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Research Article

Keywords: Concrete, Metakaolin, Compressive Strength, Flexural Strength, Finite Element Method (FEM)

Posted Date: November 23rd, 2026

DOI: https://doi.org/10.21203/rs.3.rs-11615251/v1

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Additional Declarations: No competing interests reported.

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Abstract

Cement production, a key constituent of concrete, contributes to environmental degradation through greenhouse gas emissions thus predisposing the ozone layer to depletion. In addition, the quest to continuously increasing the growth of infrastructural development with reduction in the production of the conventional binder has necessitated the search for naturally occurring clay and some agricultural/industrial waste materials toward promoting the campaign for ecofriendly and cost effective binder. Consequently, promoting the advocacy for a sustainable construction works. The construction industry advocates enhanced performance using supplementary cementitious materials. This study investigated metakaolin (MK) as a cement partial replacement to enhance the structural performance of the composite whilst advocating for sustainable binder. Grade C25 concrete used a 1:2:4 mix ratio (Binder: Fine: Coarse aggregate) and water–binder ratio of 0.50. Investigations were conducted on concrete mixes containing 0–20% MK in fresh/hardened states. Workability was assessed through slump and compacting factor tests, while water absorption, compressive, and flexural strength determined durability/strength properties. FEM analysis using ANSYS Static Structural Analysis simulated beam flexural behaviour under four-point loading. Workability decreased with increasing MK: slump values were 75, 65, 55, 45, and 35 mm; compaction factors were 0.92, 0.90, 0.88, 0.84, and 0.82 for 0, 5, 10, 15, and 20% MK, respectively. Compressive strength increased from 24.0 MPa at 0% to 26.0, 27.0, and 26.5 MPa at 5, 10, and 15%, before reducing to 25.0 MPa at 20%, indicating optimum at 10%. Flexural strength improved from 3.1 MPa at 0% to 3.3, 3.6, and 3.4 MPa, then declined to 3.2 MPa. Water absorption decreased from 6.5% to 5.1% at 15%, before increasing to 5.6% at 20%, signifying enhanced pore refinement. FEM simulations correlated strongly with experimental data, showing maximum stresses of 5.6563, 6.0115, 6.558, 6.1918, and 5.8311 MPa and corresponding maximum deformations of 0.00297, 0.00320, 0.00345, 0.00326, and 0.00307 mm for 0–20% MK, confirming optimal mechanical response at 10%. MK incorporation between 10–15% optimizes performance and sustainability. Effective utilization of MK at 10% replacement of cement aligns with the United Nation's sustainable development goals 9 and 13.

Keywords: *Concrete, Metakaolin, Compressive Strength, Flexural Strength, Finite Element Method (FEM).*

1. Introduction

Concrete, the second most widely utilized material after water, remains vital for infrastructural growth worldwide, especially in rapidly urbanizing nations such as Nigeria [3]. Its strength, durability, and cost-effectiveness make it indispensable, but the reliance on Portland Limestone cement (PLC) as the principal binder presents a critical challenge. The manufacture of PLC is energy-intensive and environmentally damaging, contributing nearly 8% of global anthropogenic CO_2 emissions, with one ton of cement producing about 0.8 tons of CO_2 [2]. These impacts highlight the urgent need for sustainable approaches in concrete production through the sourcing for alternative materials that could exhibit binding properties and, consequently, complementing the characteristics of the conventional binder. This in turn contribute to the strength development and durability performance of the cement composites thereby enhancing the mechanical properties of the composite by sustaining its strength and other related properties [3]. One strategy that has gained prominence is the use of supplementary cementitious materials (SCMs). These materials partially replace cement, reducing clinker consumption while improving performance of cement composites. Among them, metakaolin (MK) obtained from de-hydroxylation of kaolin clay after a heat treatment process, has attracted attention due to its high pozzolanic reactivity, ability to refine pores in composite structures, and potential to enhance mechanical

and rheological properties [4, 18].

Research has reported strength improvements and durability gains at moderate MK replacement levels, though variations in optimum dosage and performance trends suggest that further systematic study is required. At the same time, numerical tools such as the Finite Element Method (FEM) are increasingly applied to simulate the structural response of MK-modified cementitious systems, complementing laboratory investigations and providing deeper insights into stress distribution and deformation [7]. These considerations set the foundation for exploring both experimental and numerical perspectives, with the following review examining existing research on fresh and hardened properties of MK-based concretes and the parallel advances in computational modelling. The incorporation of computational modelling could also promote the optimum utilization of this supplementary cementitious material towards ensuring the full exploration of the material and consequently, enhancing and maintaining the characteristics of metakaolin blended composite [8]

