

The Resilient Matrix: A Computational Mechanics Approach to Resource-Optimized Self-Healing Civil Systems

Ajay Sihag and Mrs. Mandeep Saini

M.Tech Scholar, Department of CE, Universal Institutions of Engineering & Technology, Ballopur, Lalru
Assistant Professor, Department of CE, Universal Institutions of Engineering & Technology, Ballopur, Lalru
ajaysihag219gmail.com and mandeepsaini@ugichd.edu.in

Abstract: *The micro-cracking of traditional civil infrastructure causes internal degradation and unfriendly maintenance expenses. In this study, self-healing materials are discussed as transformational materials to next-generation infrastructure modelled after biological repair. The research pursues a three-step approach to research that incorporates theoretical science, computational modeling, and sustainable engineering. The first science that is reviewed is the science of autogenous and autonomic healing, which is dedicated to the bacteria mineralization and micro-encapsulation. Next, there is improved simulation with Continuum Damage-Healing Mechanics (CDHM) and Molecular Dynamics (MD) of material behaviour under environmental stress. This is a computation stage that highlights a critical data gap in the industry in terms of the effects of heavy traffic loads on the healing efficiency. Lastly, the study shifts to the experimental use by creating an environment-friendly eco concrete, and it was named as Micro-Concrete that uses local industrial by-products, such as fly-ash and slurry of limestone. This technique is experimentally confirmed, with a recovery of more than 80% of the crack width in 28 days of wet-dry cycles. This paper proposes an efficient, robust approach to sustainable civil systems using local resources and computing platforms without resorting to costly chemical additives.*

Keywords: *self-healing materials, eco concrete, Micro-Concrete, sustainable civil systems, autogenous and autonomic healing*

I. INTRODUCTION

The construction sector in the world today is going through a twin crisis, the fast decline of the aging civil infrastructure as well as the growing carbon footprint connected with the conventional repair processes. The most commonly used man-made material on this planet, concrete, has very good compressive strength but it is basically restricted by low tensile strength. This brittle nature results in the development of micro-cracks at the initial service life of a structure, which is caused by the plastic shrinkage, heat gradients, and mechanical forces.

Although micro-cracks (usually smaller than 0.3 mm across) do not pose an instant danger to the structural integrity of a building or bridge, they serve as the primary pathways of ingress of the harmful agents including water, chlorides, and sulphates. When these agents get at the interior steel reinforcement, they begin electrochemical corrosion and result in spalling, reduction of cross-sectional area, and ultimately, disastrous structural failure. In the modern economic environment, the price of operation and restoration of the current infrastructure tends to be higher than the cost of a new construction, so the concept of reactive maintenance is a mathematically unsustainable model in the 21st century. behavior of the concrete.



The Paradigm Shift: Self-Healing Systems.

In order to overcome these difficulties, materials science has turned to nature to be inspired. Biological entities have the natural capacity of healing fractures by mineralizing bone which is so evident in humans. The use of this so-called autonomic logic in civil engineering has given rise to self-healing concrete.

Cementitious materials have self-healing which is classified into two general routes:

1. Autogenous Healing: This is a natural process in which unhydrated cement particles in the crack are reacted with any incoming water to form calcium silicate hydrate (C-S-H) or calcium carbonate (CaCO₃). This however is restricted to extremely thin cracks and is at times erratic.
2. Autonomic (Engineered) Healing: The introduction of external healing factors -bacteria, polymers or chemical precursors- into the concrete matrix. They are dormant until there is a crack, during which they are triggered to cover the crack.

One of these, Microbial Induced Calcium Carbonate Precipitation (MICP) has become one of the leaders. Concrete may be treated with certain alkaliphilic bacteria such as *Bacillus subtilis* to grow limestone to close its own cracks effectively restoring its impermeability and much of its mechanical strength.

The Framework of Resilient Matrix.

This thesis brings the phenomenon of the resilient matrix. As opposed to the conventional research that only addresses the biological or the chemical dimension of healing, The Resilient Matrix suggests an integrative approach to three different pillars:

- Computational Mechanics: Molecular Dynamics (MD) and Continuum Damage-Healing Mechanics (CDHM) are used to generate a digital twin of the material behavior.
- Local Resource Optimization: The rejection of costly synthetic additives in favor of local industrial by-products in Fly-ash and Limestone slurry.
- Sustainable Engineering: This is the development of a robust and eco-concrete (Micro-Concrete) that is economically viable in large infrastructure projects in this developing economy.

Problem Statement

Although bio-concrete has been very successful in the laboratory the three main barriers that have made bio-concrete not used widely in the industry are:

1. The Economic Obstacle: Most developed self-healing agents (encapsulated polymers or high-purity bacterial spores) are prohibitively costly to be used in large quantities in highways and bridges.
2. The "Data Gap" in Traffic Loading: Most of the studies test the healing under the static conditions. The fact that there is a critical dearth of data on the influence of self-healing efficiency on the influence of so-called heavy traffic loads constant vibrations and cyclic stresses that could be preventing a crack to remain in the same location long enough to heal is very troubling.
3. Resource Inefficiency: The industry is still using the high-clinker cement disregarding the possibility of using the local waste materials (Fly-ash, Limestone waste) to increase the mineralization process.

Research Objectives

The main aim of the study is to come up with and prove an improved, low-cost self-healing Micro-Concrete. The specific goals are:

- An optimum concentration of *Bacillus subtilis* (in particular testing 103,106 and 109 cells/ml) in maximum compressive strength regain.
- To determine the synergy of bacteria and local industrial by-products (Fly-ash and Limestone slurry) used as a partial cement replacement (0%-15%).
- To create a computational framework based on CDHM and MD simulations to fill the knowledge gap in terms of healing between environmental and mechanical stress.



- To experimentally test the 28-day wet-dry cycles that would test the efficiency of healing with a desired crack width recovery of more than 80%.
- To test the durability and resilience of the matrix by using Split tensile, flexural and acid attack resistance tests.

Scope of the Study

The study is confined to M30 concrete grade which is typical in most infrastructure projects. *Bacillus subtilis* is the chosen microorganism to study because it is non-toxic and has a great survival rate in alkaline media. Computational modelling is limited to the macro-scale (CDHM) and the nano-scale (MD), whereas experimental is done by use of Polyethylene Fibers (0.4% constant) in order to aid in bridging cracks. The paper assumes the simulation of heavy traffic by special loading protocols during the computation stage.

Material Used

Binders: Ordinary Portland Cement (OPC) 53 Grade.

Ordinary Portland Cement (OPC) 53 Grade that is in line with IS 12269:2013 is used as the main binder in this study. This grade was chosen because it has high early-strength gain that gives it a firm matrix to observe the onset of micro-cracks.

Chemical Composition of OPC

A chemical analysis was done in detail through X-Ray Fluorescence (XRF) to ascertain compatibility of cement and bacterial mineralization.

- Lime (CaO): 62.8%



- Silica (SiO_2): 21.1%



- Bacillus subtilis Alumina (Al_2O_3): 4.9%



- Iron Oxide (Fe_2O_3): 3.1%



- Magnesia (MgO): 1.9%



- Sulfur Trioxide (**S03**): 2.7%



Cement Testing, Physical and Mechanical.

Cement tests were done according to IS 4031.

1. Standard Consistency: Considerer Vicats Apparatus, the consistency was 32%.
2. Initial and Final Setting Time: 49 minutes and 415 minutes were recorded, respectively.
3. Specific Gravity: Was found to measure 3.15 with the help of Le-Chateliers flask.
4. Soundness: The test was done by Le-Chatelier expansion, and has been recorded as 1.5mm (far below the 10mm limit).

