole, and a wide range of $\delta^{18}O$. In contrast, the anhydrite samples exhibit greater variability in $\delta^{34}S$ and a narrower range of $\delta^{18}O$. Sampling of the groundwater in the area allows classification of the waters as calcium-sulfate and calcium-bicarbonate types. All samples are undersaturated with respect to gypsum/anhydrite, and two of them are slightly oversaturated in calcite. The isotopic composition of $\delta^{2}H$ and $\delta^{18}O$ indicates that the samples follow the local meteoric water line.

Petrographic observations of the sulfates in the studied samples indicate that the monomineralic polycrystalline aggregates (gypsum) or polymineralic aggregates (gypsum + anhydrite), with lenticular and nodular textures, are the result of replacement. Assuming a constant-volume adjustment during the anhydrite-to-gypsum transformation would imply a release of excess sulfate and calcium into the surrounding environment. This increase in sulfate and calcium would enhance gypsum supersaturation, which in turn would facilitate the formation of fibrous gypsum veins.

The replacement of anhydrite by gypsum does not involve a change in the isotopic composition of the sulfate molecule. Thus, the lenticular anhydrite samples have $\delta^{34}S$ values consistent with those of gypsum in the area (Ortí et al. 2007). In contrast, gypsum precipitation from a solution does cause isotopic fractionation, which is greater for oxygen than for sulfur. This explains why some gypsum samples exhibit higher $\delta^{18}O$ values than dissolved sulphate. The isotopic composition of some fibrous gypsum samples is consistent with precipitation from solutions that have dissolved gypsum from the series. However, samples from greater depths (gypsum and anhydrite) show values incompatible with these hypotheses. Additionally, the nodular gypsum samples exhibit very high $\delta^{18}O$ values, which could imply various dissolution–reprecipitation processes.

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Fluorescence-based detection of crystallization pressure in microfluidic channels

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Keywords: Crystallization pressure, Finite element simulations, Mechanofluorescence, Microfluidics, PDMS.

The in-pore crystallization of salts is considered one of the major causes of degradation in construction materials, geomaterials, and built heritage. We present a fluorescence-based approach to estimate the crystallization pressure of halite in polydimethylsiloxane (PDMS) microfluidic channels. A mechanosensitive fluorescent dye is embedded in the PDMS matrix, enabling the detection of local stress through changes in fluorescence intensity. We first calibrate the fluorescence response by applying controlled uniaxial tensile stresses to fluorescent PDMS samples. We then fabricate PDMS microchannels and bond them to glass substrates. A slightly undersaturated NaCl solution is injected and allowed to crystallize through evaporation under different humidity conditions. As the crystal grows, it exerts a pressure on the surrounding PDMS, which induces a measurable decrease in fluorescence intensity. During successive imbibition–drying cycles, the fluorescence intensity in the PDMS decreases from its initial value to reach a plateau after several cycles, indicating that the crystal no more deforms the PDMS. Faster drying accelerates this process, allowing the plateau to be reached within days instead of months. We also demonstrate that the fluorescence response is reversible: dissolving the embedded crystals leads to a gradual recovery of fluorescence over several weeks. To quantify the crystallization pressure, we perform two-dimensional finite-element simulations of the system, relating the observed fluorescence change to strain in the PDMS and the corresponding applied stress. Our analysis estimates a conservative lower bound for the crystallization pressure at approximately 0.12–0.14 MPa. The simulations also indicate that localized pressures at the crystal–PDMS interface may reach significantly higher values. This fluorescence-based technique provides a practical, real-time, and non-invasive tool for estimating crystallization pressures in confined geometries, without requiring complex instrumentation. It offers new possibilities for investigating crystal-induced damage in porous materials and can be adapted to a wide range of systems and geometries.

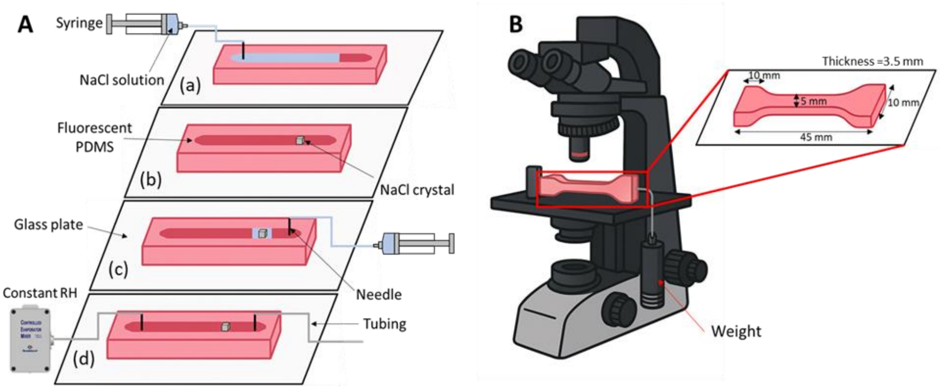

Fig 1: A-The NaCl crystallization protocol. B-The protocol used to generate calibration curve.

Crystallization Of Sodium Chloride In Microfluidic Pore Systems

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Keywords: Microfluidics, Porous Media, Salt Crystallization, SEM

Salt crystallization in porous media induced by drying involves complex coupling between drying kinetics, wettability phenomena, pore size and salt structure1. In this context, this work aims at observing sodium chloride subflorescence growth during evaporation in porous media, focusing on the shape and properties of the resulting salt structures (porosity, permeability) depending on pore size and wettability. To this end, we develop two-dimensional microfluidic chips mimicking simple porous geometries2, allowing optical microscopy observation of crystallization kinetics. The study explores the impact of geometrical confinement and wettability on salt crystallization. Different hydrophilic/hydrophobic patterns are created to stabilize the evaporative front in the model porous media and force subflorescence formation. Our microfluidic devices, designed to be reopened after drying, allow further analysis of the remaining crystals through Scanning Electron Microscopy (SEM).

