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Review

Advancements in bacteria based self-healing concrete and the promise of modelling

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ABSTRACT

In the last two decades self-healing of concrete through microbial based carbonate precipitation has emerged as a promising technology for making concrete structures more resilient and sustainable. Currently, progress in the field is achieved mainly through physical experiments, but their duration and cost are barriers to innovation and keep the number of large scale applications still very limited. Modelling and simulation of the phenomena underlying microbial based healing of concrete may provide a key to complement the experimental efforts, but their development is still in its infancy. In this review, we briefly present the field, introduce some key aspects emerged from the experiments, present the main ongoing developments in modelling and simulation of mineral and microbial systems, and discuss how their synergy may be accomplished to speed up progress in the near future.

1. Introduction

Concrete emerged as the most used construction materials around the world after the invention of Portland cement in the early 19th century. Cement is the binding component in the concrete mix, along with water and aggregates – rock, sand, or gravel. Almost two centuries later, concrete is here to stay. The world is urbanizing at an accelerated pace, with a projection that a city equivalent of New York will be built every month for the next forty years [1]. Concrete is the construction material of choice because it combines low cost with many desirable properties for a construction material, including workability, high compressive strength and durability. Global concrete production is estimated to increase by up to 23 % by 2050 [2], and, in the early 21st century alone, China has produced more cement than the United States in the entire 20th century (25.8 billion tonnes and 4.3 billion tonnes, respectively) [3].

However, concrete has a major drawback of being an important contributor to the global greenhouse gas emissions, and responsible for up to 8 % of the total anthropogenic CO_2 emissions due to its use of cement [4,5]. In this regard, the production of one tonne of Portland cement releases ~0.86 tonnes of CO_2 into the atmosphere, where ~40 % of these emissions can be associated to the burning of fossil fuels and ~60 % to the calcination of limestone to produce calcium oxide [6,7]. Decarbonizing concrete production is now high on the sustainability agenda, with innovation targeting both the production process (e.g., a switch to more sustainable fuels) and the material itself [8–13]. For the material, there is a push towards adopting new and more sustainable chemical compositions, especially to include a range of by-products for reducing reliance on calcined limestone, and to extend the service life of both existing and new concrete structures. In both cases, however, there are uncertainties around the durability of novel concretes, or of traditional concretes serving for longer periods than documented in the literature.

The durability of concrete is threatened by various processes of physical, chemical, mechanical, and biological nature. The degradation of concrete is particularly affected by the opening and propagation of cracks, especially when these trigger and accelerate the corrosion of steel rebars in reinforced concrete. To date, repairing cracks costs

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around €130/m^3, which is about double the current production cost of concrete [14]; in the United Kingdom alone, the total repair and maintenance infrastructure budget is higher than that for new works [15]. Building resilience against crack opening is thus a key pathway to ensure durability, extend service life, and thus reduce the carbon footprint and maintenance cost of concrete structures. One way to achieve such resilience is to promote the material's ability to heal its own cracks when they form. Under certain conditions, such as presence of water in the environment and absence of tensile stress, the healing of concrete can be autogenous, thanks to delayed hydration of still un-hydrated cement particles in the aged mix, or carbonation of calcium hydroxide in the material to produce calcium carbonate [16,17]. However, autogenous self-healing is restricted to microcracks smaller than 300 μm and is not sufficiently reliable as the mechanisms behind it are not well understood and its behaviour is inconsistent [18]. Therefore, researchers are considering other environmentally friendly alternatives to enable and enhance autonomous self-healing of cracks in concrete structures, such as admixtures (including microcapsules containing mineral healing agents [19] or bacterial spores [20]), shape memory polymer tendons [21,22] and vascular networks [23,24].

One of the most promising options under study is self-healing of concrete based on microbially induced calcium carbonate precipitation (MICP). MICP was first observed in *Pseudomonas calcis* [25] and occurs as a by-product of certain microbial metabolic activities, when the carbonate ions produced by microbes promote the precipitation of calcium carbonate in the presence of a calcium source. The carbonate production is influenced by numerous factors including pH, temperature, dissolved inorganic carbon or calcium ions concentration in the environment [26–28]. When used for promoting the self-healing of concrete, the microbes need to be added in the concrete matrix, normally as spores, and are usually encapsulated in a carrier since the survival of bacteria is affected by the harsh conditions during the initial mixing and by the reduction in pore sizes taking place during cement hydration and concrete hardening. The promise of this bacteria based self-healing concrete (BBSHC) is to save on labour and raw materials required for repairs, and to extend the service life of structures [29–32]. The overall process is presented in Fig. 1.

The global market for self-healing concrete is expected to expand at a compound annual growth rate of 37.0 % from 2020 to 2027 [35], but this estimation is based mainly on admixture or vascular technologies. The contribution of BBSHC is still very small because to date there is no unified or standardized approach for developing the process for large-scale applications. BBSHC is a vibrant research field, with numerous studies published in the last decade, followed by comprehensive reviews focusing on the metabolic pathways, type of microorganisms, culture media composition or test procedures for assessing the performance after healing [36–45]. However, while experimental work has progressed significantly, modelling of BBSHC is less advanced and not yet integrated in the overall process development (see Fig. 1).

A number of models exist for autogenous and autonomous self-healing of concrete, not of bacterial origin. Such models have been reviewed several times in recent years [46–49], with mentions to BBSHC being limited to the early work of Zemskov et al. [50]. These models include a description of self-healing mechanisms at the constitutive level, for a representative elementary volume (REV) of the material. This further informs larger-scale simulations which are based on various techniques, e.g. Finite Elements, Discrete Elements, and lattice models. The healing mechanisms are mostly based on reasonable assumptions directly at the REV level, and not derived from models at lower scale. In some cases, however, smaller-scale simulations have also been used, to predict microstructural changes and tailor the constitutive models to specific compositions of concrete [51,52]. By contrast, there are very few models for BBSHC, all treating the underlying mineralization process at the constitutive and at the larger, continuum, levels [50,53–55]. Therefore, the scope of this manuscript is to review the existing models and simulations of BBSHC and to identify other current modelling