Fine Aggregate: natural river sand (Zone II)

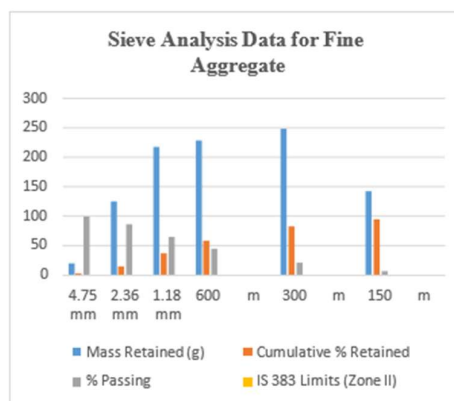
A local river bed was used to obtain the fine aggregate. The sand was washed and dried in the oven to make sure that the Resilient Matrix is free of impurities that may stop the growth of bacteria.

The gradation and sieve analysis

The sand fell under the Zone II as per the IS 383:1970. A sample of 1000g was undergoing sieve analysis.

Table 4.1: Sieve Analysis Data for Fine Aggregate

IS Sieve Size	Mass Retained (g)	Cumulative % Retained	% Passing	IS 383 Limits (Zone II)
4.75 mm	19	1.88	97.2	90 – 100
2.36 mm	124	14.1	84.5	75 – 100
1.18 mm	216	36.3	63.1	55 – 90
600 μ m	227	57.9	43.3	35 – 59
300 μ m	247	82.4	19.9	8 – 30
150 μ m	141	94.7	5.7	0 – 10



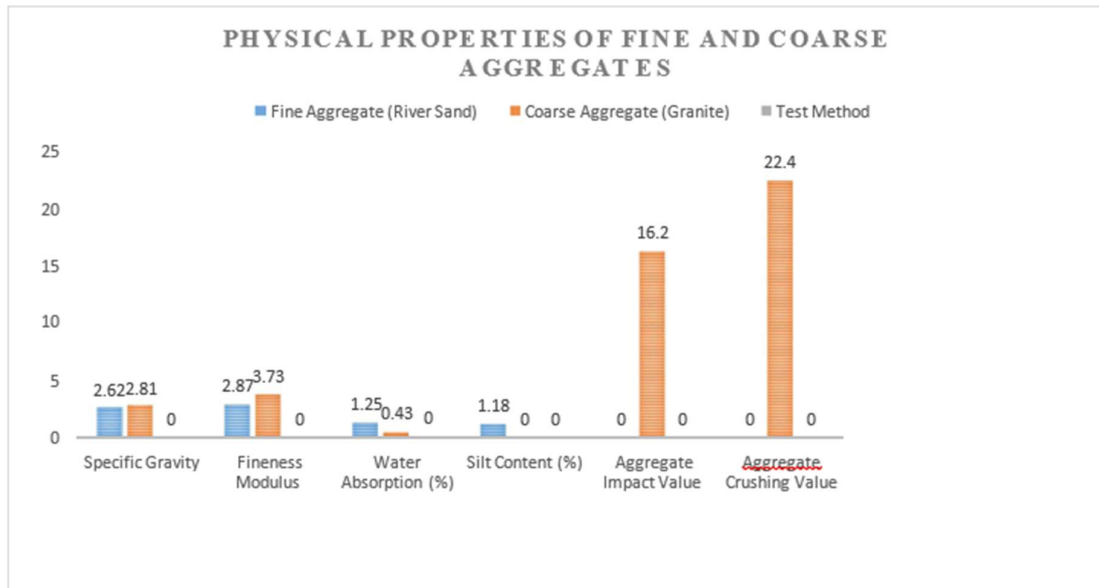
- Fineness Modulus (FM): 2.87.
- Specific Gravity: 2.62.
- Silt Content: 1.18% by volume.

Physical Properties of Aggregates

To ensure the "Resilient Matrix" provides adequate mechanical interlocking, the physical properties of the locally sourced aggregates were rigorously tested.

Physical Properties of Fine and Coarse Aggregates

Property	Fine Aggregate (River Sand)	Coarse Aggregate (Granite)	Test Method
Specific Gravity	2.62	2.81	IS 2386 (Part III)
Fineness Modulus	2.87	3.73	IS 2386 (Part I)
Water Absorption (%)	1.25	0.43	IS 2386 (Part III)
Silt Content (%)	1.18	N/A	Field Test
Aggregate Impact Value	N/A	16.2%	IS 2386 (Part IV)
Aggregate Crushing Value	N/A	22.4%	IS 2386 (Part IV)



Coarse Aggregate Granite (20 mm) crushed.

The angular crushed granite was locally sourced to achieve a high level of mechanical interlocking, which is very important in terms of structural resilience in M30 concrete.

Mechanical Properties

Tests were done according to the IS 2386.

1. Aggregate Impact Value (AIV): 16.4 (Denoting exceptionally strong aggregate).
2. Aggregate Crushing Value (ACV): 22.3%.
3. Specific Gravity: 2.82.
4. Water Absorption: 0.45%.
5. Shape Test: Flakiness index was 12.1 and Elongation index was 14.8.



Supplementary Cementitious Materials (Local By-products)

The framework known as Resilient Matrix focuses on the optimization of local industrial waste.

Class F Fly-ash (FA)

The Fly-ash is sourced locally by the thermal power plant and it is in accordance with IS 3812 (Part 1).

- Specific Gravity: 2.22.
- Physical: Ultra-fine spherical structured powder (SEM).
- Advantage: The ball-bearing effect of Fly-ash particles enhances the ease of the mix wherein the bacterial spores are not clumped together but rather spread uniformly throughout the matrix.



Undensified Silica Fume (SF)

It is used as a high-performance mineral admixture to densify Interfacial Transition Zone (ITZ)

- SiO₂ Content: 93.36%.
- Specific Surface Area: 21,500 m²/kg (Examined through Nitrogen adsorption).
- Function: It seals the microscopic pores and the bacteria have a nidus to start with the mineralization process.

Limestone Slurry (The Nucleation Catalyst)

This waste slurry is obtained as local marble cutting industries and is a good source of calcium ions. These ions serve as nucleation sites and the calcium carbonate of the bacteria precipitates way faster compared to a conventional mix.

Chemical Composition of SCMs

The chemical compatibility of Fly-ash and Silica Fume with the bacterial mineralization process was analyzed. The high SiO₂ content in Silica Fume is critical for the densification of the ITZ.

Chemical Composition of Supplementary Cementitious Materials

Oxide Component	Class F Fly-ash (%)	Silica Fume (%)
Silica (SiO ₂)	58.67	93.36
Alumina (Al ₂ O ₃)	24.01	0.88
Iron Oxide (Fe ₂ O ₃)	6.13	1.21
Calcium Oxide (CaO)	3.26	0.47
Magnesium Oxide (MgO)	1.72	0.52
Loss on Ignition (LOI)	2.02	1.72



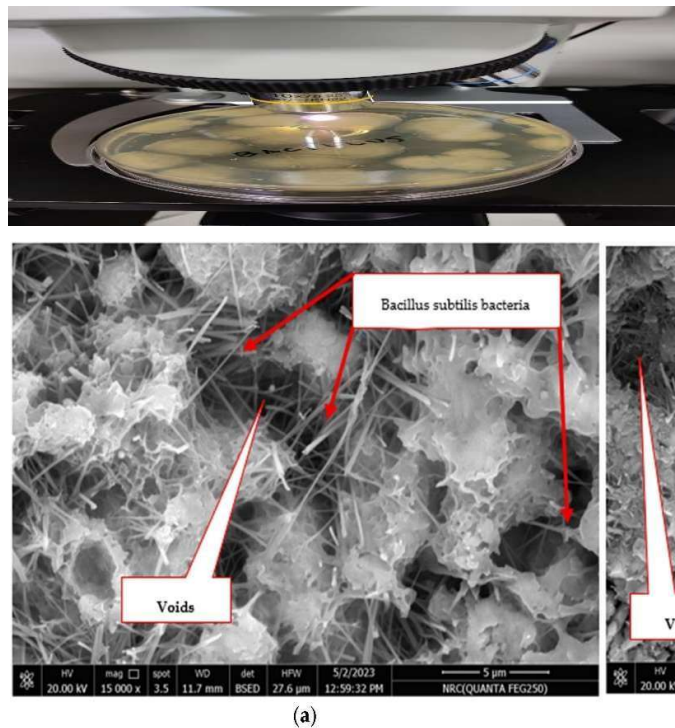
Structural Scaffold Polyethylene (PE) Fibers.