Two types of salt structures are observed: monocrystals forming in solution and porous aggregates developing in dry areas from the liquid front. The evaporation rate plays a significant role, influencing concentration dynamics in the channel and the typical size of aggregates in the dry region. Moreover, the hydrophilic nature of the crystals drives solution towards the aggregates, advancing the wet front into the hydrophobic regions. In particular, the study highlights a mechanism of dissolution of the monocrystals taking place as the salt aggregates develop in the hydrophobic region.

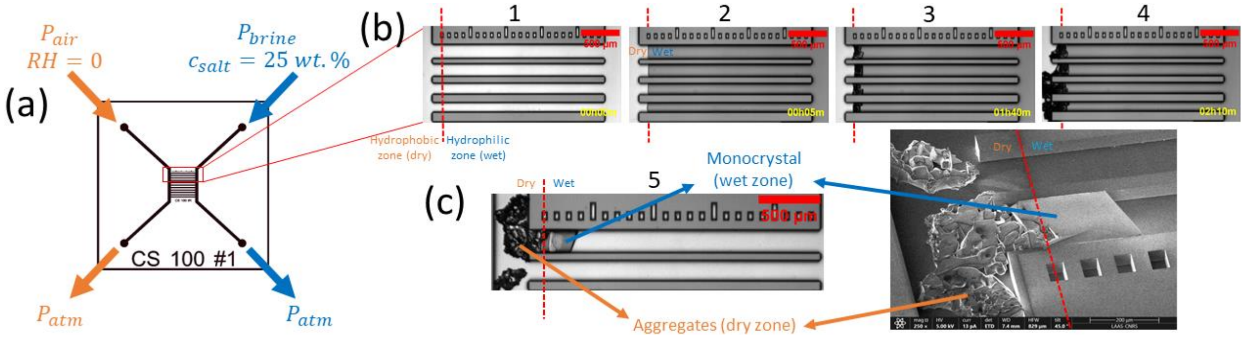

FIG. 1. Crystallization process. (a) Schematic representation of saltwater (blue) and dry air (orange) flows within the chip. (b) Zoom on channels (1), chip filling (2), crystals growth during evaporation (3,4). (c) Dried crystals after an experiment (5, t+48h), SEM image.

Acknowledgements: Financial support from project “Drysalt” funded by GIP ANR (Project: ANR-22-CE51-0041-02) is gratefully acknowledged.

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Insights on the textural and crystallographic properties of calcite obtained through MICP using scanning 3D X-ray diffraction

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Keywords: Biogenic calcite, Biocalcification, MICP, s3DXRD

The MICP (Microbially Induced Calcite Precipitation) technique is used as a reinforcement process to turn sand into a cohesive medium, inducing the precipitation of calcite crystals in the pores. This work presents a comprehensive study, using Scanning 3D X-ray Diffraction (s3DXRD) and Phase Contrast Tomography (PCT), of the morphological and crystallographic properties of bio-induced calcite, showing possible implications of calcite precipitation process on the microstructure of biocemented sand.

s3DXRD is a recently developed technique. Its peculiarity is that, compared to the more classical 3DXRD approach, it enables the isolation of diffraction spots associated with individual grains in polycrystalline aggregates allowing the reconstruction of individual sizes and shapes [1]. This specific property permits the investigation of crystallographic and morphological relationships between grains. In the case of metals, the grains usually share a similar crystallographic structure. In the case of more heterogeneous materials, such as cement or geomaterials, the presence of several different crystallographic phases complicates the system and the interpretation of the data. Since the beginning of its applications, s3DXRD has been used to investigate materials science challenges related to the field of metallurgy [2] and in one case energy storage [3]. In this talk, it will be introduced an innovative application of s3DXRD where it was used in a combined approach with phase contrast tomography to characterized the calcite precipitated by biocementation process in silica sand to investigate the role of the precipitation process of the binding phase with its microstructure. s3DXRD proved to be a powerful and versatile tool in dealing with complex and heterogeneous systems [4]. These results show the potentiality of improving the technique towards more unconventional applications.

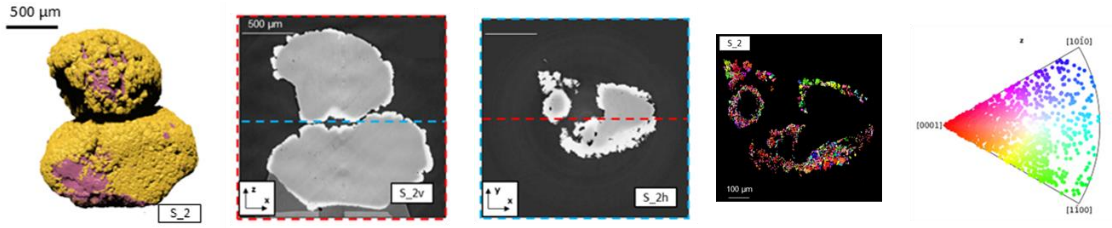

FIG. 1. From left to right: 3D visualization of the phase contrast tomography. $CaCO_3$ is in yellow and sand in purple. Vertical cross-sections of samples. Horizontal cross-sections. This section corresponds to the layers where the s3DXRD measurements were taken. Grain maps obtained from the indexing of calcite. The RGB colors are assigned based on which crystallographic direction is parallel to the z-axis of the laboratory coordinate system. Inverse pole figure

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Learning from coral biomineralization to engineer (living) materials

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Keywords: corals, biomineralization, aragonite, amorphous calcium carbonate, materials characterization

To engineer living materials (ELMs) with tailored functionalities, microorganisms can be grown, assembled, mixed, or layered synergistically with other materials to create innovative composites. A striking example of nature’s ingenuity is the ability of microorganisms to regulate biomineralization in coral reefs. Reefs are three-dimensional calcium carbonate structures constructed by marine organisms. These dynamic systems provide essential habitat for marine life, protect coastlines, and sustain local economies by supporting fisheries and tourism. Coral reefs rank among the most diverse ecosystems on Earth, hosting thousands of species of fish, invertebrates, and plants. They also serve as a source of bioactive compounds for medical research and drug discovery. As reefs grow, they enhance carbon dioxide sequestration, making them critical for climate change mitigation. Yet, climate change is driving widespread coral degradation and mortality, underscoring the urgent need for restoration strategies.

