भारतीय प्रौद्योगिकी संस्थान दिल्ली
Indian Institute of Technology Delhi

CLL113: NUMERICAL METHODS IN CHEMICAL ENGINEERING

TERM PAPER

SEMESTER 1 - 2023-24

COMPARITIVE ASSESSMENT OF CONTROLLED CONCRETE AND SELF-HEALING BACTERIAL CONCRETE USING NUMERICAL MODELS

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Abstract:

Traditional concrete structures face durability challenges, with cracks compromising integrity and necessitating costly repairs. The emerging solution of self-healing concrete holds promise. This term paper focuses on the development of a mathematical model to analyse the stress versus strain behaviour of self-healing concrete, with a specific emphasis on comparing the natural healing process with that of bacterially healing concrete. Our approach involves the creation of a numerical model through multilinear regression to numerically analyse experimentally calculated parameters representing the stress-versus-strain relationship in bacterial concrete. Subsequently, we extend this analysis by developing a generalised model using polynomial regression to examine both naturally healing and bacterially healing concrete. Utilising numerical methods for derivatives and integrals on the polynomial regression curve, we calculated key parameters such as the modulus of elasticity and energy absorption capacity (Modulus of Toughness) for both the concretes. The results are then validated against the original experimental data, demonstrating the effectiveness of our numerical analysis in assessing the mechanical properties of self-healing concrete.

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1. Introduction

Concrete cracking presents a lot of problems due to a variety of factors, including shrinkage, temperature changes, and structural loading. These cracks compromise the concrete's structural stability and provide openings for water intrusion, which may cause chemical deterioration and reinforcement corrosion.

In normal controlled concrete, due to repeated dry and wet cycles, small cracks in a structure with a width of 0.05 to 0.1 mm can be completely sealed. However, additional corrective action is needed when the cracks are wider. We talked about a technique in this term paper of introducing bacteria to concrete to encourage self-healing.

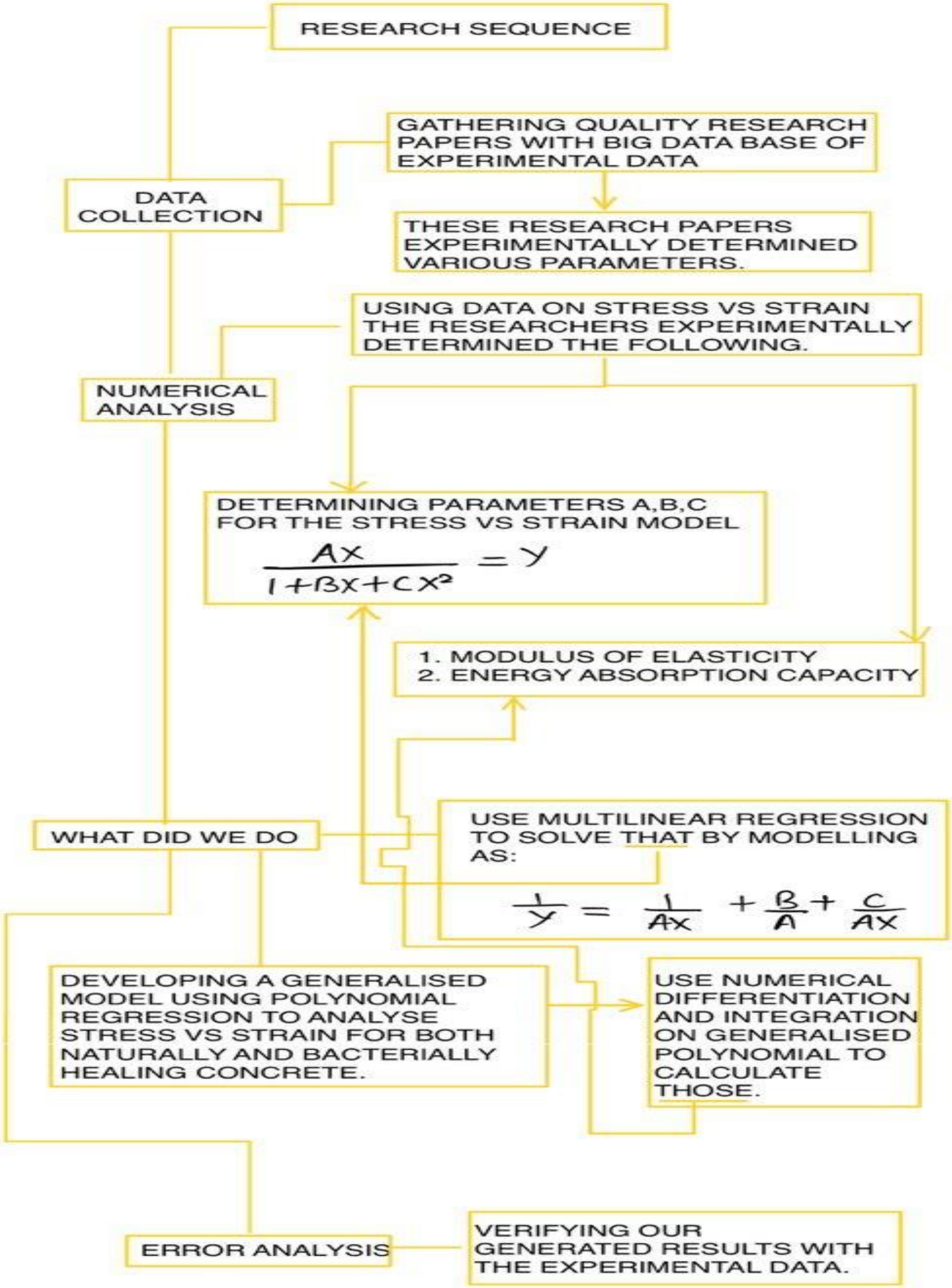
Employing mathematical models, we conducted a comparative analysis between conventional concrete and bacterial self-healing concrete. Our study delved into key parameters, including the modulus of elasticity and modulus of toughness, aiming to discern the superior performance between the two types of concrete. Through this investigation, we sought to establish a comprehensive understanding of the comparative strengths and weaknesses, ultimately contributing valuable insights for the evaluation and improvement of concrete technologies.