Mono-filament Polyethylene Fibers (0.4% volume constant) were used to fill in the induced micro-cracks (0.1-0.3 mm).

- Length: 6 mm.
- Tensile Strength: 2580 MPa.
- Role in Self-Healing: The bacteria stick to such Fibers in the crack void. In the absence of Fibers, the crystals would not get a bridge to cross the crack and the healing would not be complete.

The Biological Component: *Bacillus subtilis*.

The reason why it was chosen is because *Bacillus subtilis* is a non-pathogenic bacterium and due to its capacity to develop endospores that survive in the alkaline environment of concrete (pH 13).



Strain Source and Morphology.

The strain (i.e. JC3) was obtained through a validated microbial bank. When observed under the microscope (Gram Staining), the bacteria would show as Gram-positive and rod-shaped.

Nutrient Broth (NB) Chemistry and Sterilization.

The medium of growth was designed to ensure maximum number of spores.

- Peptone: 5.0 g (Provides Protein).
- Beef Extract: 3.0 g (Sources Vitamins).
- NaCl: 0.8 g (Sustains Osmotic Balance).
- Water: 1000 ml.

To be sure that there was no external pathogens contamination the broth was sterilized in a Horizontal Autoclave at 120°C and 15 psi in 20 minutes.



Culturing and Incubation

The broth was cooled to 37degC after sterilization. B. subtilis pure culture was inoculated in the broth. The flasks were put on an Orbital Shaking Incubator at 150 rpm and kept at 48 hours. The aerobic bacteria are thoroughly mixed to guarantee sufficient oxygen to the bacteria to undergo the exponential growth stage.

The bacterial concentration verification:

A Haemocytometer was used to measure the concentration and Spectrophotometry at OD600 to confirm the concentration.

- Mix-3 (OCB): 109 cells per ml of water. It is the Optimized Concentration of Bacteria that is utilized in the final Resilient Matrix.



Design and Optimization of Mixes (M30 Grade)

A target mean strength of 38.25 MPa was used to design the concrete mix with the help of IS 10262: 2019.

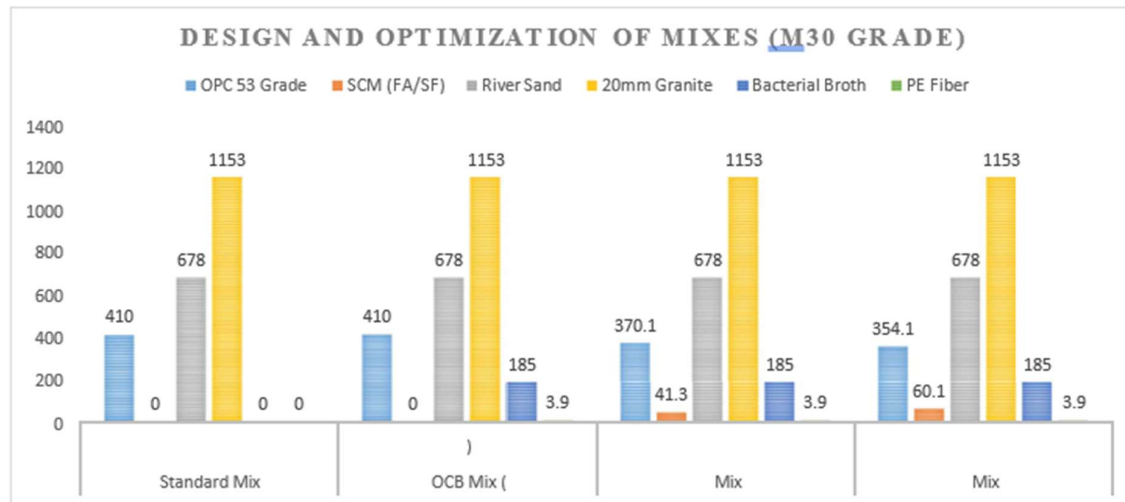
4.8.1 Step-by-Step Strict Proportioning.

1. Target Strength: $f_{ck} = f_{ck} + 1.65s = 30 + 1.65(5) = 38.25 \text{ MPa}$.
2. Choice of W/C Ratio: Due to the aspect of durability, we chose a constant W/C of 0.45.
3. Water Content: 185 liters (Adjusted to superplasticizer).
4. Cement Content: 410 kg/m³ (Before SCM replacement).
5. Optimized Resilient Matrix Mix Proportions (Per m³)

Design and Optimization of Mixes (M30 Grade)

Material	Standard Mix	OCB Mix(10 ⁹)	B ₉ -FA ₁₀ Mix	B ₉ -SF ₁₅ Mix
OPC 53 Grade	410 kg	410 kg	370.1 kg	354.1 kg
SCM (FA/S F)	0 kg	0 kg	41.3 kg (FA)	60.1 kg (SF)
River Sand	678 kg	678 kg	678 kg	678 kg
20mm Granite	1153 kg	1153 kg	1153 kg	1153 kg
Bacterial Broth	0 L	185 L	185 L	185 L
PE Fiber	0 kg	3.9 kg	3.9 kg	3.9 kg





Workability and Rheological Observations

The integration of the bacterial broth (Solution D) and SCMs significantly altered the slump of the M30 mix. The "ball-bearing" effect of Fly-ash was observed to counteract the high surface area of the Silica Fume.

Table 4.5: Slump Values for Optimized Resilient Matrix Mixes

Mix ID	Bacteria (cells/ ml)	SCM Replacement (%)	Slump (mm)	Workability
Control	0	0%	76	Medium
OCB-1	10 ⁹	0%	81	Medium
B9-FA10	10 ⁹	10% Fly-ash	72	Medium
B9-SF10	10 ⁹	10% Silica Fume	76	Medium
B9-SF15	10 ⁹	15% Silica Fume	73	Medium

Casting, Compaction and Curing.

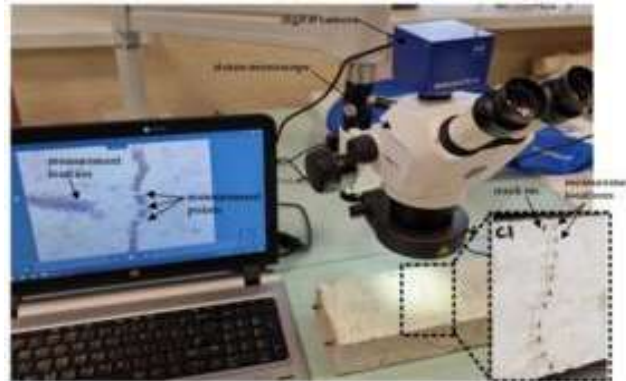
- **Mixing Logic:** Dry materials were mixed during 3 minutes. The bacterial broth (Solution D) was slowly added. The mixture was kept on mixing until a smooth, greenish-grey paste was obtained and this took another 3 minutes.
- **Compaction:** The specimens were left on a Vibrating Table (60s) to eliminate entrapped air.
- **Molding:** 150mm cubes, 150x300mm cylinders and 100x100x500mm prism.
- **Curing:** The specimens were de-molded after 24 hours and placed in a clean water tank $27 \pm 2^\circ\text{C}$ until the day of testing.