The overarching goal of our research is to deepen understanding of early-stage biomineralization and leverage this knowledge to design living materials. This project presents a unique dual opportunity: advancing the fundamental science of coral biomineralization while contributing to coral restoration from a materials science perspective. Our work focuses on reef-building scleractinian (stony) corals, specifically shallow-water, hermatypic, colony-forming species. Within our multi-institutional team, research spans larvae settlement, juvenile growth after larvae settlement, and early stage mineralization of coral fragments. The study I will highlight examines how extrinsic parameters—such as settlement substrate composition and water chemistry—influence juvenile coral growth, skeletal microstructure, and the biomineralization pathways of two species, *Diploria labyrinthiformis* and *Colpophyllia natans*. To probe these processes, we employ a suite of materials characterization techniques, including microCT, scanning electron microscopy, and energy-dispersive spectroscopy, to reveal how environmental conditions shape skeleton evolution, morphology, and microstructure.

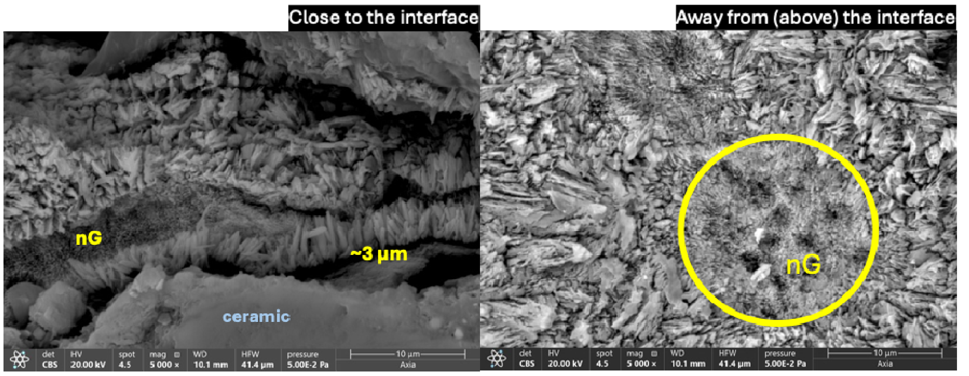

FIG. 1. Scanning electron microscopy images of 6 months old *Diploria labyrinthiformis juveniles settled on ceramic, close to the interface with the substrate and away from the interface. The basal plate consists of microsized aragonite crystals perpendicular to the substrate and region containing nanogranular* $CaCO_3$ *mineral. There are multiple centers of calcification away from the interface (circle), also rich in nanogranular* $CaCO_3$ *mineral, and space filling aragonite (acicular) crystals.*

Engineering antimicrobial calcium phosphate nanocrystals for enhanced bone regeneration

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Keywords: Bactericidal surface, Bone graft, Calcium phosphate, Hydroxyapatite, Topography

Bacterial infections remain one of the great challenges in orthopedic and maxillofacial surgery, particularly on biomaterial surfaces, where they become exceedingly difficult to eradicate. Inspired by naturally occurring biocidal surface topographies, materials with nanostructured surface features and contact-killing properties have emerged as promising strategies for reducing the risk of infection. However, their fabrication has been restricted to few substrates and the relationship between the nanofeature geometry and bactericidal efficacy remains poorly understood. In this context, we had shown that nanostructured calcium phosphate bioceramics fabricated through a dissolution-precipitation process can exhibit contact-based antimicrobial properties with gram-negative bacteria [1]. In this study, we investigated the potential for fine-tuning the nanostructures of calcium-deficient hydroxyapatite (CDHA) by adjusting the synthesis parameters including temperature, pH, duration, or nucleation seed, during the hydrolysis of α-tricalcium phosphate. From the obtained broad spectrum of topographies, three morphologies were selected: interconnected nanosheets, densely packed needles, and nest-like nanowire structures. To decouple the role of chemistry from geometry, analogous nanostructures were also replicated on titanium oxide (TiO2). All nanostructured surfaces exhibited significant bactericidal activity against *P. aeruginosa*, with no statistically significant differences between TiO_2 and CDHA, underscoring the central role of surface nanotopography. Against *S. aureus*, direct cell wall damage was not observed but metabolic activity decreased markedly, especially on needle-like surfaces, suggesting a subtler bactericidal mechanism. Our findings demonstrate that controlled processing enables the design of diverse bactericidal nanotopographies on calcium phosphate ceramics, offering new opportunities for developing antibiotic-free bone grafts combining infection prevention with regenerative capacity.

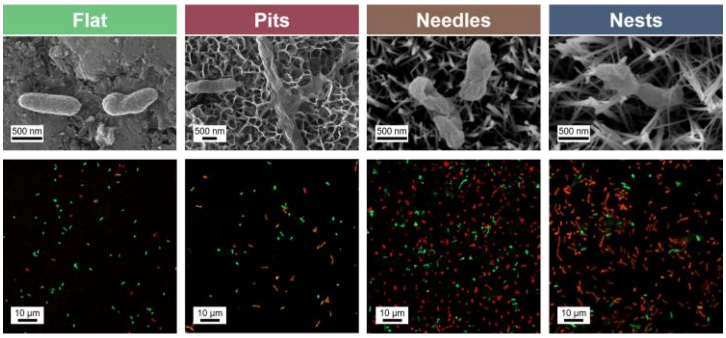

FIG. 1. Representative SEM micrographs and CLSM images of adhered *P. aeruginosa* on CaP and Ti surfaces with different nanotopographies after 15 h incubation. For CLSM images the bacteria were stained with LIVE/DEAD kit, which stains viable bacteria in green and bacteria with damaged cell wall in red.