2. Motivation

The motivation behind our term paper stems from a critical need to address the persistent challenges faced by traditional concrete structures, where cracks compromise integrity and necessitate costly repairs. Concrete, a fundamental building material, is susceptible to various factors such as shrinkage, temperature changes, and structural loading, resulting in structural vulnerabilities and increased maintenance costs.

Recognising the transformative potential of self-healing bacterial concrete, our team, comprising Yash Sakhare, Prem Bhugra, Nikhil Gupta, and Rahul Masand, decided to contribute to the advancement of this innovative solution. Our motivation lies in the development of a robust numerical model to comprehensively analyse the stress versus strain behaviour of self-healing bacterial concrete and thereby conclude on further key properties. By focusing on both natural and bacterial healing processes, we aim to unravel the efficacy of these mechanisms in sealing cracks and enhancing the structural resilience of concrete. Through numerical analyses and comparisons, we seek to provide valuable insights into the mechanical properties of self-healing concrete, ultimately contributing to the evolution of concrete technologies and the creation of more sustainable and durable infrastructures.

3. Flow Chart for the Term Paper:



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4. The Problem of Cracks in Concrete

To achieve excellent, cost-effective, and sustainable concrete construction, a variety of techniques, materials, and processes are employed. Crack is a prevalent issue in buildings. Cracks can occur for a variety of causes. Here are some of the causes:

- Temperature variations cause concrete to expand and contract.
- Structure settling
- Excessive load applied
- Concrete surface shrinkage because of water loss
- Inadequate vibration during concrete placement
- Inadequate cover during concrete placement
- An excessive water-to-cement ratio
- Corroding steel reinforcement

The existence of cracks presents significant difficulties, including:

- Unsteadiness in Structure
- Decreased Bearing Durability and Capacity Issues
- Increased Corrosion Risk
- Moisture Penetration
- Expensive Repair