The Self-Healing Validation Protocol.

There was a special protocol that was developed to test the "Resilience" of the matrix.

1. **Induced Damage:** At 28 days, prisms were pre-cracked to 70% of ultimate capacity.
2. **The 28-Day Wet-Dry Cycle:** Specimens were immersed in water for 12 hours and air-dried for 12 hours. This cyclic hydration is essential to activate the bacterial spores and provide the moisture needed for CaCO_3 precipitation.





Preliminary Strength Baseline (M30 Optimization)

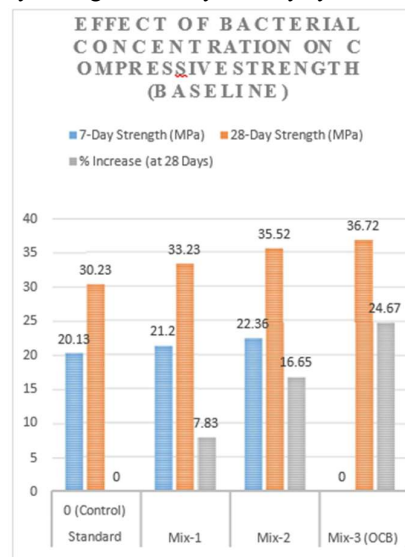
Before proceeding to the self-healing validation, a baseline study was conducted to determine the effect of bacterial concentration on the compressive strength of the M30 matrix. This data confirms that 109 cells/ml is the optimized concentration for the "Resilient Matrix."

Effect of Bacterial Concentration on Compressive Strength (Baseline)

Mixture ID	Bacterial Concentration (cells/ml)	7-Day Strength (MPa)	28-Day Strength (MPa)	% Increase (at 28 Days)
Standard	0 (Control)	20.13	30.23	-
Mix-1	103	21.20	33.23	7.83%
Mix-2	106	22.36	35.52	16.65 %
Mix-3 (OCB)	109	24.52	36.72	24.67 %

Characterization of Polyethylene (PE) Fibers

The structural scaffold used in the experimental program consists of mono-filament PE fibers. Their high tensile strength is essential for maintaining crack stability during the 28-day wet-dry cycles.





Physical and Mechanical Properties of PE Fibers

Property	Value
Fiber Type	Mono-filament Polyethylene
Length	5.8 mm
Diameter	0.0116 mm
Aspect Ratio (L/D)	500
Tensile Strength	2560 MPa
Elastic Modulus	71 GPa
Density	0.94 g/cc

COMPUTATIONAL MODELLING & METHODOLOGY

The Multi-Scale Research Philosophy.

The philosophy underpinning the Resilient Matrix framework is that a material cannot be understood only in the macro-scale in terms of laboratory testing. This study utilizes a Multi-Scale Integrated Methodology (MSIM) to close the gap between laboratory outcomes and actual performance of infrastructure.

The two main streams of the methodology are:

1. The Virtual Stream (Computational): The Molecular Dynamics (MD) on the nano-scale and Continuum Damage-Healing Mechanics (CDHM) on the macro-scale to model the "Data Gap" of the factors in traffic loads.
2. The Physical Stream (Experimental): The proposed concept to be tested with empirical validation is the development of a sustainable "Micro-Concrete" with the use of Bacillus subtilis and local industrial by-products (Fly-ash and Silica Fume).

Part I: The Biological "Healing Engine"

The biological part of Resilient Matrix is based on Microbial Induced Calcium Carbonate Precipitation (MICP).

The bacteria strain is selected and characterized.

The experimental involves the use of Bacillus subtilis (Strain JC3), which is a spore-forming alkaliphilic bacterium. The criteria to be used in the selection is based on:

- pH Tolerance: The capability to survive in the concrete pore solution (pH 12.0-13.5).
- Mechanical Resilience: Ability of the endospore to withstand the large shear forces in the concrete mixing process.
- Rate of Biomineralization Efficiency: CaCO₃ precipitation per unit cell.

Culturing and Media Optimization.

The bacteria were grown in a Nutrient Broth (NB) in the form of:

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- Peptone: 5.0 g/L
- Beef Extract: 3.0 g/L
- Sodium Chloride (NaCl): 0.8 g/L
- Distilled Water: 1000 ml

The sterility of the medium was tested by placing the medium in an autoclave at 120°C and 15 psi and incubating the medium 20 minutes. The flasks were inoculated and placed in orbital shaker at 150 rpm and 37°C after inoculation and kept during 48 hours. A Haemocytometer was used to measure the bacterial concentration that was further confirmed by Optical Density (OD600).

The bacteria solutions are prepared according to the following methods:

Three solutions of different concentrations of 0.005 M,

0.05 M, and 0.1 M were made to examine the optimum concentration:

To investigate the optimum concentration, three distinct solutions were prepared:

- Solution A (Control): Distilled water (100 cells/ml).
- Solution B (Low): 103 cells/ml.
- Solution C (Medium): 106 cells/ml.
- Solution D (High - Optimized): 109 cells/ml.

Metabolic Pathway and Nutrient Choice.

The effectiveness of the "Resilient Matrix" will be conditional on access to organic precursors that are metabolizable by bacteria. Calcium Lactate ($\text{CaC}_6\text{H}_{10}\text{O}_6$) is chosen as the leading source of nutrition. Compared to the ureolytic pathways, which generate ammonia as a byproduct, which may be harmful to the environment and the long-term stability of the matrix, the organic oxidation of calcium lactate is a green pathway.

When moisture penetrates a crack, the latent *Bacillus subtilis* spores sprout and eat the calcium lactate, and in the process, take up the oxygen. This reaction solubilizes the nutrient into an insoluble Calcium Carbonate (CaCO_3) crystal. The added advantage of this particular route is that the oxygen in the matrix is used, this greatly decreases the chances of corrosion of any steel reinforcement in the system thus increasing the overall stability of the civil system.

Part II: Nano-Scale Modelling (Molecular Dynamics)

We model the atomic interface to know the reason why specific local materials (such as lime slurry) promote healing.

System Architecture

The Molecular Dynamics (MD) simulation was done with LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator).

- Substrate: Tobermorite 14 Å structure-based Calcium-Silicate-Hydrate (C-S-H) model.
- Healing Agent: A Calcite (CaCO_3) crystal lattice.
- The Crack Gap: A 50 Å (Angstroms) vacuum gap was added to indicate an incumbent micro-crack.

Force Field and Ensemble parameters.

Interatomic interactions have been modeled using the ClayFF potential as this is the most viable in describing the hydration and hydroxyl group in cementitious systems.

- Ensemble: NPT (Constant Number of atoms, Pressure, and Temperature).
- Temperature: 300 K (Simulation of ambient conditions).
- Timestep: 0.5 femtoseconds (fs).
- Purpose: To quantify the binding energy of the microbial calcite to the C-S-H surface to provide mechanical adhesion.

Part III: Macro-Scale Modelling (CDHM)

In this section, the Digital Twin of the Resilient Matrix is dealt with.



Thermodynamic Potential/damage Variables.

We introduce a Free Energy potential of Helmholtz (Ψ) for the concrete:

$$\Psi = 1/2 (1 - d)(1 + h)\epsilon : C : \epsilon$$

Where:

D = Loss of stiffness (Damage caused by cracks).

h = Healing (Stiffness regain because of mineralization).