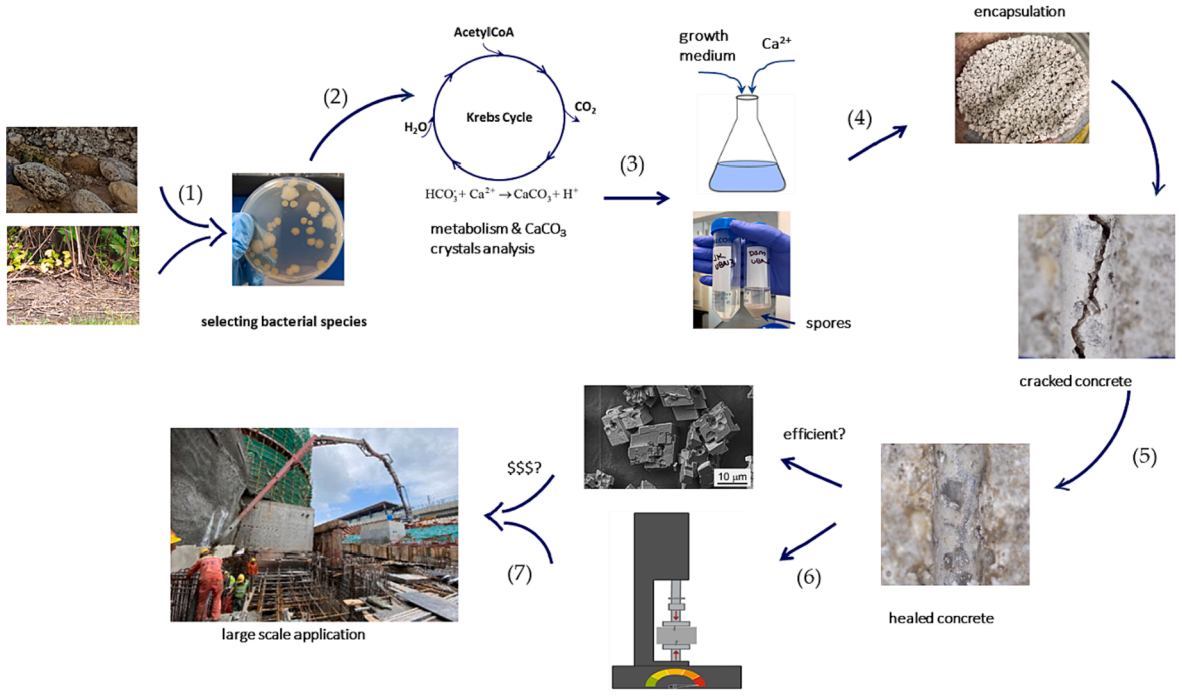

Fig. 1. Current process development for obtaining BBSHC. (1) The first step is to select a bacterial strain capable of $CaCO_3$ precipitation, appropriate for the application considered. (2) The second step is to characterize the selected strain and its carbonate precipitation efficiency. (3) Step three is to select a growth medium and to produce spores. (4) In step four there is the selection of the method for including the biological material in concrete, followed in step five (5) by testing the healing of cracked lab samples. The mechanical properties of the healed samples are evaluated in step six (6). At the end of the process and based on a rigorous economic analysis, large-scale applications are considered (7), but very few are reported to date. (Crystals picture is reproduced with permission from [33]. Large scale application picture is reproduced with permission from [34]).

techniques that, whilst still not applied to MICP, could be leveraged to advance the current state of the art. Particular emphasis is placed on simulating the co-evolution of mineral and microbial systems, as this would offer the key to predictive multiscale models of BBSHC that may significantly accelerate the development of new solutions, help reducing cost, and thus support large-scale applications. The manuscript starts with a short overview of MICP pathways and mineral formation, lab scale experimental studies, and large-scale applications. In the second part, relevant modelling-based approaches are discussed in the context of simulating BBSHC. Finally, some promising future directions are discussed.

2. MICP pathways and mineral formation

There are different pathways through which microorganisms precipitate calcium carbonate, and these pathways can be broadly classified into two groups: autotrophic (e.g., photosynthesis or methane oxidation) and heterotrophic (e.g., sulphate reduction, organic acid oxidation or nitrogen cycle), and comprehensive reviews have been recently published [43,44]. By far, reactions of the *nitrogen cycle*, and in particular *ureolysis*, are the most studied pathways for MICP. The precipitation of the mineral takes place on the cell surface and on the extracellular polymeric substances surrounding the cells, which provide nucleation sites. Mineral precipitation is actually a by-product of the microbial metabolism, which changes the local environment chemistry making it favourable for crystal formation [43].

The mineral resulting from MICP can be in any of the three polymorphs of $CaCO_3$: calcite, vaterite or aragonite, and for BBSHC applications calcite is preferred as it is the most thermodynamically stable. An important factor influencing the crystal type is the calcium source, but the morphological differences in the crystal formation are also strain specific [56], with non-ureolytic bacteria reported to precipitate mixed organic/inorganic crystals while ureolytic ones produce inorganic, homogenous crystals [57]. Different studies regarding the influence of calcium sources on MICP have been published in recent years. Some of them concluded that when ureolytic bacteria were used, calcium chloride is the best source as it gave more calcite production compared to other calcium compounds [58,59]. In contrast, other studies considering non-ureolytic bacteria concluded that the highest amount of total precipitated calcium carbonate was obtained when calcium glutamate was used, while the lowest was observed when using calcium chloride [60]. Moreover, the calcium source has also been reported to have an influence on the performance of BBSHCs, with some (calcium formate) reported to enhance the compressive strength compared to controls, while others (calcium nitrate and calcium lactate) resulting in a lower compressive strength than the controls when used with the same alkali resistant bacterial spores [61]. Nevertheless, it is not possible to generalise that the type of calcium carbonate precipitated is only related to the calcium source or bacterial strain, as many key factors (e.g., pH, availability of nucleation sites or calcium concentration) also have an important effect on the precipitation process.

3. Experimental studies of MICP

Precipitation of calcium carbonate by bacteria is considered a general phenomenon if the appropriate growth medium and conditions are provided [62]. For example, recently Reeksting et al [57] investigated a library of 74 soil bacteria, with both ureolytic and non-ureoytic species, showing that the vast majority of them (89 %) were able to produce calcium carbonate in suitable experimental conditions. However, the rate of precipitation, the quantity and the quality of the mineral obtained varied widely. This variety is reflected in the published literature on BBSHC, where there is a great diversity in microorganisms, carbon and calcium sources, ways of loading the bacteria in the cementitious matrix, and performance tests after cracking and healing. For 2020 and 2021 alone, the number of publications returned by Scopus for "bacteria based self-healing concrete" or "MICP concrete" is more than 150. A necessarily selective list of the bacterial species used in MICP, their pathways and some details of the experimental studies is presented in Table 1. Arguably, the most studied species for MICP is *Sporosarcina pasteurii,* a non-pathogenic and endospore-producing soil bacterium with high urease activity and tolerance for high pH [63].