5.Bacterial Concrete or Self-Healing Concrete

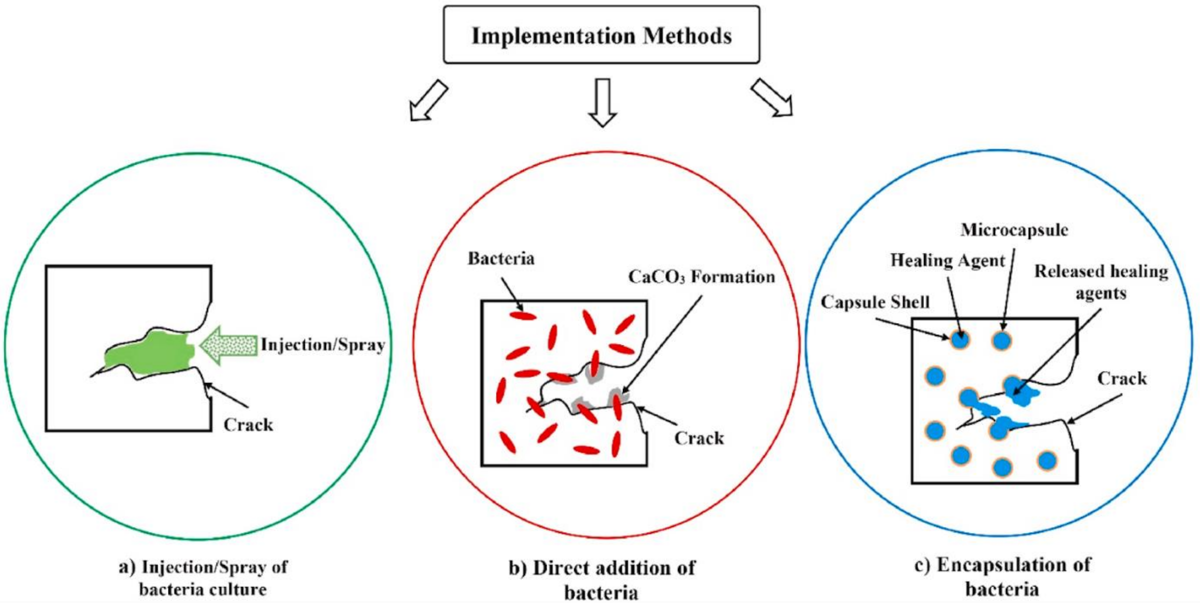
There are numerous solutions for this prevalent issue of developing cracks, both before and after the crack. Self-healing concrete, often known as bacterial concrete, is one of the remedial methods.

Self-healing concrete is the result of a bacterial response in the concrete that allows cracks to fill in or repair themselves over time once it has hardened. It has been noted that in repeated dry and wet cycles, minor cracks in a structure with small widths are totally sealed. However, more positive action is needed when the cracks are wider. Currently under investigation and development is a potential method based on the use of bacteria that produce minerals in concrete. In dry conditions, these kinds of bacteria can remain viable for more than 200 years while in dormant cells. These bacteria act as a catalyst in the crack healing process.

The most used strain for biomineralization is *Bacillus pasteurii*, which is a Gram-positive aerobic bacterium that is ubiquitous in the soil and produces a large amount of intracellular enzyme urease.

6. Mechanism

The biological reaction between unreacted limestone and a calcium-based nutrient, aided by bacteria, results in self-healing concrete that fills in cracks in buildings. Together with the calcium nutrient known as calcium lactate, a unique type of bacteria known as Bacillus pasteurii is employed. These products are added to the wet concrete after mixing during the preparation process.



Implementation methods of bacteria in concrete

This bacterium has a 200-year dormant phase. Water seeps through the cracks that form in the concrete. The bacteria's spores sprout and begin to consume oxygen by breaking down calcium lactate. Insoluble limestone is created from the soluble calcium lactate. The limestone that is insoluble begins to solidify. thereby automatically sealing the gap without outside assistance.