Funding: ERC project BAMBBI (No101055053)

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On the role of $BaCO_3$ on preventing sulfate attack on Portland cement concrete

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Keywords: $BaCO_3$, ettringite, OPC concrete, sacrificial aggregate, sulfate attack, thaumasite

Current measures to protect Portland cement based-materials (mortars, concrete) from sulfate attack include: the use of cements with low C3A ($3CaO·Al_2O_3$) content that prevent ettringite ($3CaO·Al_2O_3·3CaSO_4·32H_2O$) precipitation but not thaumasite ($CaSiO·CaSO_4·CaCO_3·15H_2O$) formation; the use of supplementary blends materials to consume the portlandite needed for the precipitation of expansive salts (Hossack et al. 2015); or the correct compaction and curing to prevent the ingress of aggressive solutions with the occasional help of protective membranes or coatings.

This study aims to explore an additional measure, using $BaCO_3$ (crushed stone) as a sacrificial aggregate and additionally as a filler (Carmona-Quiroga et al. 2021) to prevent sulfates from reacting with cement paste by precipitating nearly insoluble $BaSO_4$. For that purpose, five concrete mixes were prepared. Two of them were elaborated with a commercial sulfate-resistant cement (CEM I 52.5 N/SR5 with low C3A content) with either siliceous or barium carbonate aggregate. In the remaining three with $BaCO_3$ aggregate, CEM I 52.5 R was partially replaced by fly ash (20 wt%) or slag (64 wt%) and/or $BaCO_3$ filler (20 wt%).

The sulfate resistance of the concrete mixes was assessed in a standard concentrated Na_2SO_4 solution at 23 ºC and 8ºC for 6 months. Mass, ultrasonic velocity and compressive strength of the cylindrical specimens were periodically recorded and at the end of the exposure period, the mineralogy of the samples was inspected through XRD and the composition and pH of the dissolutions analysed, the former via ICP-OES.

Results reveal that at 23ºC, samples bearing barium aggregate perform better than the reference concrete made with the commercial sulfate resistant cement and conventional (siliceous) aggregate. At lower temperature, mixes with the barium aggregate deteriorate instead, apart from the blend with the lower cement content (64 wt% of slag), as a result of both thaumasite and ettringite precipitation (FIG. 1) linked to the hindered dissolution of $BaCO_3$.

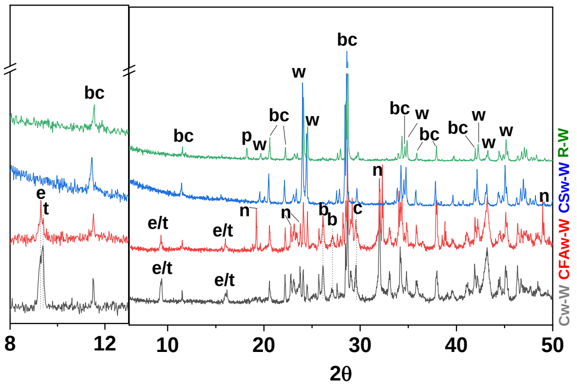

FIG. 1. 6 month XRD patterns for specimens soaked in sulfate solution at 8ºC (i= illite; e=ettringite, t=thaumasite, bc=barytocalcite; h=hydrotalcite; mc= calcium monocarboaluminate hydrate; p= portlandite; n= Na2SO4; w=witherite; q=quartz; c=calcite; f= feldspar).

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Assessment of the durability of bio-cemented sand exposed to acidic conditions by X-Ray µ-tomography

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Keywords: Bio-calcification, dissolution, X-ray µ-tomography, reactive flow

The microbially induced calcite precipitation is a reinforcement technique that uses the bacteria activity to turn sand into a cohesive medium, inducing the precipitation of calcite crystals in the pores that bond grains together [1]. One of the challenges for its industrial spreading is characterizing the durability of this reinforcement and in particular, predicting how the mechanical behaviour of a biocemented media evolves in an acidic environment (acid rain, industrial pollution…). Indeed, initial work performed by our group has shown that exposing a biocalcified material to an acidic solution rapidly reduces the strength of this material [2].

To understand better the interactions between transport, chemistry, and mechanics, this study has been complemented by in-situ X-ray tomography dissolution experiments at Ghent University and at the synchrotron facility SOLEIL. Dissolution of biocemented granular media was performed under different flow rates and pH in order to understand the temporal and spatial changes in calcite distribution within the media with a special interest in the evolution of the cohesive contact surface area that creates the cohesion.

First observations (Figure 1) show that preferential pathways along which calcite rapidly dissolves, appear when the flow rate is high and the pH is low, whereas a flat dissolution front forms when the flow rate is low and the pH is close to seven. Once the evolution of the cohesive contact area will be extracted, they will be used as input parameter in a Discrete Element Model we have developed [3] in order to predict the evolution of the strength of the material.

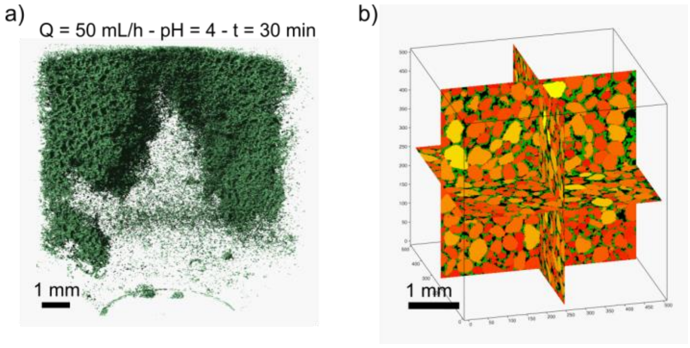

FIG. 1. a) 3D image of the calcite (sand removed) after 30 min of dissolution. b) Segmented cross sections of a biocemented granular column (green: calcite, black: porosity, hot color map : sand). The color map represents the cohesive contact surface area of each grain.

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Crystallization phenomena in the pore network of lime binders incorporating natural additives

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Keywords: Lime mortars; Additives; Crystallization; Durability; Heritage conservation; Pore Network

Ancient lime mortars were rarely composed of lime and sand alone. Builders systematically incorporated natural or artificial additives—such as pozzolans, ceramics, ashes, fibers, sugars, proteins, and fats—to enhance performance and adapt mortars to local conditions. This study investigates the influence of both traditional and modern additives on lime binders, focusing on their role in crystallization phenomena within the pore network. Two representative modern additives, polydimethylsiloxane (PDMS) and Acril 33, selected due to their widespread application in conservation. PDMS provides hydrophobicity, elasticity, and biological resistance, while Acril 33 improves adhesion, flexibility, and vapour permeability. Their performance was compared with traditional organic additives (egg white, casein, starch), aiming to assess mechanical strength, porosity, durability, and compatibility with historical substrates.