In most experimental studies bacteria, as either vegetative cells or spores, are encapsulated in a carrier to retain their viability for a longer time inside the concrete matrix. The tested encapsulation materials include aerated concrete granules (ACG) [67], ceramsite [70], silica gels [71], polyurethane [85], hydrogels [93] and expanded clay particles [90] (more are listed in Table 2). The addition of the carriers affects the strength of the BBSHC [102,103]. Earlier reports indicated that the presence of bacterial cells in concrete increases the strength of the structure through the deposition of calcite, which decreases water permeability and provides resistance to acids [68,69,104]. More recent research argues that any strength improvement is due to the presence of bacterial cells *per se*, but not because of any activity by the bacteria (e.g., by providing nucleation sites for cement minerals or behaving like organic fibres reinforcing the matrix) [105]. At the same time, cell debris resulting from the vegetative cells can negatively affect the compressive strength of the concrete, by making it more porous over time [32,82,106].

Most laboratory experiments to date have used reagent grade chemicals and pure cultures. However, this is probably neither sustainable nor cost-effective for large-scale applications. Alternative ways to produce BBSHC were also tested, involving mixed cultures [107,108] and industrial by-products as growth media (e.g., the effluent from the dairy industry [109], corn wet milling processes [110], or from a biogas plant [111]) or calcium sources (e.g., from chlor-alkali industrial waste [112]), but with mixed results on improving the process performance.

4. Large-scale industrial applications of self-healing concrete using MICP

Despite the abundance of laboratory experiments of BBSHC, there have been relatively few large-scale industrial site trails or published applications of the technology. The pioneer company in manufacturing BBSHC is Basilisk©, established in 2015 by TU Delft in collaboration with the Dutch company Corbion. BBSHC has been commercially available since 2017. Basilisk© produces BBSHC for construction as well as a mortar and a liquid solution for repair of old existing buildings. The first large-scale applications to test BBSHC under environmental conditions were done in the Netherlands for a wastewater purification tank and a water reservoir, which have been in operation since August 2016 and July 2018, respectively. The results are not yet conclusive as more time is needed for concrete to age and develop cracks [113], but so far there are no evident negative effects of incorporating the biological mix in the concrete matrix. Prior to this, the same research group had a pilot scale study in a parking garage concrete deck and showed that the bacteria-based healing mixture sprayed on the surface of previous existing cracks in the concrete slabs reduced water leakage [29].

In October 2015, the first large-scale self-healing concrete trial in the United Kingdom was conducted by Davies et al. [114] as part of the Materials for Life (M4L) project. They constructed concrete panels with four different healing techniques, one of them being bacteria-infused expanded perlite particles, as a part of the Valleys Highway upgrading project. For the BBSHC, the panel was successfully cast using standard concrete practice with no negative effects observed on its setting or hardening properties. However, no significant self-healing that could be attributed to MICP was observed at the end of the trial, likely due to cold temperatures, a suboptimum ratio of spores to growth media or an unevenly distribution of spores throughout the concrete matrix [115]. The study concluded that different methods must be investigated to find a reliable autonomous self-healing solution for a given damage mechanism.

Table 1
Selective examples of experimental studies using MICP.

No	Species	Pathway	Material	Comments	Reference
1	*ACRN3 & ACRN5*	Ureolysis	Cement	Cement samples including ACRN5 had reduced chloride ion permeability and increased electrical resistivity and compressive strength of concrete	[64]
2	*Alkalihalobacillus pseudofirmus*	Ureolysis	Cement	After 10 days of curing, viable spores in the cement stone were 7 % of the ones in the original spore suspension	[65]
3	*Bacillus cereus*	Deamination	Concrete	Reduced water permeability; potentially pathogenic species.	[66]
4	*Bacillus cohnii*	Organic acid utilization	Cement	Use of endospore forming bacteria for MICP	[65,67,32]
5	*Bacillus licheniformis*	Ureolysis	Concrete	Wheat bran used as substrate	[68]
6	*Bacillus megaterium*	Ureolysis	Concrete	Used dairy industry waste as nutrient medium	[69,68]
7	*Bacillus mucilaginous*	Ureolysis	Cement	Immobilized using ceramsite	[70]
8	*Bacillus sphaericus*	Ureolysis/ Denitrification	Mortar/Concrete	Studied effect of multiple protection materials Immobilization of bacteria using biochar	[71,72,73,74]
9	*Bacillus subtilis*	Organic acid utilization	Concrete	Bacterial spores immobilized using light weight aggregates and graphite nano platelets	[75]
10	*Diaphorobacter nitroreducens*	Nitrate reduction	Concrete	Reduced setting time	[72]
11	*Lysinibacillus bornitolerans*	Non-ureolytic	Mortar	Used alternative nutrient source including malt powder, corn syrup, rice bran and $(NH_4)_2SO_4$	[76,77]
12	*Myxococcus xanthus*	Deamination	Limestone	Produced vaterite	[78]
13	*Proteus mirabilis* *Proteus vulgaris*	Ureolysis	Concrete	Cannot survive under high pH in concrete. *P. mirabilis* is a human pathogen	[79]
14	*Pseudomonas aeruginosa*	Ureolysis	Portland cement	No significant effect of compressive strength and a pathogen	[63]
15	*Shewanella spp*	Ureolysis	Cement	Formed silicate contributing in compressive strength	[80]
16	*Sporosarcina pasteurii*	Ureolysis	Limestone, Portland cement	Bind sand columns in oil field, Increased compressive strength, Using live cells affected the strength of concrete. Vegetative cells retained viability for around 330 days in hardened mortar samples	[81,82,83,84,578586]

Table 2
Encapsulation techniques used for bacteria before they are included in the cement-based matrix.