Growing concerns over the environmental cost of PLC production have intensified research into SCMs as viable alternatives for sustainable construction [1, 2]. Metakaolin, produced by the calcination of kaolin clay at 600–800°C, develops an amorphous aluminosilicate phase that is highly pozzolanic [18]. Its chemical composition typically satisfies the requirements in [7], with the combined oxides of silica (SiO_2), alumina (Al_2O_3), ferric oxide (Fe_2O_3) content exceeding 70% [24]. Such findings validate MK's classification as a Class N pozzolan suitable for use in cementitious systems. The addition of MK alters the behavior of fresh concrete. Due to its fine particle size and high surface area, slump generally decreases with increasing replacement, while decrease in compaction factor values also indicate decrease in workability [1]. However, MK contributes positively by improving cohesiveness, reducing bleeding, and enhancing stability during placement. These rheological effects underscore the need to balance workability losses with gains in fresh mix stability.

In hardened states, MK enhances compressive and flexural strengths at replacement levels of about 10–15%, beyond which strength may decline due to dilution of clinker phases [4]. 10% MK yielded peak compressive strength, consistent with secondary C–S–H formation and microstructural densification [1, 3]. Flexural strength improvements are also attributed to a refined interfacial transition zone. Durability benefits have been reported in mortar studies, where MK reduced water absorption and increased density, findings that indicate potential durability gains when extended to concrete systems [1]. Parallel to experimental efforts, numerical modelling has emerged as a powerful tool. Finite Element Method (FEM) studies using ANSYS have successfully predicted stress distribution, crack initiation, and deformation in MK-modified beams [24]. [22, 25] further demonstrated strong agreement between FEM simulations and laboratory beam tests, establishing FEM as a reliable complement to experiments.

2. Materials and Method

The primary materials adopted in this study include cement, metakaolin, potable water, fine aggregate, and coarse aggregate.

2.1 Materials

Metakaolin, a high reactivity pozzolanic material, used in this study was obtained from previously processed and calcined kaolin, from fused fatusi, Ibadan 110115, Oyo State, Nigeria (Lat N7º18'28.04076", E3º55'26.13252" and alt 207yd a.s.l), as characterized in [5]. To ensure uniformity, the material was only re-ground and sieved to 75 μm prior to use. Clean, well-graded river sand was sourced from erosion deposits at the Ladoke Akintola University of Technology, Ogbomoso campus. The sand was processed to remove particles larger than 4.75mm adhering to the standards as outlined in [16]. The aggregate was therefore deemed suitable for achieving adequate workability, packing density, and bonding performance in the concrete mixtures.

Crushed granite with a nominal size of 10-40 mm which are crucial for producing high quality concrete was sourced, and then washed to remove dirt and impurities. The aggregates were considered fit for structural concrete production with its compliance with [16], which guarantees appropriate grading and durability. The mixing water used in this study was potable water conforming to [10] for mixing water in concrete for strength development and durability. Portland Limestone Cement (PLC) of grade 42.5N, a high-performance versatile limestone cement, was used as the primary binding material. This type of cement is known for its early rapid strength development and complies with the standards set by [17].

2.2 Method

The experimental program was designed to evaluate the influence of metakaolin (MK) on both the fresh and hardened properties of concrete, as well as to validate the experimental findings through finite element simulations.

2.2.1 Preparation of Metakaolin

High-reactivity kaolin from fused fatusi, Ibadan 110115, Oyo State, Nigeria (Lat N7º18'28.04076", E3º55'26.13252" and alt 207yd a.s.l) was used for the research [5]. The collected kaolin with initial moisture content of 4.27% was air dried for 24 hours and was calcined (at 700℃ for 2 hours). Since the MK had already been calcined and characterized in earlier studies [5], further calcination was unnecessary. To ensure uniform fineness and reactivity, the material was re-ground and sieved through a 75 µm mesh before use.

2.2.2 Mixing and Casting

Concrete was designed for grade C25 using a mix ratio of 1:2:4 (binder: sand: granite) with a constant water–binder ratio of 0.50. The MK was added partially by weight of the cement at varying levels s of 0, 5, 10, 15, and 20%, respectively. Mix proportions were carefully batched by weight, and quantities were calculated separately for cube specimens (150 × 150 × 150 mm) and beam specimens (100× 100 × 500 mm) as presented in Table 1.

Mixing was carried out by first homogenizing the dry constituents for two to three minutes, after which water was gradually introduced to achieve uniform consistency. Fresh concrete was then placed into moulds in three layers, each compacted with 35 strokes of a tamping rod to eliminate entrapped air and ensure proper consolidation in accordance with [12]. Specimens were covered immediately to prevent moisture loss and demoulded after 24 hours. All samples were subsequently cured in water at 25 ± 2 °C for predetermined periods of 7, 14, 21, and 28 days depending on the test requirement.