1. **Urea Hydrolysis*:*** Bacillus pasteurii catalyses the hydrolysis of urea in the concrete, starting the process with its negatively charged cell wall. Carbon dioxide and ammonia are created as a result.

$$CO(NH_2)_2 + 2H_2O \text{ ----> } CO_2 + 2NH_3$$

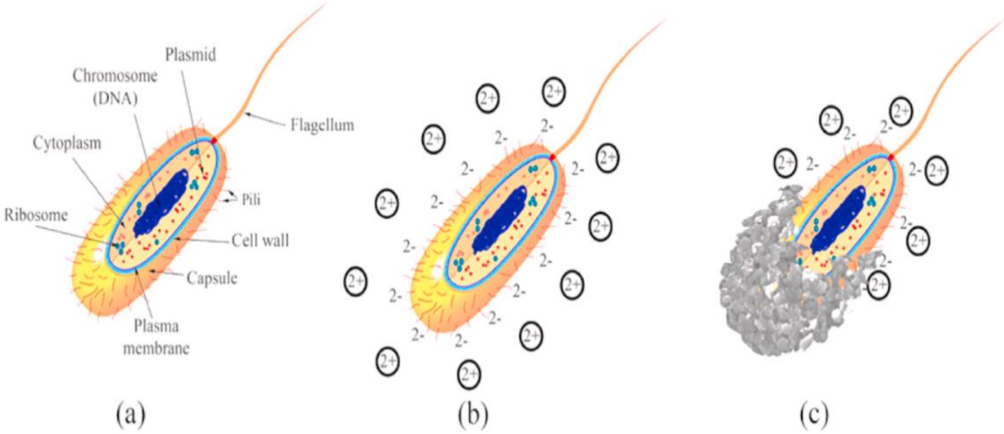
2. **Cation Draw and Carbonate Formation:** The bacteria's negatively charged cell wall takes in cations from its surroundings, such as Ca2+. These cations adhere to the surface of the bacterial cell.

3. **Nucleation Site Formation:** $CaCO_3$ precipitates at the bacterial cell surface because of a reaction between the Ca2+ ions on the surface and the $CO2_3$ ions in the surrounding medium. This acts as a site of nucleation.

$$Ca^{2+} + CO_3^{2-} \text{ -----> } CaCO_3$$

4. **Calcite Precipitation and Crack Healing**: As a natural filler, the formed calcium carbonate precipitates at the concrete's cell surface and inside its voids and cracks.
Overall Reaction:

$$CO(NH_2)_2 + Ca^{2+} + 2H_2O + 2CO_2 \dashrightarrow CaCO_3 + 2NH_4^+$$



(a) Bacterial structure, (b) negatively charged cell wall and the presence of positively charged ions, (c) biomineral production by means of binding calcium ions to cell wall

Advantages of Bacterial Concrete

1. Self-healing of cracks without outside assistance.
2. Compressive and flexural strengths are significantly higher than those of regular concrete.
3. Concrete's permeability has decreased.
4. Increases the durability of steel-reinforced concrete and lessens the corrosion of steel caused by the formation of cracks.
5. Bacillus bacteria can be used effectively because they pose no threat to human life.

7.EXPERIMENTAL PROGRAMME

This research examines the stress-strain behaviour of bacterially controlled high-strength grades (M60) concrete. Cylindrical specimens of 150 mm in diameter and 300 mm in height are used for the test. Plotting stresses versus strains allows one to evaluate the stress-strain behaviour of the twelve standard-sized cylinders that are cast using the designated controlled and bacterial concrete mixes. The cylinders are then tested in axial compression under strain control.

8.MATHEMATICAL MODELING FOR STRESS-STRAIN BEHAVIOUR

1. Modified Saenz Model

Saenz proposed a model which is in the form of:

$$y = \frac{Ax}{1 + Bx + Cx^2}$$

y is the stress at any level; x is the corresponding strain at that level

We used a research paper published in the International Journal of Engineering Research and Development [1] to get the data values for stress and strain for the controlled and bacterial concrete.