No	Encapsulation technique	Bacterial species used	Reference
1	Aerated concrete granules (ACG)	*Bacillus cohnii,*	[67,87]
2	Air-entraining admixture	*Bacillus cohnii*	[88]
3	Calcium alginate beads	*Bacillus subtilis*	[89]
4	CERUP, Clay, ACDC, Activated carbon	*Bacillus sphaericus, Diaphorobacter nitroreducens*	[72]
5	Ceramsite	*Bacillus mucilaginous*	[70]
6	Diatomaceous earth	*Bacillus mucilaginous*	[31]
7	Expanded clay particles	*Bacillus spp (unspecified)*	[90]
8	Expanded perlite	*Bacillus cohnii*	[91]
9	Fly ash	*B. megaterium*	[92]
10	Hydrogel	*Bacillus sphaericus*	[93]
11	Magnetic iron oxide particles	*Bacillus licheniformis, Bacillus sphaericus*	[94]
12	Melamine microcapsule	*Bacillus sphaericus*	[95]
13	Natural fibres	*Bacillus subtilis, Bacillus cohnii, Bacillus sphaericus*	[96]
14	Polyurea	*Bacillus pseudofirmus*	[97]
15	Polyurethane	*Sporosarcina pasteurii*	[85]
16	Recycled coarse aggregate, Virgin fine aggregate, Iron oxide nano/micro particles, Bentonite nano/micro particles	*Bacillus subtilis*	[98,99]
17	Silica fume	*Sporosarcina pasteurii*	[81]
18	Silica gel	*Bacillus sphaericus*	[100]
19	Zeolite	*Sporosarcina ureae, Sporosarcina pasteurii*	[101]

A more recent large-scale application installed in Antwerp, Belgium [116], consists in a roof slab made of BBSHC including a mixed ureolytic culture and anaerobic granular bacteria. The monitoring of the slab is ongoing as in one year no cracks have been observed; the site test is accompanied by control samples in the laboratory, whose cracks indeed got sealed after wet and dry cycles.

The closest description of an industrial production of BBSHC was reported in the last couple of years in China, where it was applied in the construction of a metro station [34] and a lock channel wall [117]. The reported studies used spore powder obtained through spray drying and capsule-based healing agents and both showed good efficiency in healing early cracks in concrete. In those works, the authors stress the difficulty of integrating microbial healing agents (which need to be protected from humid environments to avoid early germination) in the existing production lines of commercial concrete.

Regarding the use of commercial bacteria-based healing agents (i.e., granular Basilisk© healing agent), two very recent projects include an underground parking garage (Rotterdam, Netherlands) and a water tank (Sapporo, Japan). The latter is part of a main water purification project and will require 5000 m^3 of BBSHC when completed [118].

5. Limitations of BBSHC and scope for modelling

After more than two decades since its first reported application, MICP is considered a process that may be conveniently exploited in building materials, but it does not provide yet consistent and cost-effective solutions [119,120]. Despite the relatively extensive set of reported experimental results, there are still various aspects of MICP in concrete that are not fully understood, due to the complexity of the underlying mechanisms, and indeed there are conflicting results in the literature for similarly performed experiments, as remarked also by other authors [42]. Extensive research is required to understand the genetic factors associated with MICP for different pathways, as this will guide the selection of the most suitable species for a particular application [121]. Spore production and encapsulation are expensive processes, so it is necessary to find low-cost solutions to make BBSHC an accessible product [14,34]. Many studies report improved mechanical

properties of BBSHC after cracking and healing, but they draw this conclusion mostly based on compressive strength and water permeability tests, which are not necessarily representative measures as they do not reflect the more complex stress states in concrete structures [37].

Currently, the development and improvement of new and existing BBSHC solutions relies entirely on experiments, which are rather expensive and necessarily slow, due to the long timescales of concrete degradation, especially in field trials and large-scale applications. Another aspect that is slowing down progress is that different research groups often use different experimental set-ups and protocols for testing self-healing solutions and for measuring their effectiveness. This lack of standardization is currently a key barrier for the development and commercialization of BBSHC [122,123]. All these aspects create scope for modelling and simulation to complement the experimental efforts. Albeit still scattered to some extent, the current body of experimental results have largely uncovered the main mechanisms in biomineralization, creating the basis for modelling to rationalize these mechanisms across different experimental protocols and include them into predictive tools that can help integrate, validate, and even design future experiments. Indeed, it has been recognized that realistic numerical simulations could significantly accelerate the development of microbial self-healing technologies [36]. Such models and simulations would have to address the multiple length and time scales of biomineralization and concrete degradation, to ultimately optimize the cost, production, and efficiency of BBSHC, towards a wider and faster adoption in construction.

6. Mathematical modelling approaches

The current paucity of realistic numerical simulations of MICP is largely due to the complexity of the process, which takes place across multiple time and length scales, and involves coupled biological, chemical, mechanical, and hydraulic phenomena. In this section we present independent developments in molecular simulations [<10 nm] of mineral phases and bio-relevant systems, such as proteins and membranes. We then move up to the mesoscale [< 100 μm], presenting again separate developments for mineral and biological systems. The mesoscale approaches provide the starting point to consider coupled simulations aiming to describe the representative elementary volumes (REV) for MICP and BBSHC systems. The current literature only features a couple of mesoscale simulations of MICP, not yet applied to BBSHC, which offers an opportunity for future contributions. Subsequently we present current macroscale simulations [greater than100 μm] of MICP; also in this case there are very few works, none of which addresses BBSHC despite a richer literature exists on other types of self-healing concrete [46,49].

The transition from mesoscale to macroscale models highlights the current paucity of methods to develop constitutive laws for MICP simulations. A few contributions in this area are identified and presented in some detail. At the macroscale, we are including also some microbial self-healing models which were proposed and tested mainly for sand columns or soils as some of their findings are relevant also for cementitious materials; indeed, many of the underlying physical processes governing the self-healing response are common between the two materials. The question on how to derive constitutive laws from scaling-up results of mesoscale simulations is thus presented, in general for self-healing processes in concrete, but also particularly for MICP and BBSHC. Finally, we provide an overview of current machine-learning approaches to address the complexity of MICP, to potentially enhance and, in some cases, even replace altogether the demanding, physics-based simulations.

6.1. Models at molecular scale

At the molecular scale there is an established literature on atomistic models and simulations of cement minerals, including anhydrous and hydrated phases and with emphasis on calcium – silicate – hydrates (C—S—H), which are the main binding phase in ordinary cement pastes [124], see Fig. 2 (A). The main techniques at this scale range from full *ab-initio* simulations to atomistic simulations based on force fields, to coarse-grained approaches still with molecular resolution, such as the primitive model. Many properties have been computed using these techniques (see recent reviews, e.g. [129–131]), also for cement phases beyond C—S—H [132–135]. In the context of self-healing concrete, albeit not for MICP, the most relevant efforts are those concerned with interfacial properties and interactions between cement minerals and other phases, typically organic ones. The interested reader can find a brief review of molecular simulations of the interactions between C—S—H and carbon nanotubes here [48], a more extensive review of the interactions between cement minerals and admixtures here [136], and simulations of interactions between cement minerals and polymers leading to self-healing capabilities here [137]. The lack of molecular simulations of cement minerals in the context of MICP is probably due to the complexity of the process and of the molecules and reactions involved. However, there may be scope to explore some fundamental parts of the process, such as how the cement minerals interact with extracellular polymeric substances or with selected portions of a bacterium's membrane.