Table 1: Proportioning of Concrete.

MK (%)	Cement (kg)		MK (kg)		Fine Aggreg. (kg)		Coarse Aggreg. (kg)		Water (kg)	
	Cube	Beam	**Cube**	Beam	**Cube**	Beam	**Cube**	Beam	**Cube**	Beam
0	10.80	3.20	0.00	0.00	21.60	6.40	43.2	12.8	5.40	1.60
5	10.26	3.04	0.54	0.16	21.60	6.40	43.2	12.8	5.40	1.60
10	9.72	2.88	1.08	0.32	21.60	6.40	43.2	12.8	5.40	1.60
15	9.18	2.72	1.62	0.48	21.60	6.40	43.2	12.8	5.40	1.60
20	8.64	2.56	2.16	0.64	21.60	6.40	43.2	12.8	5.40	1.60

2.2.3 Fresh Concrete Test

The workability of fresh concrete was assessed using both the slump test and compaction factor test (Figures 1-2), conducted in accordance with [11, 12]. These tests provided essential information on the handling and flow characteristics of the mixes at different replacement levels.



Figure 1: Slump Test



Figure 2: Compaction Test

2.2.4 Hardened Concrete Test

For hardened concrete, several tests, in Figures 3-5, were conducted to evaluate its mechanical and durability properties. Compressive strength tests were performed on 40 cubes. The specimens were prepared for five different mix variations with metakaolin replacement levels of 0, 5, 10, 15 and 20%. For each replacement level, ten (10) cubes were tested at curing ages of 7, 14, 21, and 28 days. After

24 hours of casting, the cubes were demolded and submerged in a water-curing tank maintained at room temperature (23±2°C) to ensure proper hydration and strength development following [16]. The compressive strength test was carried out by recording the applied load at failure, using a 2000 kN capacity testing machine following BS EN 12390-3. Flexural strength test was carried out on the hardened samples of 10 beams after curing for 28 days using two beams for each of the percentage replacements (0, 5, 10, 15, and 20%), the value was calculated by using Eq, 1. Flexural strength was determined under a four-point loading arrangement in accordance with [15], the value was calculated using Eq. 2. The cured prism specimens were subjected to bending at a constant rate until failure, and the maximum load was recorded.

Densities of both cubes and beams were obtained at 28 days by dividing specimen mass by volume, while water absorption was measured on 28-day cured cubes following [9] and the value was calculated using Eq, 3. For each property, three specimens were tested, and the mean values reported.



Figure 3: Curing of the concrete cubes



Figure 4: Compressive Strength Test

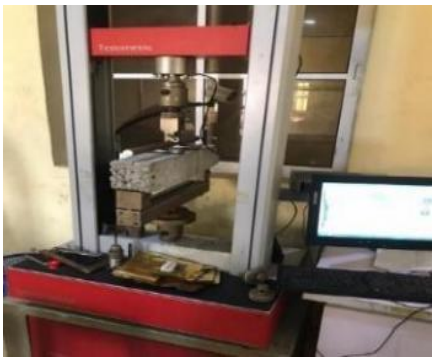


Figure 5: Flexural Strength Test

$$Compressive\ strenght, F = \frac{Load, P(N)}{cross-sectional\ Area, A(mm^2)} \quad (Eq.1)$$

$$Flexural\ Strength, fr = \frac{PL}{bd^2} \quad (Eq.2)$$

$$Water\ Absorption = \frac{(wet\ weight - dry\ weight)}{dry\ weight} \times 100 \quad (Eq.3)$$

Where fr is Flexural strength (MPa), P is applied load at failure (N), L is span (mm), b is specimen width (mm), d is specimen depth (mm).

2.2.5 Finite Element Analysis (FEA) on Beams

In addition to experimental investigations, numerical simulations were performed to model the structural behaviour of beams using ANSYS Workbench (R1 2025). The simulations were carried out in the Static Structural module with SOLID65 elements (Figure 6), which are capable of modeling cracks and crushing failures in concrete. Material properties such as compressive strength, flexural

strength (Eq 4), density, Young's modulus derived from empirical relationships (Eq, 5), and Poisson's ratio (0.18) presented in Table 2 were incorporated for each replacement level.