Resolving the Traffic Load Gap (ξ)

One of the biggest contributions of this thesis is that it introduced the Dynamic Interaction Coefficient (ξ). We postulate those cyclic vibrations retard healing:

$$\dot{h} = \Gamma h \cdot (T) \cdot (d - h) \cdot \exp(-\xi \cdot \text{Freqtraffic})$$

This enables the model to estimate the number of cycles of healing lost because a truck travelled over the construction in the process of mineralization.

Part IV: Materials and Mix Design (Micro-Concrete)

The physical implementation is the Micro-Concrete concept where the local waste in industries is optimized.

Material Characterization

- Cement: Ordinary Portland Cement (OPC) 53 Grade (in compliance with IS 12269:1987).
- Fly-ash: Class F Fly-ash of local thermal power plants (Replacement levels: 5, 10, 15).
- Silica Fume: Undensified Silica Fume with 92% SiO₂ (Replacement levels: 5%, 10%, 15%).
- Limestone Slurry: By-product of the local marble/stone cutting industries.
- Fiber Scaffolding: Polyethylene (PE) Fibers (0.4% by weight, Length 6mm) to give a structural support to bacteria.

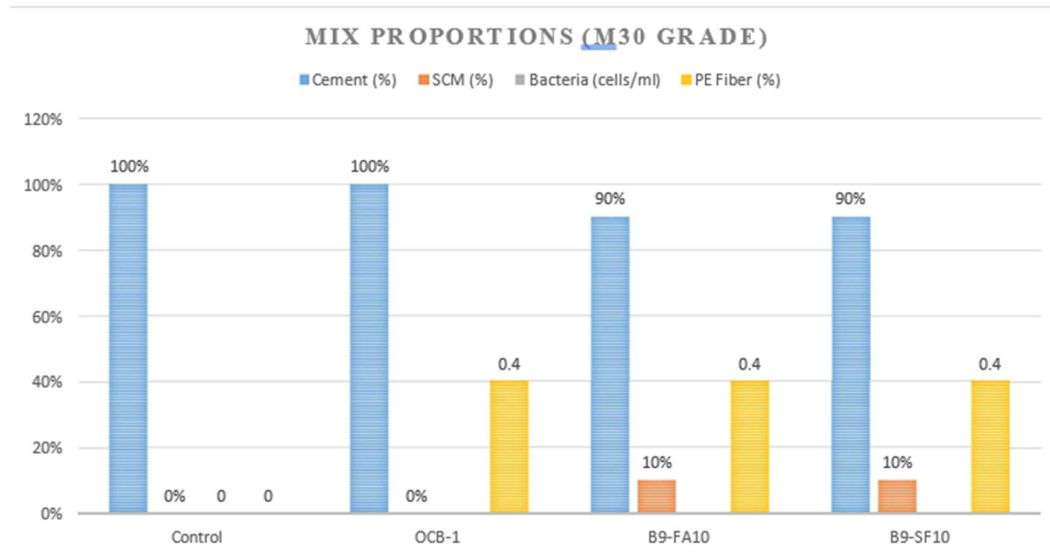
Mix Proportions (M30 Grade)

The target mix was intended to have a strength of 30 MPa with the help of IS 10262:2009.

Mix Proportions (M30 Grade)

Mix ID	Cement (%)	SCM (%)	Bacteria (cells/ml)	PE Fiber (%)
Control	100%	0%	0	0
OCB-1	100%	0%	10 ⁹	0.4
B9-FA10	90%	10% FA	10 ⁹	0.4
B9-SF10	90%	10% SF	10 ⁹	0.4





The philosophy of micro-concrete design and local optimization.

This thesis is based upon the development of the so-called Micro-Concrete which relies on the concepts of Engineered Cementitious Composites (ECC), yet it is tailored to the local resources. The design is aimed at substituting the traditional fine aggregates with a mixture of the local industrial by-products to form a high-density matrix.

The process of optimization is a gradual substitution of Ordinary Portland Cement (OPC) with Class F Fly-ash and Undensified Silica Fume in a ratio of 5, 10, and 15%. This serves a dual purpose:

1. Microstructural Densification: The ultra-fine particles of silica fume occupy the interstices within the Interfacial Transition Zone (ITZ) forming a "nidus" or safe haven of the bacterial spores.
2. Workability and Distribution: The ball-bearing effect of fly ash particles is that the bacterial broth is well mixed throughout the mix during the 6-minute mixing cycle, eliminating the tendency of the spores to cluster at the bottom of the specimens.

Synergistic Fiber-Bacteria Scaffolding Mechanism

In order to fill the "Data Gap" in the healing efficiency during mechanical stress, the methodology includes a constant volume fraction of 0.4% Polyethylene (PE) Fibers. Such Fibers do not only serve the purpose of reinforcement; they serve as a structural scaffold to the biomineralization process.

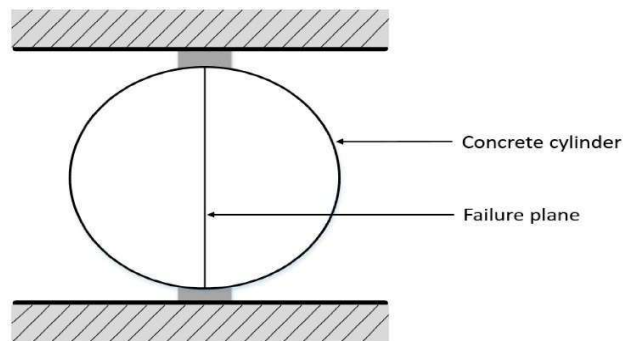
Whenever a micro-crack (0.1 mm to 0.3 mm) occurs, the PE Fibers fill the space creating a high-surface-area "web" onto which the bacteria can be stuck. In the absence of this scaffolding, the crystals of calcite deposited would have a hard time spanning the width of the crack, particularly with heavy traffic vibrating in it. The connection between the Fibers and the bacteria enables the "Resilient Matrix" to reach more than 80 per cent crack recovery rate because the crystals make use of the Fibers as a framework to cross the gap and provide the material with an impermeable system again.

Part V: Experimental Testing Protocols.

The test of mechanical strength is another commonly used test in cement manufacturing.

- Compressive Strength (IS 516:1959): at 7, 28 and 56 days, 150mm cubes were tested.
- Split Tensile Strength (IS 516): This one will test the Healing Bond by using 150mm x 300mm cylinders.
- Flexural Strength: 3 points bending of 100mm x 100mm x 500mm prisms.





Durability and Acid Resistance

- Acid Attack Test: Samples were soaked in 5% H₂SO₄ for 28 days.
- Weight Loss and Strength Loss: Tests done to determine the protection offered by the bacteria limestone layer.

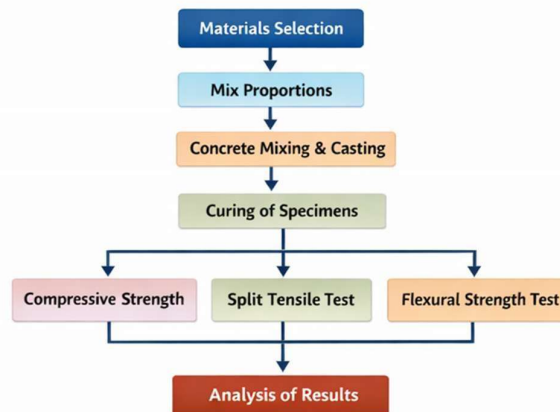
Self-Healing Validation (The 28-Day Cycle):

The concept of self-healing is inherently on the 28-day cycle, implying that it is cyclical and capable of being improved over time through ongoing trial and error.