A series of lime specimens incorporating these additives were prepared and tested under environmental stressors such as freeze–thaw cycles, salt crystallization, and wetting drying. The microstructural and mineralogical evolution of the mortars was analysed using X-ray diffraction (XRD), infrared spectroscopy (FTIR), and synchrotron X-ray microtomography. Results indicate that natural additives modify crystallization pathways within the pore network, enhancing cohesion and mitigating shrinkage-induced cracking, whereas synthetic additives significantly improve hydrophobicity and long-term durability. However, issues of compatibility and reversibility remain critical for conservation practice.

Overall, this work provides comparative insights into traditional and modern additive strategies, highlighting the potential of combining heritage-compatible approaches with advanced materials to design sustainable, durable, and reversible interventions in lime-based restoration mortars.

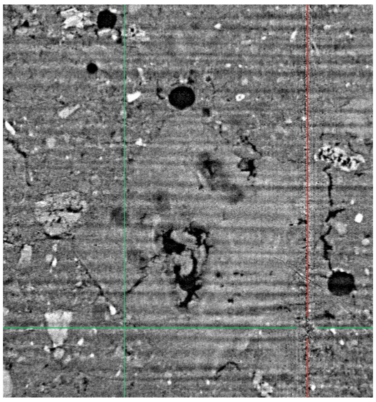

Figure 1. Pore network of lime reference samples

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Zeolite Crystallization within Pores as a Disruptive Method for Developing Advanced and Sustainable Construction Materials

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Keywords: Construction materials; Hydrothermal synthesis; Pore crystallization; Zeolite

A new approach to the development of more advanced, sustainable and energy-efficient construction materials is presented. The method, based on the work of Moreno-Maroto and Alonso-Azcárate (2024) and Moreno-Maroto *et al*. (2024), consists of firing macroscopic specimens from an aluminosilicate-rich precursor (such as clays, construction waste, etc.) at a lower temperature than conventional, favouring an initial open porosity that allows the permeation of an alkaline solution used in a subsequent hydrothermal treatment. It has been shown that increasing the initial porosity by adding porogenic components (*e.g*., rubber powder, plastic, etc.), promotes a higher degree of zeolitization of the sample after the hydrothermal treatment (Fig. 1). This generally entails an increase in mechanical strength, as well as the development of decontamination capacity, obtaining satisfactory results in ammonium retention.

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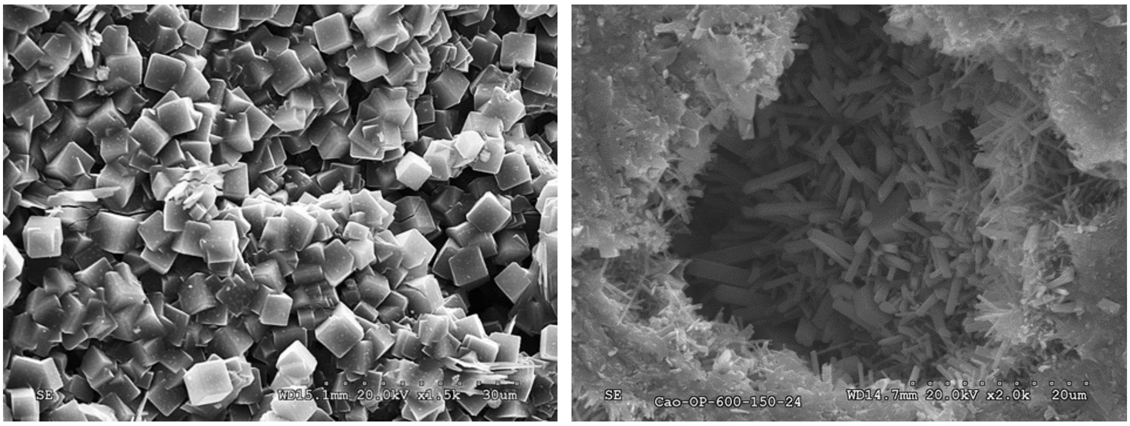

FIG. 1. Zeolite A crystals (left) and nepheline and cancrinite crystals (right) formed inside the pores of some developed materials from kaolin-based specimens as major raw materials.

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Deliquescence and Hygroscopic Properties of Salt Mixtures

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Keywords: Deliquescence, Hygroscopicity, Salt mixtures, Water films, Water vapor sorption

Deliquescence is the process that occurs when the vapor pressure of a saturated aqueous solution of a substance is less than the vapor pressure of water in the ambient air (Calvert 1990). In this case, water vapor is collected by the pure solid compound and a saturated solution is formed. The water activity of this saturated aqueous solution equals the relative humidity (RH) of the atmosphere in contact with it. Thus, a crystalline salt particle deliquesces when the relative humidity surpasses a characteristic value, the so-called deliquescence point or deliquescence humidity (DRH). The minimum relative humidity in which a multicomponent mixture can deliquesce is known as mutual deliquescence relative humidity (MDRH). The MDRH is always lower than the lowest DRH of any of the single salts present in the mixture. Below the MDRH a mixture of solid phases is stable and a solution phase does not exist. Above the MDRH, saturated solutions and solid phases can coexist. Thus, in salt mixtures deliquescence occurs across a range of RH (Godts et al. 3023).