On the modelling of bacteria, molecular dynamics (MD) was used for simulating protein structural dynamics that are intrinsic to biological processes or the complex membranes or bacterial flagellum [126,138,139]. These models consist of tens of thousands of protein molecules and tens of different kinds of proteins (see Fig. 2 (C)). Systems with even further complexity may be attained through developments in coarse-grained molecular simulation [140] and with the progress of computing power; however, increasing the complexity of the simulations may not be needed for simulating bacteria in MICP models. By contrast, the analysis of subsystems with limited size and complexity may suffice to understand mechanisms and processes and, eventually, to inform larger-scale simulations. For example, one aspect which may be of interest to simulate by MD is the extrapolymeric substances and the pili on the surface of the cells, since the interaction between bacterial cells and minerals is dominated by interfacial processes, whereas the internal structure of a cell plays only a minimal role.

6.2. Models at mesoscale

The mesoscale between 10 nm and 100 μm is crucial for microstructure development and degradation in the cement paste, which largely control the macroscopic properties of concrete. The paste is a multi-phase systems and various models have focused on simulating the spatial, kinetic evolution of solid and liquid phases during hydration and aging. The seminal review in [141] provides a good introduction of some of the main models addressing microstructure development. An important limitation of these models, however, is that they do not predict the evolution of mechanical stress and deformations accompanying the chemical transformations. Such mechanical aspects are essential to describe degradation phenomena (and thus self-healing) in concrete, e.g. crystallisation pressure [142], eigenstress relaxation during creep [143,144], and drying shrinkage [145]. A focus on mechanical interactions and related processes characterizes a more recent class of particle-based, mesoscale simulations of cementitious materials [146]. These simulations are based on a rigorous statistical mechanical framework, coarse-graining the interactions between millions of atoms into potentials of mean forces between larger coarse-gained units or, in other words, effective interaction potentials between nanoparticles. To date, particle-based simulations have focused almost exclusively on C—S—H, capturing a wide range of structural, physical, and mechanical properties for this phase. Extension to other cement minerals is however well in reach of current capabilities, e.g. [147] on interactions between C—S—H and fly ash particles. In a recent development, chemical transformations between aqueous and solid phases, modelling

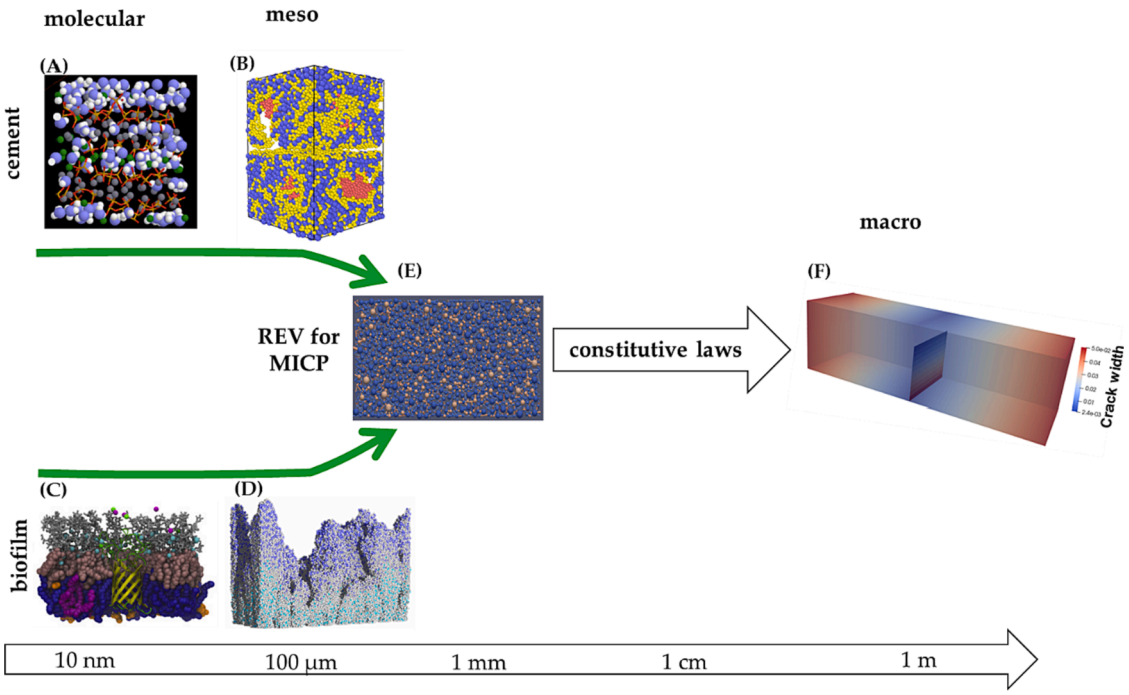

Fig. 2. Scales for representing the MICP process. (A) A molecular model of calcium – silicate – hydrate (C—S—H): the blue and white spheres are oxygen and hydrogen atoms of water molecules, respectively; the green and gray spheres are inter and intra-layer calcium ions, respectively; yellow and red sticks are silicon and oxygen atoms in silica tetrahedra (reproduced with permission from [124]). (B) Kinetic Monte Carlo simulation of autogenous healing (blue C—S—H; red CH; yellow $CaCO_3$) (reproduced with permission from [125]). (C) Molecular dynamic simulation for the outer membrane of Gram-negative bacteria (reproduced with permission from [126]). (D) Bacterial growth as biofilm under limited oxygen conditions, as it may develop inside a cement crack: blue spheres are bacteria, cyan spheres are inert particles, and grey spheres are extracellular polymeric substances secreted by bacteria (reproduced with permission from [127]). (E) Pore-scale distributions of the biofilm volume fraction in a packed sand porous media used to simulate MICP (reproduced with permission from [128]). (F) Simulation of a crack plane in the centre of a concrete beam with a contour of the crack width. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

microstructural evolution, have been implemented alongside mechanical interactions in particle-based simulations, exploiting the Kinetic Monte Carlo framework [148]. Thus far, these new chemo-mechanical simulations have addressed C—S—H precipitation [149], dissolution of tricalcium silicate [150], and recently carbonation of a C—S—H / $Ca(OH)_2$ system [125], as a first example of autogenous self-healing mechanisms in concrete. In all these endeavours, however, the biological component is still absent.