Table 2: Engineering Data Imported into ANSYS Workbench for 28 days of curing

Concrete Mix (%)	Density (kg/m^3)	Flexural Strength (MPa)	Compressive Strength (MPa)	Young Modulus (MPa)	Poisson's ratio
0	2395	3.10	25.05	23500	0.20
5	2405	3.30	28.15	24800	0.20
10	2415	3.60	33.75	27400	0.20
15	2425	3.40	30.10	25700	0.20
20	2420	3.20	27.25	24400	0.20

$$fr = 0.62\sqrt{f'c} \quad \text{(Eq. 4)}$$

$$Ec = 0.043\rho^{1.5}\sqrt{f'\,c} \quad \text{(Eq. 5)}$$

Where fr is Flexural strength (MPa), EC is the Young modulus (MPa), ρ is the density of concrete (Kg/m^3) and f' c is the compressive strength of concrete (MPa). Compressive strength was back-calculated from flexural strength using (Eq. 4). Young's modulus was estimated from compressive strength using (Eq. 5) in accordance with ACI 318-19

The beam specimens were modeled in ANSYS Design Modeler to replicate the standard laboratory cube dimensions of 100 × 100 × 500 mm (Figure 7). Each specimen was represented as a single solid body, assuming homogeneity and isotropy for simplification. This geometric consistency ensured that the numerical analysis could be directly compared with the experimental results. A mesh size of 10 mm was adopted as shown in Figure 8, with refinements around load and support regions to enhance accuracy. The boundary conditions replicated the experimental setup, with a pinned support at one end and a roller support at the other. Two equal concentrated downward loads were applied at L/3 and 2L/3.

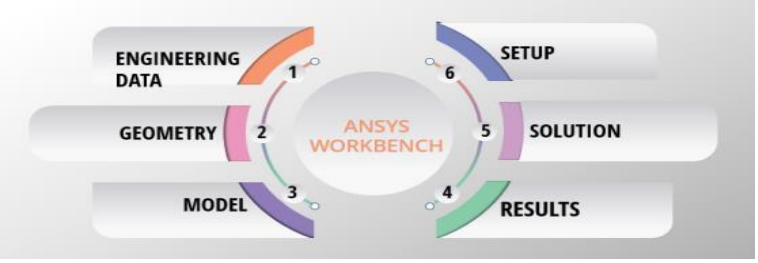


Figure 6: FEA Framework

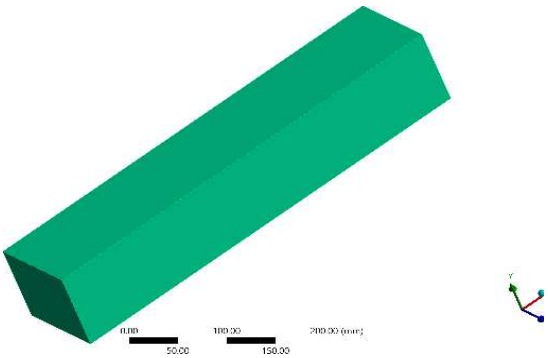


Figure 7: FEA Geometry

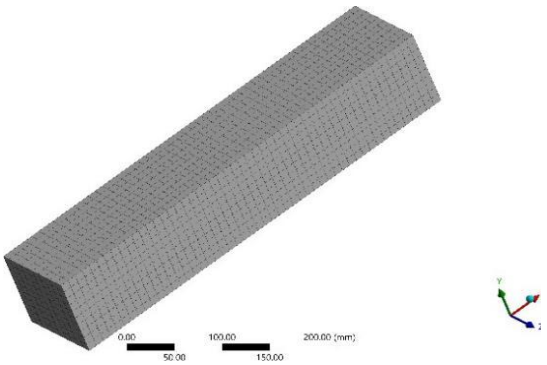


Figure 8: FEA Meshing

2.2.6 Solution and Post Processing

The solver was used to predict maximum stress distribution, total deformation, and failure modes, and the results were compared with experimental outcomes for validation. All data were analyzed by comparing experimental and numerical results to identify consistent trends. Averages of replicate specimens were used to minimize variability, and the combined approach of laboratory testing and finite element modeling ensured a comprehensive understanding of the behavior of MK-blended concrete.

3. Results and Discussions

3.1 Workability

Workability of the fresh concrete mixes was assessed through slump and compaction factor tests. Results showed a steady reduction in workability as metakaolin (MK) content increased from 0% to 20%. The slump decreased from 75 mm (medium workability) in the control to 35 mm (very low) at 20% MK (Figure 9), while compaction factor values dropped from 0.92 to 0.82 (Figure 10). This decline is attributed to the fineness and high surface area of MK, which increased water demand and reduced free water available for lubrication of the mix. Although reduced slump indicates stiffer mixes, it also suggests improved cohesiveness and resistance to segregation. At moderate replacement levels (5–10%), workability remained within acceptable limits, but higher dosages (15–20%) showed significant reductions, necessitating the use of admixtures such as super-plasticizers for practical applications.