Deliquescence of crystals is a common phenomenon in natural environments significantly influencing the physical and chemical stability of salts and their mixtures and is, thus, relevant in various fields of research and application, including the chemistry of atmospheric aerosols, cloud formation and climate change, the Martian water cycle, food storag, powder engineering, thermochemical heat storage and damage processes in building materials. Initially, at low relative humidity (RH), a nanoscale water film on a crystal surface consists of adsorbed water molecules which gradually evolves into a brine film with increasing RH, a process known as pre-deliquescence (Ewing 2004). The presence of this liquid film on the crystal surface not only induces the deliquescence of soluble electrolytes and causes powder agglomeration, it also facilitates solid–solid reactions of salt particles, such as hydration reactions. This process involves the dissolution of the educt phase and nucleation of the product phase within the nano- or microscale water film (Sögütoglu et al. 2019).

In this study, dynamic water vapor sorption, Raman spectroscopy, and environmental scanning electron microscopy (ESEM) were used to probe the role of a water film in phase transitions of the reciprocal quaternary salt system, $Na^+–Cl^-–K^+–NO_3^-–H_2O$. The goal was to elucidate the contribution of the water film to the mutual deliquescence of ternary salt mixtures, and to understand its role in the transformation of the metastable salt pair according to $KCl + NaNO_3 \rightarrow NaCl + KNO_3$. The influence of relative humidity of the latter solid state reaction is particularly interesting as water is not involved in the reaction equation. The findings provide a detailed explanation of the mechanisms of vapor–solid and solid–solid reactions in analogous systems. Further examples presented include the deliquescence of incongruently soluble double salts (Hamze et al. 2024), applications in thermochemical heat storage where mutual deliquescence of salt mixtures is used to accelerate hydration reactions and hydration–deliquescence processes involving metastable reaction pathways (Wang et al. 2024).

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Multi-Scale Investigation and Modeling of Alkali-Silica Reaction in Concrete under Confinement

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Keywords: Alkali-Silica Reaction, Chemo-Mechanical Modeling, Triaxial Confinement

Alkali-Silica Reaction (ASR) is a deleterious chemical reaction that affects the durability and structural integrity of concrete, characterized by the formation of expansive reaction products within the material's microstructure. While the influence of environmental and compositional factors on ASR has been widely studied, the role of mechanical stress—particularly multiaxial and confinement stress states—remains insufficiently understood. To address this gap, recent research has adopted both experimental and modelling approaches at multiple scales.

At the macro scale, experimental investigations on concrete specimens subjected to controlled triaxial confinement reveal a clear dependency of ASR expansion behaviour on the applied stress state. Using a custom-designed loading apparatus, ASR-induced volumetric expansion was measured under different compressive stress configurations. Results demonstrate that increased volumetric compressive stress substantially inhibits overall expansion, while also redistributing strain—leading to increased expansion in the least confined direction and reduced expansion along the most confined axes. These findings highlight the complex, anisotropic nature of ASR development under real-world loading conditions and emphasize the need for stress-aware modelling techniques.

At the meso- and micro-scale, a novel experimental methodology was developed to isolate and study ASR mechanisms at the interface between individual aggregate particles and the cementitious matrix. Using soda-lime glass discs embedded between cement paste or mortar layers, the setup replicates a simplified interface and accelerates ASR through exposure to alkaline solutions at elevated temperatures. Observed expansions, reaching approximately 30 μm before debonding occurred, offer valuable insight into the initiation of cracking at the aggregate-matrix boundary. SEM/EDS analysis of the ASR products indicates calcium-to-silica molar ratios between 1.0 and 1.5, supporting a chemically-driven mechanism involving pressure build-up from product accumulation. Based on these observations, a qualitative reaction-expansion mechanism is proposed, as a basis for subsequent numerical modelling efforts.

To integrate and simulate these experimental observations, a coupled chemo-mechanical (C-M) finite element model has been developed to capture ASR-induced damage at the meso-structural scale. The model employs zero-thickness interface elements to represent cracks and discontinuities within the concrete matrix, where ASR products accumulate and generate internal pressure. This framework includes a new diffusion-reaction formulation adapted for interface elements and a specialized mechanical constitutive law that accounts for expansion-driven crack propagation. The model effectively reproduces observed behaviors such as stress-dependent expansion suppression and anisotropic deformation patterns. Furthermore, the numerical implementation separates the structural governing equations from the chemical constitutive relations, enabling efficient and modular analysis.

Together, these contributions provide a comprehensive, multi-scale perspective on ASR in concrete, combining novel experimental techniques with advanced modeling strategies. The findings not only deepen the understanding of ASR mechanisms and their interaction with stress fields but also offer practical insights for predicting, mitigating ASR damage in concrete infrastructure under service loads.

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Sulphate attack and chemical damage in concrete structures in deep geological repositories for nuclear waste storage

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Keywords: Concrete alteration, concrete-clay interaction, deep geological repository, sulphate attack.

Concrete structures in the future deep geological disposal facility for radioactive wastes in France, named Cigéo, will interact with the surrounding barriers. In particular, sulphates in clayey materials, such as Wyoming bentonite or oxidized Callovo Oxfordian rock to be used as engineered barriers, could be detrimental to the performance of the concrete liners and plugs in the sealing system. Sulphates can diffuse into the cementitious matrix and form expansive products, mainly ettringite. These expansive products can cause microcracking (diffuse damage) and, if sustained in time and under certain conditions, macrocracking. Sulphate attack is generally coupled with calcium leaching and other diffusing species in underground structures, these need to be considered simultaneously.

The hydro-chemo-mechanical behaviour of concrete under sulphate attack is simulated considering explicitly: (1) reactive transport between the cementitious matrix and the surrounding materials (not limited to sulphates and including the reactions of cement hydrates and precipitation of secondary minerals); (2) the expansions based on ettringite volume fraction and available pore space; (3) a chemical damage model to account for the impact of chemical reactions on the mechanical properties; and (4) a mechanical damage model of concrete to account for the impact of mechanical loads, based on Mazars (1986), with a regularization method to eliminate mesh dependence of the results.

Additionally, the effect of calcium leaching and carbonation is considered by explicitly solving the reactive transport processes and the associated chemical damage. The effect of transformation and neutralization of the cement hydrates on the mechanical properties can be considered through an isotropic chemical damage variable (d_c). This non-dimensional scalar variable, varying between 0 (intact material) and 1 (fully damaged material), is a measure of the level of chemical degradation due to calcium leaching. The chemical damage model is calculated using a multi-scale homogenization model originally developed by Stora et al. (2010) and further adapted to the chemical studied system.