Individual-based Models (IbM) of microbial systems employ a discrete modelling framework analogous to that of the above-mentioned particle-based simulations of minerals. IbM is arguably-one of the most promising frameworks to include the bacterial component in BBSHC modelling. In IbM, bacteria are represented as rigid discrete particles, each of which is associated with a set of properties such as mass, position, and velocity [112,127]. These properties are affected by internal or external processes (e.g., diffusion), resulting in microbial growth, decay, motility, etc. The models represent the interaction of bacteria with each other and with the environment (Fig. 2(D)). The individual representation of bacteria allows the inclusion of a specific metabolism [151] or genetic circuits and metabolic pathways [152], and the calculation of the local pH, an important factor in self-healing.

6.3. The REV for BBSHC

The previous sections 5.1 and 5.2 have discussed separate developments in simulations of mineral and biological systems. The next step is to combine these models of MICP and BBSHC at a mesoscale that is sufficiently large to extract constitutive behaviours for larger scale models, viz. to simulate a representative elementary volume (REV).

One biomineralization model which explicitly includes the biofilm development at the REV scale was proposed by Zhang and Klapper [153]. The model consists of three phases (calcite, biofilm and solvent; calcite and biofilm are considered viscous fluids), each represented by its own volume fraction, which satisfies conservation of mass and momentum laws with addition of a free energy of mixing. In the computational domain were included the solvent (unspecified), biofilm, dissolved urea, and calcium chloride. Urea hydrolysis is catalysed by ureolytic bacteria and the subsequent carbonate species distribution leads to the formation of carbonate ions. In the presence of soluble calcium ions, calcite precipitation occurs once its saturation state exceeds a critical level. The 2D numerical simulations qualitatively reveal essential temporal and spatial features of biofilm induced calcite precipitation, as well as the significant impact of flow on its distribution (Fig. 3). Their model does not include the cement component of BBSHC.

A second example of MICP simulations was developed for a packed sand porous media by Qin et al. [128] and includes a comprehensive pore-network model which includes ureolytic biofilm evolution, considering its growth, decay, attachment and detachment. They have used a novel pore generator by initially randomly filling predefined pore bodies in a given computational domain. Their results showed that the calcite precipitation is dependent on the biofilm distribution (Fig. 4). This suggests that the models including a constant ureolysis rate may not give a fair representation of the MICP process.

The two simulation works presented in this section are the only ones in the literature addressing MICP at the REV level as we defined it here; mesoscale simulations of BBSHC instead are still to be attempted. One common limitation of the aforementioned simulations, in the context of BBSHC, is that the mineral part of the domain (except for the $CaCO_3$) is not evolving during the simulation, accompanying the evolution of the biofilm and of the solution chemistry. To include this coupling between mineral and biological components, future endeavours could leverage the developments on discrete mesoscale models of mineral and biofilms

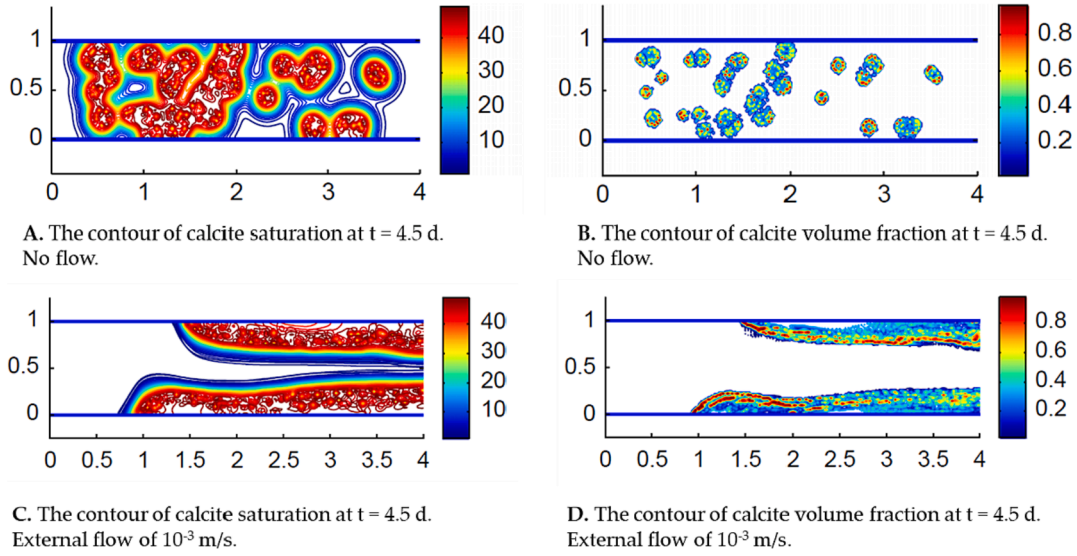

Fig. 3. *Top*: a 2D simulation of biofilm induced calcite precipitation without external flow, ureolysis rate coefficient $k_{urea} = 0.2\ day^{-1}$. The contour of calcite saturation peaks (A) and the contour of calcite volume fraction (B) coincide closely with the biofilm colonies. *Bottom*: a 2D simulation of biofilm induced calcite precipitation with external flow of 10^{-3} m/s, $k_{urea} = 0.2\ day^{-1}$. The calcite saturation peaks (C) and the calcite volume fraction (D) coincide with the biofilm region but the external flow impacts both. Computation domain size 1 mm by 4 mm. (reproduced with permission from [153]).