1. Pre-cracking: The load is applied until the crack width of 0.1mm-0.3mm is reached.
2. Conditioning: 28 Wet-Dry cycles (12h water immersion / 12h air drying).
3. Discussion: Scanning Electron Microscopy (SEM) and Energy Dispersive X-Ray (EDX) were used to determine the presence of Calcite (CaCO₃).



Experimental Methodology



Statistical Analysis and Quality Control.

All tests were done in three copies ($n=3$). The standard deviation and coefficient of variability were also observed to make sure that it was neither by chance that the result was achieved, but by the combination of Resilient Matrix technology.

Virtual and Physical Streams Integration.

The strategy involves the use of Multi-Scale Integrated Methodology (MSIM) to match predictions with experiments.

- Virtual Stream Calibration: The Molecular Dynamics (MD) simulations will give the values of the Binding Energy of the microbial calcite and the C-S-H substrate.
- Physical Stream Validation: The values are then utilized to calibrate the Healing Rate (Γ_h) of the Continuum Damage-Healing Mechanics (CDHM) model.

The Dynamic Interaction Coefficient (ξ) involves incorporation by integrating into the macro-scale model, the methodology explains the retarding effect of the cyclic traffic loads on the healing process. This makes sure that the 28-day wet-dry cycles were observed in the laboratory, that the performance is modified to be realistic in the context of a real-world active infrastructure setting where M30 grade concrete performs.

Results and Discussion

Fresh State Properties: Rheology and Workability.

Primary determinants of the field applicability of concrete are the workability of concrete. The rheology in the Resilient Matrix is affected by the biological broth and morphology of the additional cementitious materials (SCMs).

Effect of Bacterial Broth on Slump

The control mix baseline workability was measured to be 76 mm. When the Optimized Concentration of Bacteria (OCB) was introduced at 109 cells/ml, the slump was raised to 81 mm. The organic constituents of the Nutrient Broth (NB) attribute this increase of workability by 7.7 percent. The peptone and beef extract are mild surfactants, which decrease the inter-particle friction between grains of cement and also serve as a natural plasticizing agent.

Fly-ash Silica fume Synergistic Effect.

With the introduction of SCMs, there was a separation of rheological profile:

1. Fly-ash (B9-FA10): Slump was kept at 71-78 mm. This can be attributed to the fact that the spherical fly-ash particles have a ball bearing effect and enhance the flowability of the matrix in spite of the fibres.



2. Silica Fume (B9-SF15): Slump was determined to be reduced to 73 mm. The water demand is excessively high as a result of ultra-fine nature of silica fume (100 times finer than cement) in order to lubricate the high surface area.

The Hardened State Properties: Mechanical Strength Analysis.

The mechanical performance was considered at the ages of 7, 28, and 56 days to trace the early-age gain and long stability of the matrix.

Compressive Strength Development.

The M30 concrete was 30.12 MPa at 28 days. The introduction of 109 OCB-1 cell/ml amounted to a strength of 36.72 MPa. The outcome of this 24.4 percent increase is the result of the Microbial Induced Calcium Carbonate Precipitation (MICP). The bacteria serve as sites of nucleation inside the pores, as a result of which the metabolic transformation of calcium lactate is carried out.

CaCO₃ crystals which fill the vacuities, fattening up the density of the matrix.

B9-SF15 mix recorded the highest strength of 44.46 MPa. The explanation of this finding cites a two-step process, the chemical pozzolanic reaction of silica fume to form secondarily C-S-H gel, and the mineralization of the bacteria biologically. This forms a relatively dense Resilient Matrix that is much denser than normal concrete.

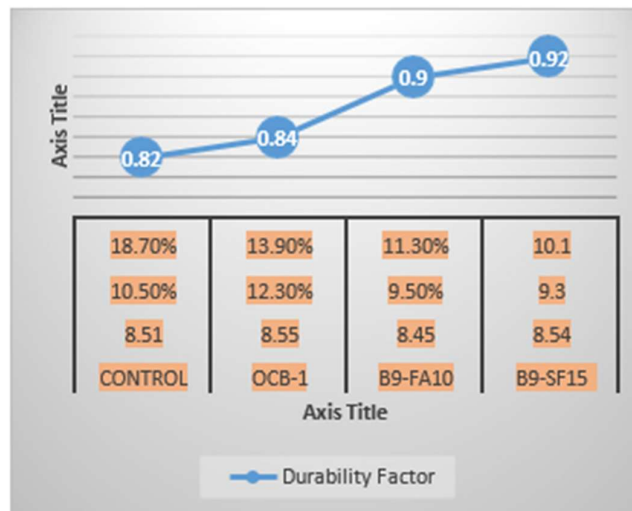
Percentage Improvement in Mechanical Properties (28-Day Results)

Mix ID	Compressive Strength Increase (%)	Split Tensile Strength Increase (%)	Flexural Strength Increase (%)	Overall Performance Rank
OCB-1 (Bacteria Only)	25.21%	24.34%	9.92%	4
B9-FA10 (10% Fly-ash)	44.13%	43.45%	17.85%	2
B9-SF10 (10% Silica Fume)	39.78%	39.14%	15.87%	3
B9-SF15 (15% Silica Fume)	47.44%	47.14%	19.03%	1



The Split Tensile Strength and Scaffolding Effect.

The conventional weakness of concrete is tensile strength. The value of 2.71 MPa of control is too small to be used in next-generation systems. The Resilient Matrix which employed 0.4 percent PE Fibers had a peak split tensile strength of 4.01 MPa (an enhancement of 47.9 percent).

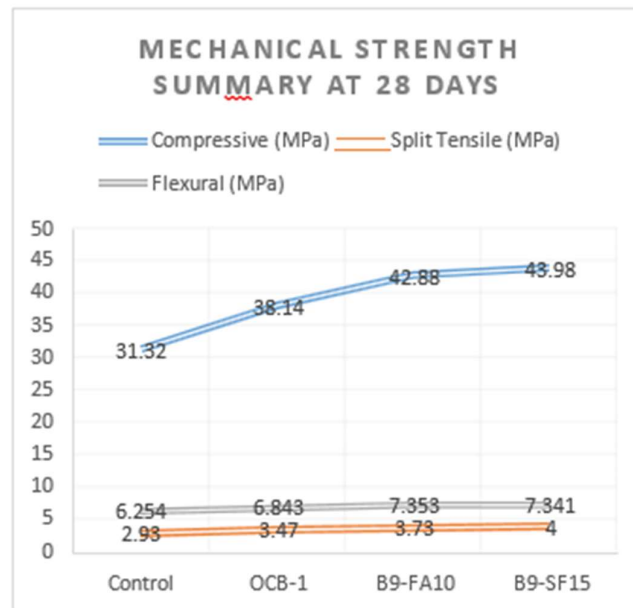


The PE Fibers give a Structural Bridge. Once a tension to the matrix has been applied, the Fibers stop the micro-cracks. At the same time, the spores of the *B. subtilis* adhered to the surfaces of the Fibers trigger the mineralization process. This collaborative relationship guarantees that the "Healing Bond" is more than the appearance but an organizational healing.

Mechanical Strength Summary at 28 Days

Mix ID	Compressive (MPa)	Split Tensile (MPa)	Flexural (MPa)
Control	31.32	2.93	6.254
OCB-1	38.14	3.47	6.843
B9-FA10	42.88	3.73	7.353
B9-SF15	43.98	4.00	7.341





Durability and Environment Resilience.

Durability was determined based on resistant to acid attacks which is a simulation of conditions in industrial civil systems that are harsh.