The mechanical constitutive model considers the impact of mechanical loading as well as the chemical processes. Considering an isotropic scalar damage variable, the stiffness tensor follows a multiplicative decomposition approach accounting for the mechanical (d_m) and chemical (d_c) damage variables. The main source of expansion at repository conditions is ettringite reprecipitation at concrete structures outermost bands (FIG. 1). However, the associated decrease in material stiffness shows to have no noticeable consequence on the sealing system function.

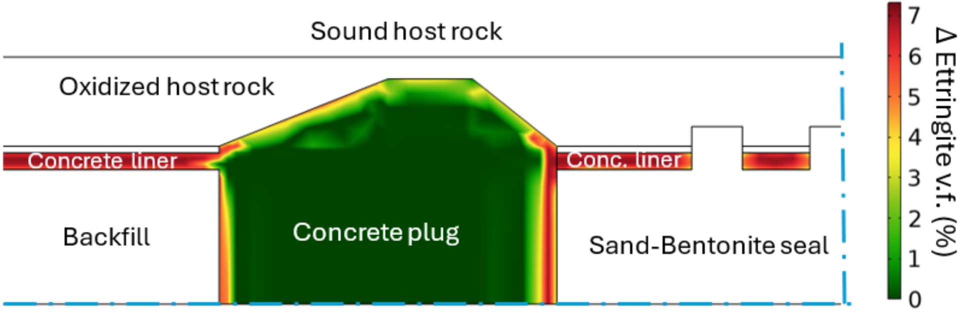

FIG. 1. Precipitation of ettringite in concrete structures after 10 ky of repository closure.

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Sulphate Attack in Cement-Stabilized Materials: Influence of Slate-Containing Recycled Aggregates

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Keywords: Ettringite; Foliation planes; Natural rock fraction; recycled concrete aggregates¸ Slate; Sulphate attack.

This study investigates how the type of natural aggregate rock present in recycled aggregates (RA) from demolition waste influences their durability, depending on their application. Previous research by the group established that the mechanical behaviour and durability of mixed recycled concrete aggregates (MRCA) are generally inferior to those of recycled masonry aggregates (MRMA). To improve the quality of MRCA, producers have incorporated fragments of various rock types originating from construction and demolition waste. In the studied region, unbound natural aggregate is often composed of slate, originating from the demolition of building materials. The presence of gypsum represents a key weakness for the use of recycled aggregates in applications such as subbases or cement-treated gravel, as gypsum content in mixed recycled aggregates—typically the most common type—can vary between 0.5% and 6.7% by weight. The study demonstrates that sulphate attack durability decreases in MRCA containing natural metamorphic rock fragments such as slate or shale. This degradation is particularly significant when these fragments are contaminated with construction gypsum. To evaluate the behaviour and stability of the slate fraction in MRCA, three systems were analysed: slate and water (S), slate with gypsum (SG), and slate with gypsum and cement (SGC). Two temperatures (5°C and 21°C) and pH were also considered as variables. To maintain consistent pH conditions across systems, NaOH was added to the S and SG systems. The combination of gypsum and alkaline conditions in contact with natural aggregate (slate) leads to the formation of ettringite in the SG system, with aluminium supplied by the slate. In the SGC system, significantly more ettringite is formed, and potentially thaumasite as well, although only at low temperatures. In both systems, slate is attacked by sulphate derived from gypsum. The characterization of the slate, carried out using scanning electron microscopy (SEM) (FIG. 1), reveals the growth of sulphate crystals between the foliation planes of the slate.

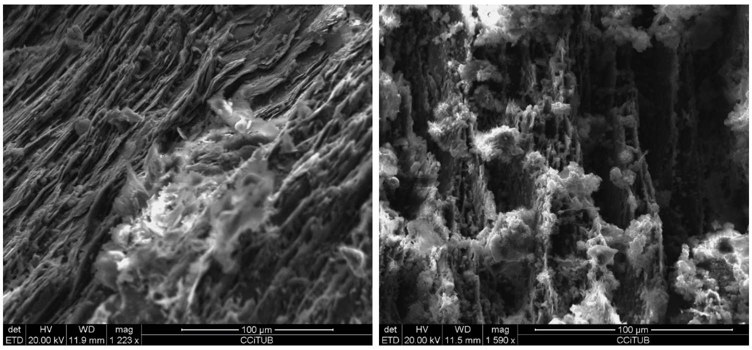

FIG. 1. (left) attack forms over the slate and (right) ettringite into the foliation of the slate.

Based on the results of this study, it can be concluded that recycled concrete aggregates containing unbound slate particles are susceptible to sulphate attack in the presence of gypsum. Gypsum may be present as a contaminant in demolition waste and often appears in variable amounts in recycled aggregates.

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Pore Crystallization in Carbonated Low-Clinker Cements Reinforced with Nonwoven Textile Fibers

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Keywords: Carbonation, Crystallization, Low-clinker cements, Porosity, Textile fibers durability.

In addition to other potential future applications, at present the reutilization of post-consumer textiles in construction materials offers an innovative pathway toward sustainable development. This study employs the carbonation of low-clinker mortars reinforced with textile fibers wastes as a strategy to improve their durability and as a result of this process we examine the crystallization phenomena within their pore network.

The carbonated composites were characterized using X-ray diffraction (XRD), Fourier-transform infrared spectroscopy (FTIR), and scanning electron microscopy (SEM). Calcium carbonate polymorphs—primarily calcite, with minor vaterite—were detected by XRD, partly occluding the pore space and altering transport properties and mechanical strengths.

In addition, the microstructural evolution of the fibers was observed after 28 days of carbonation. Importantly, carbonation exerts a dual effect: (i) it enhances CO2 sequestration, beneficial for climate change mitigation, and (ii) it reduces the alkalinity (pH) of the cement matrix, potentially compromising the long-term durability of textile fibers. Mechanical tests revealed that carbonation improves compressive strength in fiber-containing mortars, offsetting the initial porosity increase from fiber addition.