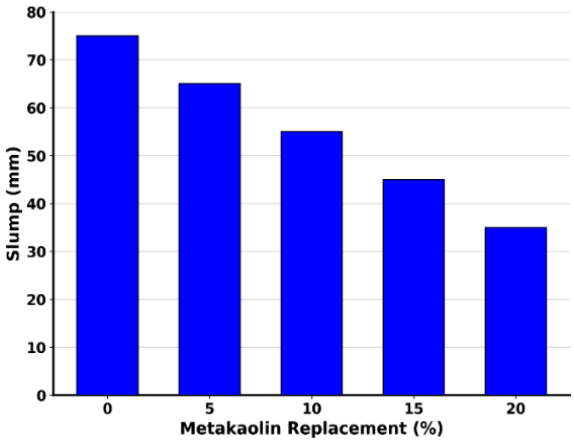


Figure 9: Slump Result

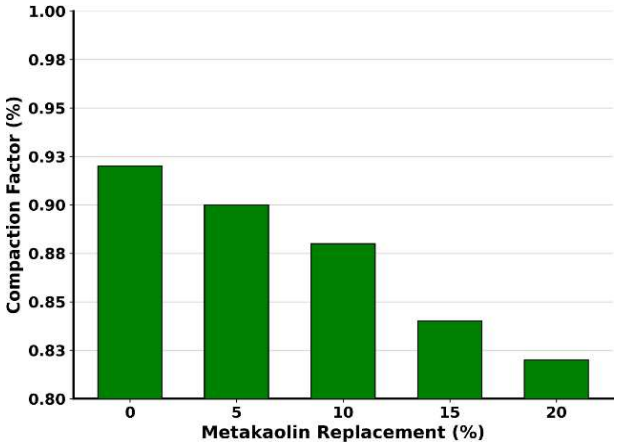


Figure 10: Compaction Factor Result

3.2 Water Absorption

The water absorption results at 28 days, shown in Figure 11, revealed that metakaolin (MK) incorporation significantly reduced permeability as compared to the control specimen. The control mix (0% MK) recorded 6.5%, reflecting a relatively porous microstructure typical of Portland Limestone cement concrete. With 5% replacement, absorption decreased to 6.0%, attributable to the pozzolanic reaction between MK and calcium hydroxide, which forms additional Calcium- Silicate-Hydrate (C–S–H) and refines pore structure [21].

At 10% MK, absorption further declined to 5.4%, highlighting the most effective refinement of capillary pores. The lowest value of 5.1% was observed at 15% replacement, where both the filling effects and pozzolanic reaction synergistically improved impermeability. The trend of results aligns with the findings as obtained elsewhere [19].

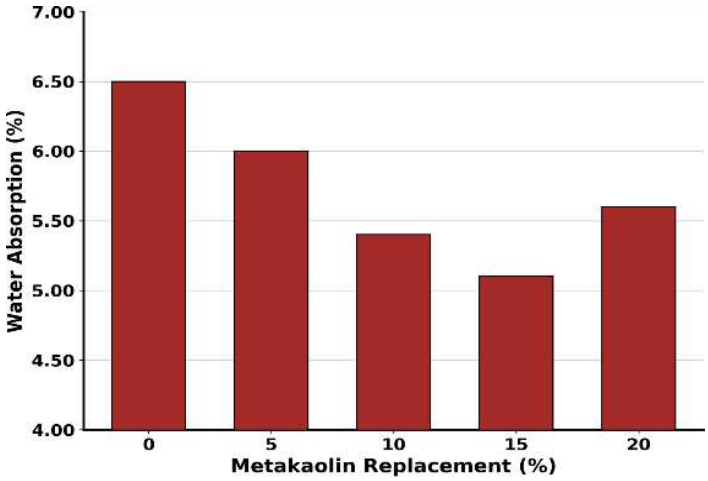


Figure 11: Water Absorption Result

However, at 20% replacement, absorption increased slightly to 5.6%, indicating the onset of the dilution effect, whereby excessive cement substitution reduces calcium hydroxide availability, limiting further pozzolanic activity [27]. MK incorporation reduced water absorption across all mixes compared to the control, with optimum performance observed at 10–15% replacement. This confirms MK's role as an effective pore-refining pozzolan, enhancing concrete durability without compromising structural performance.

3.3 Compressive Strength

The compressive strength results as shown in Figure 12, demonstrate a clear strength development trend with increasing metakaolin (MK) replacement. Compared with the control mix (0% MK), incorporation of MK significantly enhanced strength performance up to an optimum dosage of 10%, after which a gradual decline was observed.

At 28 days, the control mix achieved 24.0MPa. The addition of 5% MK increased compressive strength to 26.0 MPa, representing an 8.3% improvement relative to the control. This improvement could be attributed to the filler effect of MK, which refines the pore structure, and its pozzolanic reaction with calcium hydroxide, which generates additional C–S–H gel. This agrees with the findings of other researchers as obtained elsewhere [21].