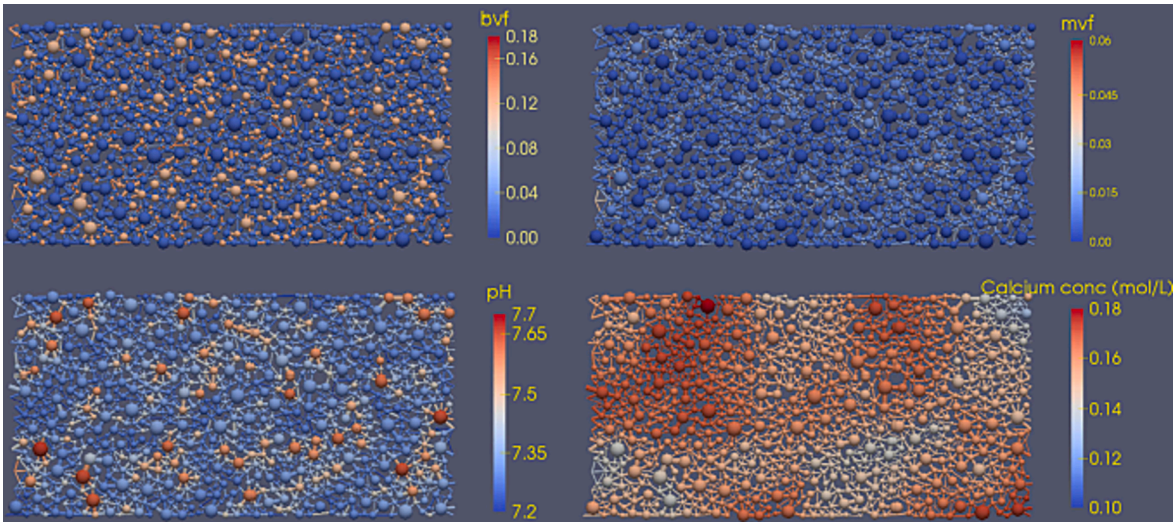

Fig. 4. Pore-scale distribution of biofilm volume fraction (bvf), calcite volume fraction (mvf), pH value, and calcium concentration in the simulation domain 40 mm < x < 60 mm. (reproduced with permission from [128]).

presented in the previous section 5.2. Such a combination has indeed been recently proposed for BBSHC as part of the EPSRC project EP/S013997/1 *Engineering Microbial-Induced Carbonate Precipitation via meso-Scale Simulations* [154], where that Kinetic Monte Carlo was used for the mineral and IbM for bacteria. Mesoscale simulations will likely be computationally expensive but may allow testing a wide combination of cement chemistries and bacterial metabolisms before experimentation, moving the BBSHC from being mostly lab driven to a cycle of design-build-test-learn as used now in Synthetic Biology [155].

6.4. Models at the macroscale

Modelling MICP at the macro scale requires the selection of a reasonable model-domain size, initial and boundary conditions, and determining the initial distribution of porosity and permeability [156].

Nassar et al [157] aimed to predict MICP under controlled conditions in a metre-scale tank with transient nonuniform transport in a natural soil, using independently determined parameters. The governing equations for the multicomponent reactive transport model were solved with an established simulator (PHT3D; [158]). They have concluded that a simplified bacterial growth, with the microbes considered exclusively sessile and with constant activity, will give a good representation of the process leading to nonuniform calcite precipitation. However, Minto et al. [159] have showed that, in the systems where there is a significant flow as, for example, in porous systems with multiple injection cycles, it is necessary to model the bacterial attachment as a function of fluid velocity rather than considering them strictly sessile. Their field-scale reactive transport model of MICP [159] captures the key processes of bacteria transport and attachment, urea hydrolysis, $CaCO_3$ precipitation, and modification to the porous media housing the bacteria (e.g. soil or concrete) in terms of porosity and permeability.

Wijngaarden et al. [160] examined four different reaction models in the simulation of MICP in a 5 m column. The results of the simulations showed that whilst all four models captured the average final calcite

concentration, there were large variations in the predicted profiles. The authors concluded that to better capture the experimentally observed behaviour, more advanced models are required. Wang and Nackenhorst [161] performed numerical analyses of the coupled mechanisms in MICP for soil treatment and showed that the spatial distribution of the precipitated calcite is heavily dependent on the bacterial distribution and the relation between the reaction rate and mass transport rate. In further work, Wang and Nachenhorst [162] extended their model to include both the mechanical behaviour of the medium, including the increase in stiffness with MICP, and micro-structural effects on the reaction kinetics. The comparison of simulations with experimental data showed that the coupled bio-chemo-hydro-mechanical model gave a reasonable prediction of the test results.

Zemskov et al. [50] proposed a simple two dimensional model to describe bacterial crack healing. Bacteria and the nutrients (calcium lactate) were considered embedded in a clay capsule which breaks at the appearance of a crack (Fig. 5). The model considers a circular capsule section of radius *R* broken in two equal parts by a streak of width *w* representing a crack that passes through the centre of the capsule (one quarter of the domain is solved due to symmetry; the number of bacteria doubles each hour). The simulations showed that the crack is completely healed after 72 h, though no details are included on the chemistry of the cement side. Previous work of the same research group has reported an analytical model to represent the probability that a crack hits an encapsulated particle, allowing to estimate combinations of crack lengths, capsule size and mean intercapsule distance in order to analyse the potential of bacteria to act as a catalysis of the self-healing process [51]. Their results showed that a fully random distribution requires the placement of fewer capsules compared to a layered random allocation. Their work was followed by other models focused on the probability that a crack will hit the capsules containing spores/bacteria and their nutrients [163,164]. A different approach for simulating calcite precipitation in a crack considered that only urea was contained in a capsule, while bacteria, nutrient and calcium where assumed to exist in the concrete matrix and distributed homogeneously [55]. In further work on a related theme, Romero Rodríguez and co-workers [165] used a 2D lattice model to explore the changes that occur in the interface zone around polylactic acid (PLA) capsules containing bacterial spores of *Bacillus cohnii*-related strains and nutrient inorganic salts. The results showed that the mechanical properties were lower in the interface zone in the self-healing samples than in plain cement-paste specimens but that the properties varied greatly depending on the shape of the PLA particle. It was concluded that the model would be useful for optimising the interface properties for particular damage scenarios.

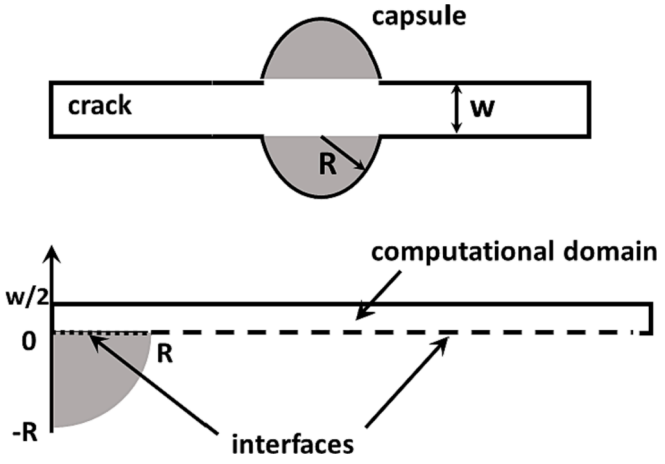

Fig. 5. Schematic representation of a crack of width w hitting a capsule section of radius R filled with bacteria and nutrients and the computational domain for the 2D model (adapted from [50]). Solved for R = 1.5 mm, w = 1 mm.