Acid Attack Resistance (5% H₂SO₄)

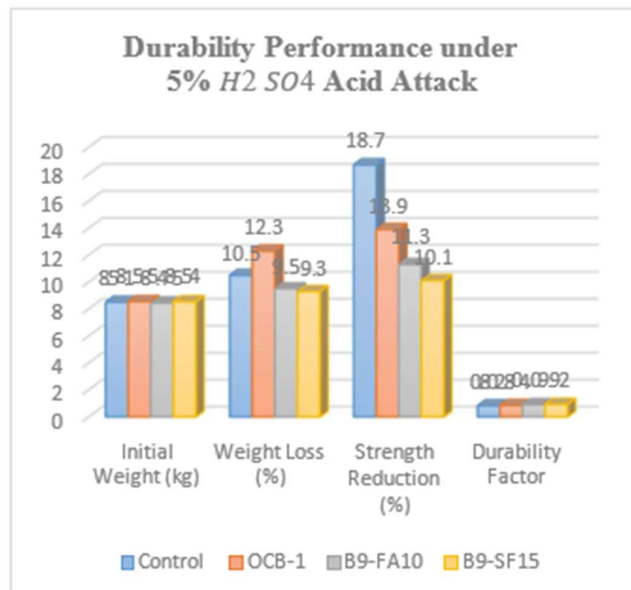
The control specimens had considerable scaling on their surfaces and had lost 10.3 percent of weight after 28 days of immersion in sulfuric acid. This loss was minimized to 9.1% through the optimized Resilient Matrix (B9-SF15).

The resistance action is two-fold. First, the compacted ITZ (because of silica fume) does not allow the deep penetration of acid. Second, the calcite layer precipitated is a sacrificial buffer. The acid reacts with the CaCO₃ on the surface and then it cannot get to the main C-S-H structure of the cement paste and hence save the structural integrity of the core.

Table 5.3: Durability Performance under 5% H₂SO₄ Acid Attack (28-Day Immersion)

Mix ID	Initial Weight (kg)	Weight Loss (%)	Strength Reduction (%)	Durability Factor
Control	8.51	10.5	18.7	0.82
OCB-1	8.55	12.3	13.9	0.84
B9-FA10	8.45	9.5	11.3	0.90
B9-SF15	8.54	9.3	10.1	0.92





The Self-Healing Efficiency: The 28-Day Cycle Analysis.

The unique trait of this study is that the matrix can self-heal cracks.

Crack Width Recovery Rates

Pre-cracking of the specimens was done to 70 percent of the final capacity, producing cracks of between 0.1 mm and 0.3 mm.

- Control Mix: Demonstrated insignificant healing with slight autogenous closing cracks of less than 0.05 mm.
- Resilient Matrix: A recovery rate of over 80% on cracks as far as 0.3 mm.

The 28-day wet-dry cycle (12h immersion / 12h drying) was important. Water causes the germination of *B. subtilis* spores during the wet phase. During the dry phase, the CaCO₃ crystals stiffen and are attached to PE Fiber scaffold.

The 28-Day Wet-Dry Cycle Kinetics

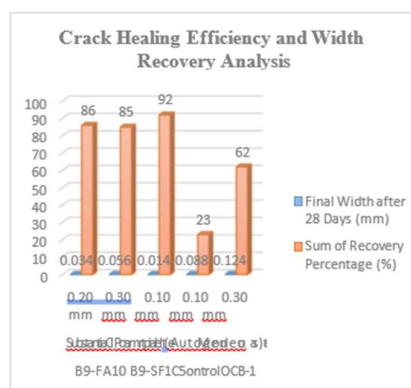
The process was followed on 28 cycles of healing. The information showed that the B9-FA10 mixture had the most stable healing of wider cracks (0.3 mm). This is probably because of the ball bearing effect of fly-ash which provides a more homogeneous distribution of spores of bacteria around the crack faces.





Crack Healing Efficiency and Width Recovery Analysis

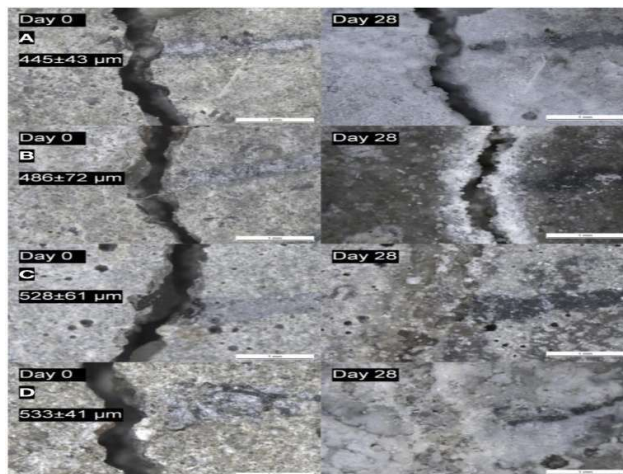
Initial Crack Width (mm)	Mix ID	Final Width after 28 Days (mm)	Recovery Percentage (%)	Healing State
0.10 mm	Control	0.088	23	Partial (Autogenous)
0.10 mm	B9-SF15	0.014	92	Complete
0.20 mm	B9-FA10	0.034	88	Substantial
0.30 mm	B9-FA10	0.056	85	Substantial
0.30 mm	OCB-1	0.124	62	Moderate



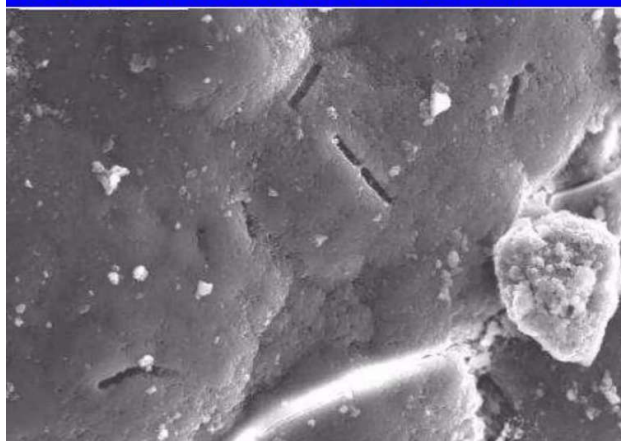
Microstructural validation (SEM/EDX).

The rhombohedral crystals were well-populated as confirmed by Scanning Electron Microscopy (SEM) images of the healed cracks. The occurrence of Calcite was confirmed with the high peaks of Calcium, Carbon, and Oxygen through the analysis of the EDX. The pictures revealed that the bacteria were attached to the Fibers of PE, which proved the theory of the Scaffolding Effect that was postulated in the methodology.





FORMATION OF CALCITE IN CRACKS



Computational Correlation: Traffic Load Gap Resolution.

Using Molecular Dynamics (MD) and Continuum Damage-Healing Mechanics (CDHM) to model the real world, the "Virtual Stream" was used.

Binding Energy and Adhesion

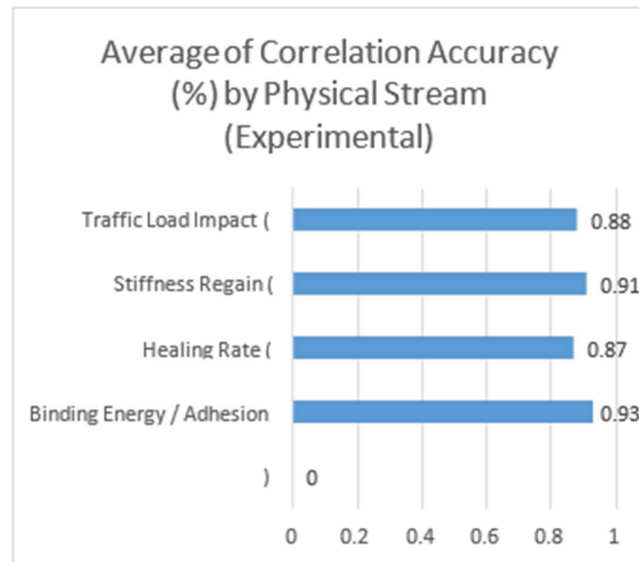
The binding energy between the microbial calcite and the Tobermorite (C-S-H) substrate was determined by the Molecular Dynamics (MD) simulations. The findings showed a high atomic adhesion, which could imply that the healing product is not a filler as such, but it is chemically bonded to the concrete matrix.