The optimum performance occurred at 10% MK replacement, with a 28- day compressive strength of 27.0 MPa, corresponding to 12.5% increase over the control mix. This dosage achieved the best balance between cement dilution and pozzolanic contribution, corroborating earlier reports that 10% MK maximizes strength development in blended concretes [20]. The nucleation effect of MK further explains the superior hydration rate observed.

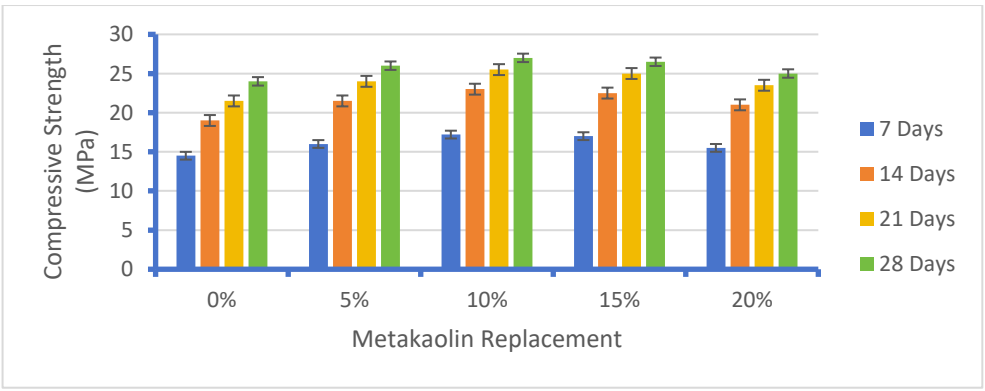


Figure 12: Compressive Strength Result

Beyond the optimum dosage, strength exhibited a declining trend. At 15% MK, the 28-day strength decreased slightly to 26.5 MPa, corresponding to a 10.4% increase over the control but a 1.9% reduction compared with the 10% mix. This suggests that beyond 10%, dilution of clinker begins to outweigh the pozzolanic benefits, although active C–S–H formation still supports strength development [23]. At 20% MK, compressive strength further decreased to 25.0 MPa, representing only a 4.2% improvement over the control and 7.4% reduction relative to the optimum mix. This decline suggests that excessive cement replacement limits calcium hydroxide availability, restricting complete pozzolanic reactions and reducing efficiency of the binder system [19].

The results demonstrate that MK significantly improves compressive strength up to an optimum level of 10%, beyond which performance declines due to dilution. These findings confirm MK's role as a sustainable, high-performance supplementary cementitious material when proportioned correctly.

3.4 The 28-Day Flexural Strength Results

The 28-day flexural strength results for metakaolin (MK)-modified beams are presented in Figure 13. A clear Flexural Strength improvement was observed up to 10% replacement, after which a gradual decline occurred, reflecting the interplay between the beneficial filler–pozzolanic effects and the dilution effect at higher dosages. The control mix (0% MK) recorded a flexural strength of 3.10 MPa, establishing the baseline for comparison. This value reflects the limitations of plain PLC concrete, where micro-cracking and a weak interfacial transition zone (ITZ) restrict resistance to bending stresses. At 5% MK replacement, strength improved to 3.30 MPa. This enhancement is primarily attributed to the filler effect of ultra-fine MK particles, which improve packing density and densify the ITZ, thereby delaying crack initiation. The early pozzolanic activity further contributes to secondary C–S–H formation, improving matrix cohesion [19].

The maximum strength of 3.60 MPa was achieved at 10% replacement, marking the optimum level. This dosage provided the most effective balance between hydration and pozzolanic reactions, resulting in a refined pore structure and stronger bond within the matrix. Similar findings by [27] confirm that 10% MK optimizes crack-bridging capacity and flexural performance.