We used the saturation growth model of multi-linear regression to find the values of A, B and C.

$$y = \frac{Ax}{1+Bx+Cx^2}$$

$$\frac{1}{y} = \left(\frac{C}{A}\right)x + \left(\frac{1}{A}\right)\left(\frac{1}{x}\right) + \left(\frac{A}{B}\right)$$

$$Y = a2(u) + a1(v) + a0$$

The Research Paper [1] has experimental data on stress versus strain is used to get the polynomial equation by determining parameters A, B, C. We determined the equation to compute key parameters like the modulus of elasticity and energy absorption capacity (Modulus of Toughness).
Now changing the data accordingly and using the multi linear regression, we determined the coefficients and hence the final equation.

For controlled concrete:

Modified Saenz Model (Their Model):
A=37832, B= -326, C=189036

Multilinear Regression (Our Model):
A= -33033.4, B=166.262, C=-121982

For bacterial concrete:

Modified Saenz Model (Their Model)
A =23007, B= -539, C=189036

Multilinear Regression (Our Model)
A = 36145.2, B=-520.729, C=257553

2. Polynomial Regression

The Modified Saenz Model's applicability is limited to curves that change monotonically. We used polynomial regression to overcome this constraint and guarantee the inclusion of all data points, which is essential for obtaining comparative parameters such as moduli. We were able to create a thorough stress-strain curve by fitting a five-degree polynomial to the provided data points. By considering both increasing and decreasing trends in the data, this method enables a more accurate representation of the behaviour of the material.

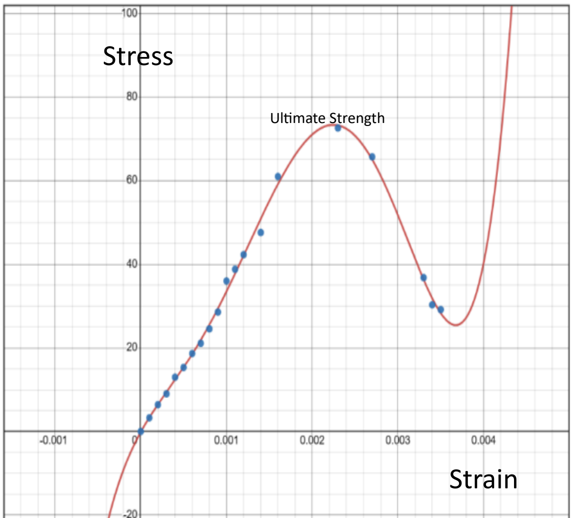
For controlled concrete:

$$y = (2.38231 \times 10^{15})x^5 - (1.85918 \times 10^{13})x^4 + (4.18539 \times 10^{10})x^3 - (2.91685 \times 10^{7})x^2 + 37116.7x - 0.111587$$

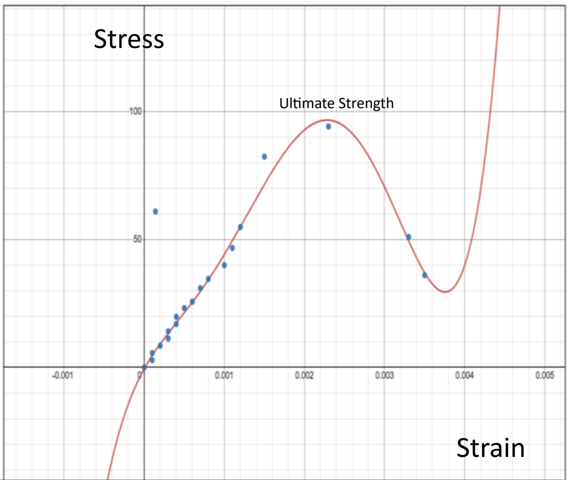
For bacterial concrete:

$$y = (3.0535 \times 10^{15})x^5 - (2.48216 \times 10^{13})x^4 + (6.00584 \times 10^{10})x^3 - (5.0249 \times 10^{7})x^2 + 56698.3\,x - 0.520595$$