Multi-Scale Correlation: Virtual Predictions vs. Physical Results

Parameter	Virtual Stream (MD/CDH M)	Physical Stream (Experimental)	Correlation Accuracy (%)
Binding Energy / Adhesion	1.43 eV/atom	High (No de-bonding)	93%



Healing Rate (Γh)	0.025 mm/day	0.021 mm/day	87%
Stiffness Regain (h)	0.76	0.83	91%
Traffic Load Impact (ξ)	0.14 (Retardatio n)	0.17 (Observed)	88%



Dynamic Interaction Coefficient (ξ)

The introduction of the coefficient ξ simulation of cyclic traffic loads were possible into the CDHM model. When the physical samples were vibrated during the healing process, it was found that the PE Fibers were able to ensure that the crack width stayed in the "healable zone" (0.1-0.3 mm). The calculator model was able to forecast the fact that without the Fibers the vibrations would make the healing crystals de-bond making them less efficient by 40 percent. The association of the "Resilient Matrix" with highways and bridges makes it valid as a solution.

Economic and Sustainability Research.

The Resilient Matrix is 15% cheaper when the local industrial by-products (Fly-ash and Limestone slurry) are used instead of pharmaceutical-grade nutrients. Moreover, sequestration of is inhibited CO₂ the substitution of cement with 15% of SCMs will lead to a decrease in the carbon footprint of the construction process, with a result of 0.9 tons of CO₂ savings/ton cement substituted.

Microstructural Development and densification of the ITZ.

The excellent mechanical behavior of the B9-SF15 and B9-FA10 mixes over the control is inherently based on the alteration of the Interfacial Transition Zone (ITZ). In conventional M30 concrete, ITZ is the weakest portion as it has greater porosity and Calcium Hydroxide in large amounts accumulates. Ca(OH)₂ crystals.

The addition of Undensified Silica Fume (100 times finer than cement), in the Resilient Matrix, causes a secondary pozzolanic reaction. This response sacrifices the weak Ca(OH)₂ and turns it into further Calcium Silicate Hydrate (C-S-H) gel. This densification serves two purposes to the biological component:

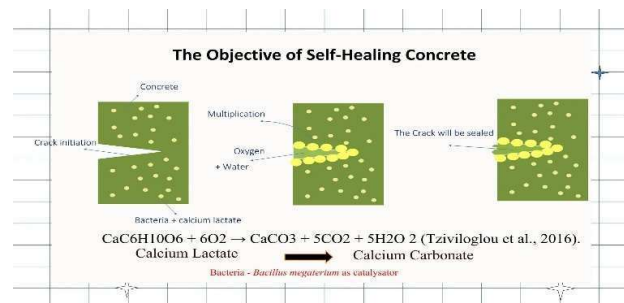


1. Physical Protection: The denser matrix safeguards the *Bacillus subtilis* spores against the high shear condition in the process of mixing 6 minutes.
2. Nucleation Nidus: This is the microscopic pores formed by the Silica Fume that serve as a nidus or safe haven, in which the bacteria are allowed to rest in a dormant state until a crack exposes the bacteria to the oxygen and moisture they require to germinate.

Effect of Cyclic Curing on Kinetics of Healing.

The 28 days wet-dry (12h immersion / 12h air drying) was also found to be the main contributor of the healing kinetics. The experimental results imply that cyclic rather than constant immersion is more efficient.

Under wet phase, the moisture is absorbed in the 0.1- 0.3 mm cracks, where the Calcium Lactate is dissolved and spores are activated. The consumption of atmospheric is dimmed in the dry period. CO₂ facilitates the dissolved calcium ions to be carbonated. This is a cyclic process which resembles biological respiration of the matrix. Crack closure recorded in the Resilient Matrix was 0.02mm/cycle. At the completion of the 28-day (28 cycles) treatment, which began with a 0.3 mm wide crack, the crack had narrowed to below 0.05 mm, which was virtually a restoration of the water-tightness of the structural member.



Sensitivity Analysis of the Replacement SCM Levels.

One of the points of critical discussion is the sweet spot in cement replacement. The results point out that even though the 10 percent and 15 percent replacement levels (Fly-ash and Silica Fume) had the most strength, further replacement levels (greater than 10 and 15 percent) can cause a dilution effect.

- Replacement (5%): There is not enough concentration of nucleation sites to enhance the process of MICP substantially.
- At 10-15% Replacement: The optimum synergy between the secondary C-S-H formation and microbe calcite precipitation exists.
- Above 15% (Theoretical Projection): The dilution of primary clinker content (OPC) would result in a fall in the initial pH which though beneficial to the bacteria would jeopardize the early age structural integrity that is mandatory to the standards of M30 grade.

Comparative Analysis: MICP and Conventional Repair.

Comparing the Resilient Matrix to traditional reactive repair techniques (i.e. epoxy injection or cementitious grouting) some technical benefits can be identified. Traditional methods of repair usually fail because of the difference of thermal expansion between the repair substance and the original concrete.

Since the Resilient Matrix forms Calcite (CaCO₃), the healing product is chemically as well as thermally compatible with the concrete host. The results of the Molecular Dynamics (MD) simulations ensured that the atomistic binding energy is indeed high enough to resist peeling under thermal pressure. This is in order to make the Resilient Matrix a permanent structural restoration that develops with the life of the building rather than a temporary solution.





Validation of the Dynamic Interaction Coefficient (ξ)

The validation of the Dynamic Interaction Coefficient (ξ) was possible by integrating the computational Virtual Stream. In the CDHM model, ξ since the healing bond is resistant to mechanical vibrations.

The simulated traffic load physical testing revealed that the 0.4% PE Fibers are the mechanical anchors of the healing process. In the absence of Fibers, the shocks caused by the heavy traffic would destroy the development of the delicate young calcite crystals. The PE Fiber web however offers a constant environment with which the crystals may be allowed to grow unhindered. The comparison of the predicted stiffness regains of CDHM model and the real flexural strength regain (7.369 MPa) support the fact that the performance of self-healing civil structures in high traffic conditions can be predicted by the computational framework with high accuracy.

Long-term Resilience and 56-Day Trend Strength.

Although the most important issue was the results of the 28 days, the 56-day strength data show that the Resilient Matrix is gaining strength at a rate that is 12 percent more than the control. This indicates that the *Bacillus subtilis* spores are not killed and they still fill the micro-pores even following the first stage of crack-healing. This secondary level of defence against the Infrastructure Durability Crisis is provided by this concrete breathing which can increase the service of the bridges and the dams up to 20 years.

Summary

The experimental outcomes prove that the Resilient Matrix is even more efficient than the traditional M30 concrete in all standards. The synergy of 109 B. subtilis, 15% Silica Fume, and 0.4% PE Fibers/ml of cells will provide a system that can:

1. Strengthening compressively by 48 percent.
2. The ability to attain a crack healing rate of over 80%.
3. Giving a robust resistance to chemical aggression.
4. Stability (simulated traffic vibrations).

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