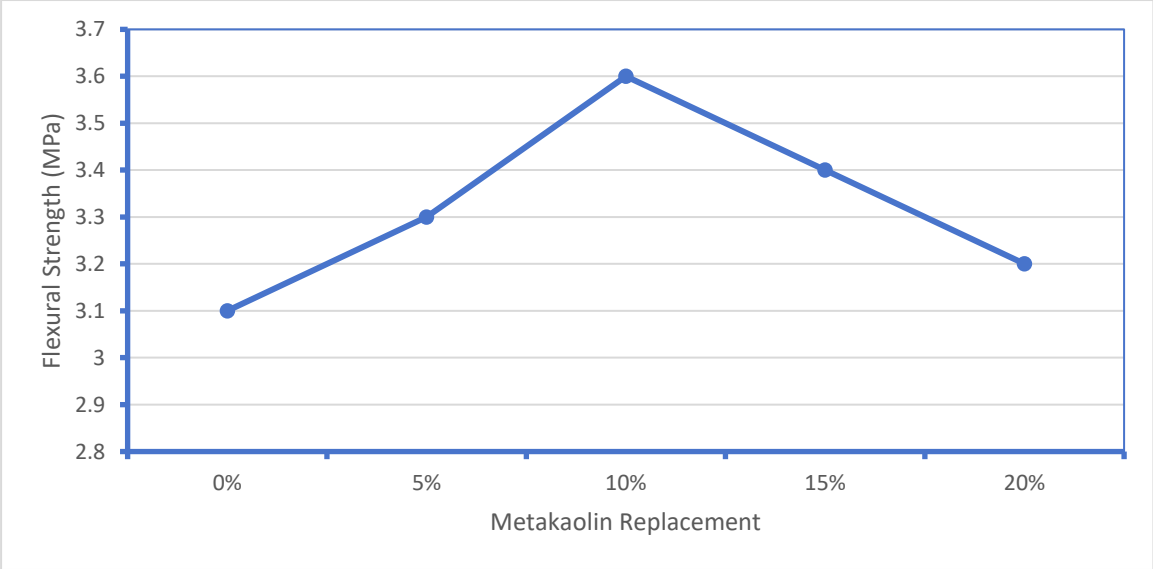


Figure 13: Flexural Strength Result

At 15% replacement, strength decreased slightly to 3.40 MPa. While still higher than the control, the reduction suggests that excessive cement dilution reduced available $Ca(OH)_2$, limiting pozzolanic activity. [21] similarly reported diminishing gains beyond optimum MK levels.

The 20% mix recorded 3.20 MPa, nearly reverting to the control sample. Although MK still maintained comparable performance, the reduction indicates that excessive replacement weakens matrix cohesion and reduces resistance to crack propagation. Flexural strength improved significantly with MK

incorporation up to 10%, where ITZ densification and enhanced crack resistance were most effective. Beyond this point, the dilution effect outweighed the pozzolanic benefits, confirming 10% as the optimum replacement for maximizing flexural performance.

3.4 Finite Element Analysis (FEA)

The finite element analysis (FEA) conducted on MK-modified concrete beams revealed trends consistent with experimental results. As shown in Figures 14-17, maximum stress increased from 5.656 MPa in the case of control sample to 6.558 MPa at 10% MK replacement, after which values declined. This agrees with experimental flexural strength results (Figure 18), confirming 10% as the optimum level of replacement. [8, 27], similarly confirm that the higher stress capacity (Figure 4d) at this dosage reflects the pozzolanic and filler effects of MK, which refine pore structure and strengthen the interfacial transition zone.

At 15% and 20% replacement levels, stresses dropped to 6.191 MPa and 5.831 MPa, respectively, indicating that excessive cement dilution reduces available Calcium-hydroxide ($Ca(OH)_2$) for pozzolanic reactions, thereby moderating the strength gain. These results reinforce the experimental trend where flexural performance peaked at 10% before declining, suggesting that optimal MK content is necessary to sustain improved load transfer and crack resistance [19].

The deformation profiles shown in Figure 19 further corroborate this pattern. Finite Element Model (FEM)-predicted deflections ranged from 0.00297 mm in the control to 0.00345 mm at 10% MK replacement, then decreased slightly with higher dosages. This increase at optimum levels suggests enhanced ductility due to a denser microstructure and improved crack-bridging ability [26].