Overall, the aim of these models was to give directions for the manufacturing of self-healing materials with embedded capsules containing the healing agent, but they give little or no consideration to the cement chemistry or to the details of the biological component.

In their work, Xin et al. [166] focused on MICP in discrete cracks and the associated regain in mechanical properties in ceramic and cementitious materials. The MICP process was modelled as the nucleation of calcite crystals around bacteria located on the crack surface, that then grow to form pillar-like structures that bridge the crack. The decomposition of urea, production of urease, precipitation of calcite and changing concentration of bacteria were considered. The results of the bio-chemical model fed into a cohesive zone model that described the mechanical damage-healing behaviour. Despite some simplifying assumptions made in the bio-chemical model, simulations of a three-point bending test showed a good match to experimental data in terms of both pillar diameter, area coverage and mechanical regain.

An important limitation of the existing models is their complexity, leading to high computational costs which limit the size of numerical simulations and force the authors to simplify them even further in order to make them amenable for field-scale application [156,167,168]. Some authors argue that small-scale parameters may not be relevant when modelling at larger scale [157] and propose the elimination of much of the complexity of bacterial growth. However, oversimplifying the bacterial component can lead to unrealistic models which will not be useful in design. This highlight the need to construct targeted constitutive laws at the relevant REV scales, which is an area whose development for MICP in BBSHC is still in its infancy.

The computational cost associated with such models was investigated by Feng et al. [169], who compared the performance of an operator splitting (OS) approach, that splits the problem into two parts, a transport step and a reaction step, to a fully coupled globally implicit (GI) approach. The authors found that whilst the GI approach was computationally more efficient, it also required a greater amount of computer storage than the OS approach. In their work, Scheurer et al. [170] addressed the issue of model complexity through the application of Bayesian model selection (BMS) to the MICP problem. Three models of varying complexity were considered and their performance in simulating a column experiment was evaluated. The results of the BMS revealed that, for this problem, the most comprehensive model was not the optimum choice, due to the trade-off between accuracy and model complexity (BMS follows the principle of Occam's razor).

Models at the crack scale show just one possible approach to develop constitutive models for larger-scale analyses. Other approaches exist and some have been used to derive constitute equations for self-healing concrete, albeit not from MICP, e.g., computational homogenization techniques and inverse continuum damage models. The frontier now is to leverage these techniques in combination with simulations at the REV level, for a bottom-up workflow leading to constitutive laws that capture the role of the chemical composition and microstructure of the material. This would complete the multi-scale description of BBSHC and provide a method to support and enhance the development of such solutions in the future.

6.5. *Models using machine learning approaches*

One of the barriers in developing physical, multi-scale simulations of MICP and BBSHC lies in the complexity of the processes, which involve a large number of species and reactions. The large amount of available experimental data addresses how some combinations of materials and exposure conditions translate into self-healing behaviours. However, reproducing all those scenarios consistently through physical simulations is a challenge that is still far from being met. One way to enhance the physical simulations and rationalize the large amount of experimental data is to take advantage of machine learning (ML) techniques. This was attempted first with autogenous healing, with one of the first examples being given by Suleiman and Nehdi [171] who have predicted

the efficiency of autogenous healing (measured as the closing of the initial crack) with artificial neural networks (ANN) and genetic algorithms (GA). They have used a database with 1462 data points and selected eleven input parameters to train the ANN. The selected parameters encompass the factors controlling self-healing in cementitious materials including water to cement ratio, initial crack width and healing time. The output of the model was one single neuron representing the final crack width. Their work was followed up by more sophisticated ML approaches [172] based on a similarly large experimental data sets from literature (1417 data points), when six algorithms were compared for their ability to predict the autogenous healing performance of concrete. A similar example was very recently reported by Chen et al. [173], with the difference that they have generated their own experimental data. This ensured more uniformity of the training data, but the number of data points was smaller.

ML approaches were further used for evaluating the crack repairing capacity of BBSHC. Using a dataset of 1223 cases from literature, Zhuang and Zhou [174] have predicted the crack repair based on the number of bacteria, the healing time and the initial crack width. Because of the scattered experimental results and the lack of data on other variables influencing the crack healing, their results have limited applicability. However, such approach can be used in concrete design. Another interesting approach is to use ML models only for some of the processes involved in BBSHC, as recently ANN were considered for modelling the contribution of bacterial cells as nucleation centres in MICP [175]. ML models can also be employed as 'surrogates' for complex or computationally demanding models. Oyebamiji et al. [176] presented a surrogate model of the IbM presented in [127], based on Gaussian process emulation. The aim of the work was to show how microscale processes could be considered in macroscale models in a computationally efficient way. Once fitting was complete, the authors found that the surrogate model was around 220 times more efficient in terms of computational cost than the IbM. Scheurer et al. [170] employed surrogate models based on arbitrary polynomial chaos expansion in their BMS to reduce the computational demand and therefore ensure the feasibility of their analysis.

These pioneer papers for prediction of self-healing performance of concrete based on ML show that multiple algorithms would need to be used to cross-validate the calculations and that extensive data sets are needed for a robust model. Such models can put the numerous experimental data at good use and help reconcile the apparently contradictory results. Moreover, advancement in ML should encourage the researchers to add their experimental results in centralized databases, similar to the ones used for genome and protein sequencing. Such a database would undoubtedly help with data-sharing and save significant time for individually screening the hundreds of experiments reported in literature.

7. Future perspectives/conclusion

So far, the biological self-healing of materials has brought a lot of optimism, but limited engineering progress was made in this area. If we want to understand and predict the true limits of this process, we will need effective, reliable, and detailed models to complement experimentation and practice at larger scales. A mathematical/design tool able to capture the main characteristics of the process and simulate the different conditions developed in the cement matrix is essential for making rapid progress in this area. The current macroscale models of BBSHC are informed at the constitutive level by simple models, typically at the single-crack level, which oversimplify the MICP process. The field however is now mature for individual based simulations of bacteria and cement minerals to be combined into more detailed and predictive simulations of coupled processes in MICP at the REV level. While the coupling is possible already, more progress is needed both on the mineral and on the biological simulations side to address the complexity of the processes at play. Molecular dynamics can help providing fundamental quantities informing the mesoscale simulations, especially on the interactions at the interface between the biological and mineral components, e.g. during $CaCO_3$ nucleation and growth. Finally, the handshake between experiments and simulations will be challenging and machine learning techniques could help. Ideally, the emerging field of BBSHC will be able to borrow the design-build-test-learn approach for engineering problem solving used in Synthetic Biology, at least in the initial development phases.

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Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

No data was used for the research described in the article.

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