These results underscore the dual benefit of combining low-clinker cements with textile fibers—not only for valorization of waste streams but also for the controlled management of pore crystallization, with implications for CO2 uptake, durability, and sustainable construction.

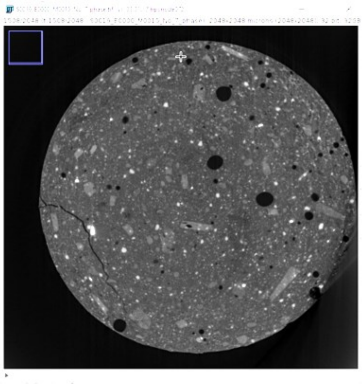

FIG. 1. Porosity of samples

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High Performance Pore Scale Reactive Transport Model for Cement-Claystone and Cement-Iron Interface Interactions

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Keywords: Reactive Transport Model, Machine Learning, Cement, Claystone, Iron, Pore Scale

Pore scale Reactive Transport Modelling (RTMs) provides detailed insight into the the time-evolution of the microstructure, its transport properties, and mineral phases reactivity with aqueous pore solution. However, such simulations are often limited to small domains and cover very short evolution period due to the necessary fine temporal and spatial discretization, and thus, high computational costs. Two methods have been developed and benchmarked in this work to circumvent the time scale limitations of conventional pore scale modelling approaches. First, machine learning is used to replace the iterative geochemical solver by a neural network surrogate model trained on the specific chemical system (Prasianakis et al., 2021). This is an already established method and leads to overall acceleration factors up to 50 times for the simulations of this work. Second, a novel adaptive time-stepping scheme is presented that takes advantage of the multi-scale nature of the studied reactive transport processes, which leads to an additional acceleration factor up to 9’000 times with an accuracy remaining well below 2% compared to the reference simulations. Both methods combined lead to acceleration factors up to 450’000. This allows the efficient simulation of cement-claystone interface processes at the pore scale and it will in a next step also be used to investigate cement-iron interface interactions. The developed simulation approach was applied to study the evolution of porosity and diffusivity at cement-claystone interface caused by the counter-diffusion of aqueous $Ca(OH)_2$ and SiO_2 and subsequent precipitation of Calcium-Silicate-Hydrate (C-S-H). C-S-H is a semi-crystalline cementitious phase modelled by a quaternary solid solution (Kulik, 2011) to consider the varying structure and chemical composition present in the same system. Unprecedented acceleration of numerical simulations compared to the conventional models allow to realistically simulate the conditions leading to the clogging phenomena and eventually derive macroscopic parameter of interface evolution which can be used for parametrisation of continuum scale simulations. Following the successful simulations of cement-claystone interface, the model is being extended to describe pore scale RTM at iron-cement interface.

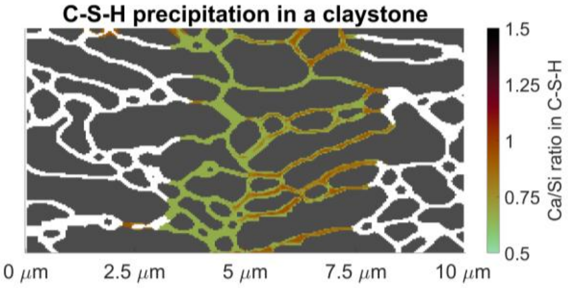

FIG. 1. Simulation of the C-S-H precipitation in claystone macropores. Grey are clay minerals and white are fluid filled macropores. The C-S-H precipitates are coloured according to the Ca/Si ratio.

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Salt crystallization modifiers in porous media contaminated with salt mixture

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Keywords: ceramic, heritage preservation, salt crystallization, salt mixture, stone.

Salt crystallization is frequently found as one of the main causes of built heritage decay. The best approach to this problem is still in question for many authors, who in the last decades have taken on the study of crystallization modifiers, introducing these additives as possible heritage preservation treatments. The present research is focused in the behaviour of modifiers when faced with salt mixtures within porous media, specifically ceramic and stone since both of them have been historically used in built heritage. Stone damage by means of salt crystallization and the use of modifiers in this material has been studied in more depth than ceramic, but results from a previous study carried out by the corresponding author seem to prove that salt crystallization modifiers could be as effective. Salt decay test and different analytical techniques will be used in order to characterize both porous materials, as well as the chosen salt mixture and modifiers. These tests would be repeated on the outside, if the modifiers were to be proven effective in the laboratory, in order to determine whether they could be used in different and variable conditions or not, considering the contamination of the surroundings.

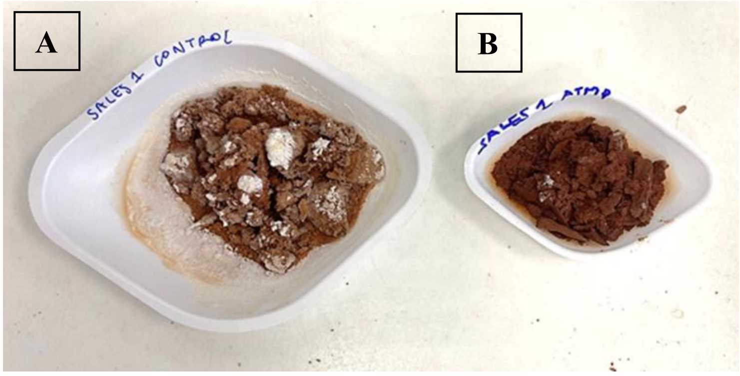

FIG. 1. Results from previous study carried out by the corresponding author. From left to right: A) salt efflorescence on fragments from ceramic contaminated with salt mixture and without the studied modifier, which were filtered and weighed at the end of 3 weeks of salt decay tests, after 24h of drying under normal conditions; and B) salt efflorescence on fragments from ceramic contaminated with salt mixture and the studied modifier, which were filtered and weighed at the end of 3 weeks of salt decay tests, after 24h of drying under normal conditions. Also note that the amount of material loss is remarkably less in the case of the ceramic with the modifier.

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