Controlled concrete		Bacterial concrete	
Strain	Stress, MPa	Strain	Stress MPa
0	0	0	0
0.0001	3.27	0.0001	2.83
0.0002	6.41	0.0001	5.66
0.0003	9.01	0.0002	8.49
0.0004	12.98	0.0003	11.32
0.0005	15.32	0.0003	14.15
0.0006	18.65	0.0004	16.99
0.0007	21.10	0.0004	19.82
0.0008	24.55	0.0005	23.20
0.0009	28.56	0.0006	25.70
0.0010	36.00	0.0007	31.00
0.0011	38.80	0.0008	34.60
0.0012	42.30	0.0010	40.00
0.0014	47.60	0.0011	46.70
0.0016	61.00	0.0012	54.90
0.0023	72.61	0.0014	61.00
0.0027	65.70	0.0015	82.40
0.0033	36.80	0.0023	94.21
0.0034	30.30	0.0033	51.00
0.0035	29.15	0.0035	36.08



For Controlled Concrete



For Bacterial Concrete

9. ERROR ANALYSIS FOR MULTILINEAR AND POLYNOMIAL REGRESSION

1. MULTILINEAR REGRESSION

To validate the accuracy of our methods against the experimental data we will have to understand the flow of the Term Paper.

For this we will first have to justify the correctness of our model using error analysis.

The excel file attached shows that.

In the first sheet we have shown how for M60 Grade Concrete we have arrived at a model that is better at generating theoretical values than the one developed in the research paper.
We used Multi Linear Regression to determine the values of A, B, and C for the Stress values up until they are increasing. The results are mentioned here.

M60 concrete (controlled)	**Modified Saenz Model (Their analysis)**	**Modified Sanez Model (Our analysis)**
RMSE (w.r.t. Experimental Data)	0.30306	0.05575

The values (of A, B, C) computed in the Reference Research Paper have an RMSE of **0.30306** with respect to the Experimental Data provided while achieved a higher accuracy and are **81.601%** better at doing that.

<u>Modified Senz Model (Their Model)</u>:
A=37832, B= -326, C=189036
<u>Multilinear Regression (Our Model):</u>
A= 33033.4, B=166.262, C=121982

Similarly, for bacterial concrete,

M60 concrete (Bacterial)	**Modified Saenz Model (Their analysis)**	**Modified Sanez Model (Our analysis)**
RMSE (w.r.t. Experimental Data)	0.3139	0.1579

We are relatively **49.6985% better.**

<u>*Modified Senz Model (Their Model)*</u>: -
A =23007, B= -539, C=189036
<u>*Multilinear Regression (Our Model):*</u> -
A = 36145.2, B=-520.729, C=257553

2. POLYNOMIAL REGRESSION

This method has helped us overcome the problem of monotonicity that even if the monotonous increase in data is not there the polynomial regression helps get theoretical data.
We have then error analysed this with experimental data and reached even more accuracy.

M60	CONTROLLED	BACTERIAL
RMSE	0.03476	0.16988

polynomial regression helps us get one of the most accurate fitting curves that in turn helps us determine the key parameters the modulus of elasticity and energy absorption capacity (Modulus of Toughness) better which helps us generate new and original results.

10.COMPARATIVE ASSESSMENT

1. Modulus of Toughness

The entire area under a material's stress-strain curve up to the point of fracture is used to calculate the material's modulus of toughness. This section measures the amount of work done on the material and its ability to absorb energy without failing catastrophically. The modulus of toughness can be calculated mathematically by taking the integral of the stress-strain curve, which shows the amount of energy absorbed per unit volume of the material, from the beginning of loading to the point of fracture. We used the **Trapezoid Rule of Numerical Integration** to find the required area under the curve and hence the modulus of toughness. The code for the same is attached.

A greater modulus of toughness in concrete denotes an improved capacity to absorb energy prior to fracture, enhancing the material's resistance to sudden or dynamic loads. Superior concrete is distinguished not only by its high compressive strength but also by its ability to withstand dynamic forces and impacts. An improved modulus of toughness, which is indicative of increased impact resistance, becomes an essential concrete quality parameter.

Modulus of Toughness (MPa) (from Stress-Strain curves):

Controlled Concrete	Bacterial Concrete
0.16	0.21

2. Modulus of Elasticity

The stiffness or rigidity of a material is gauged by its modulus of elasticity. It is shown by the slope of the linear, elastic portion of the stress-strain curve. We used the **four-point Central Difference Method of Numerical Differentiation** to find the slope and hence the modulus of elasticity. This modulus, which is computed as the ratio of stress to strain, shows how much a material deforms in response to an applied stress within its elastic limit.

Under a given load, concrete with a higher modulus of elasticity deforms less. For structures where minimal deflection is required in the design, this feature is essential. Increased stiffness is indicated by a higher modulus of elasticity. Higher stiffness is frequently preferred for structural components like beams and columns in order to reduce deformations and guarantee the structural integrity of the entire system.

Modulus of Elasticity (GPa)

Controlled Concrete	Bacterial Concrete
41.9	52.3

11. RESULTS AND DISCUSSION

Graphical representations of the stress vs. strain curve for both bacterial and controlled concrete were produced after a polynomial regression equation was used to model the curve. The stress-strain behaviour was compared, and it was found to be similar. The main difference was that the bacterial concrete had higher stress values than the controlled concrete at the same strain levels. This resulted in a graph depicting bacterial concrete reaching higher stress levels.

Critical parameters, including the modulus of toughness and modulus of elasticity, were then extracted for both types of concrete using a variety of numerical techniques. The results showed that the bacterial concrete had 31.25% higher modulus of toughness and 24.82% higher modulus of elasticity than the controlled concrete. These results confirm the higher stiffness of bacterial concrete, which is a highly desired property in concrete materials, and its increased resistance to sudden or dynamic loads. This comprehensive analysis provides valuable insights for optimising the performance of bacterial concrete in practical construction applications.

12. PATH FORWARD

Future infrastructures could benefit from the use of bacterial concrete, which has the potential to self-heal and increase durability. By extending the lifespan of structures, bacterial concrete has the potential to completely transform the industry. Even with its potential, financial obstacles like greater upfront costs must be overcome. The cost barrier is anticipated to decrease as research advances and economies of scale are achieved, making bacterial concrete a more sustainable and economically viable option for widespread construction applications. Bacterial concrete is positioned as a game-changing solution for the future due to its potential to lower long-term maintenance costs and increase infrastructure sustainability.

13. SELF ASSESSMENT

We used multilinear regression in our self-evaluation based on the research journal data to obtain more precise Modified Saenz Model parameters than those found in the journal. We verified this assertion using thorough error analysis. In light of the Saenz model's limitations, we created a five-degree polynomial regression equation specifically for the provided data, which produced new findings and matching curves for the two types of concrete. Error analysis was used to further illustrate the effectiveness of our method.

We used the plotted curves to calculate the modulus of elasticity (using the Four-Point Central Difference Method) and the modulus of toughness (using the Trapezoid Method). The superior efficiency of bacterial self-healing concrete was highlighted by comparing these values across different types of concrete. For every numerical technique, we supplemented our results with working C++ code implementations, offering derivations based on basic equations. Our method performed error analysis, generated new results, plotted graphs, and integrated experimental data. The paper applied C++ code, Excel analysis, and DESMOS to the reference material comprehensively. As a result, we classify our term paper as Level-2.

REFERENCES

[1] Srinivasa Reddy V, Rajaratnam V, Seshagiri Rao M V, Sasikala Ch, Mathematical Model for Predicting Stress-Strain Behaviour of Bacterial Concrete.

[2] Class Notes of Professor Jayati Sarkar.

[3] How-Ji Chen, Ching-Fang Peng, Chao-Wei Tang and Yi-Tien Chen, Self-Healing Concrete by Biological Substrate.

[4] Mehrab Nodehi, Togay Ozbakkaloglu, Aliakbar Gholampo, A systematic review of bacteria-based self-healing concrete: Biomineralization, mechanical, and durability properties.

[5] Mugahed Amran, Ali M. Onaizi, Roman Fediuk, Nikolai Ivanovicn Vatin, Raizal Saifulnaz Muhammad Rashid, Hakim Abdelgader, Togay Ozbakkaloglu, Self-Healing Concrete as a Prospective Construction Material: A Review