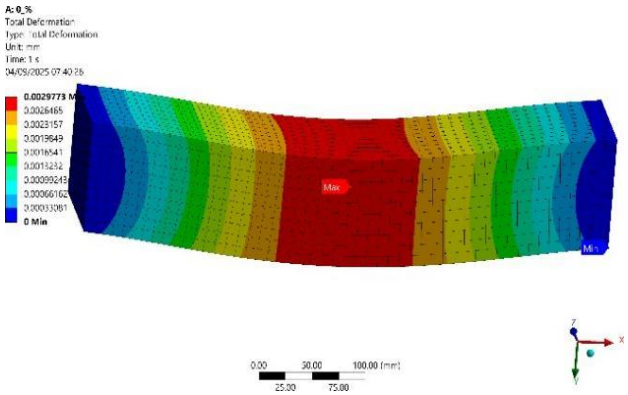


Figure 14: Total Deformation at 0%

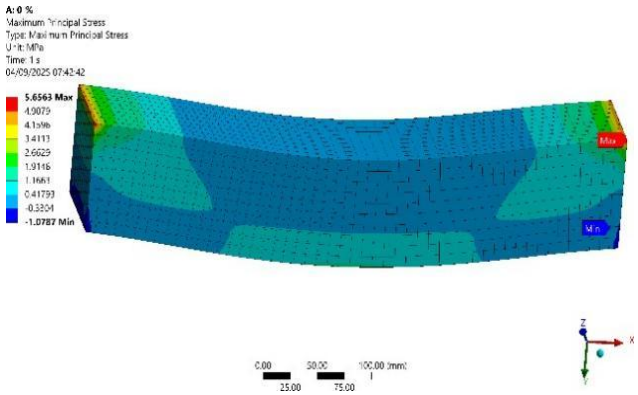


Figure 15: Maximum Stress at 0%

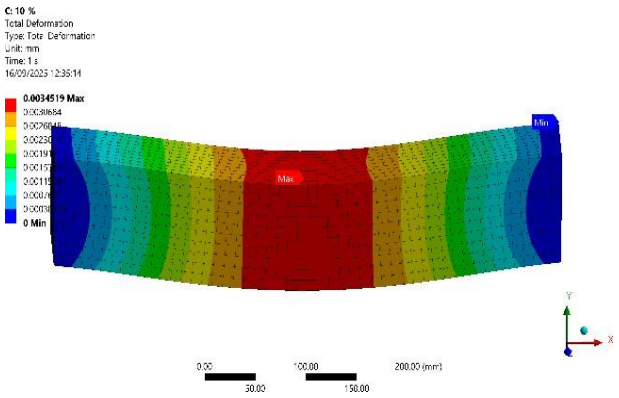


Figure 16: Total Deformation at 10%.

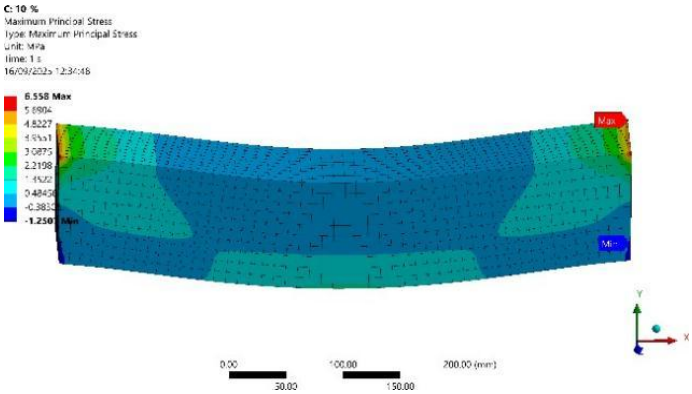


Figure 17: Maximum Stress at 10%

It was also observed that FEM consistently predicted higher stress values compared to experimental tests. This discrepancy arises from the idealized assumptions of finite element model (FEM), including perfect bonding and homogeneity, which do not fully capture real micro- cracking, voids, or ITZ

weaknesses present in laboratory specimens. Despite this, the close agreement in trends across Figure 4 to 5 demonstrates that FEM is a reliable tool for validating experimental outcomes and predicting beam performance under flexural loading.

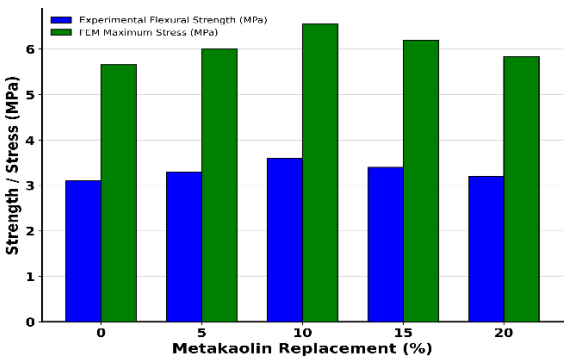


Figure 18: Flexural Strength vs FEM Stress

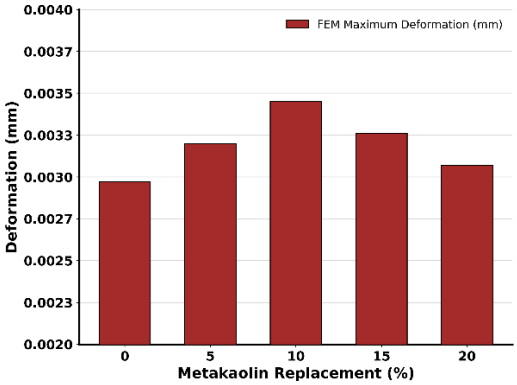


Figure 19: FEM Deformation

The consistency of experimental and FEM results validates the numerical model as a predictive tool for MK-based concretes. This dual approach not only enhances confidence in the mechanical characterization of MK concretes but also demonstrates the potential of FEM to reduce experimental workload in future optimization studies.

Conclusions

Based on the experimental and numerical investigations carried out in this study, the following conclusions are drawn:

i. The workability of concrete decreased progressively with the incorporation MK, as shown by reductions in slump and compaction factor values. However, moderate replacement levels (5-10%) maintained acceptable workability for practical application.

ii. Mechanical and durability properties improved significantly at 10% replacement, with peak compressive and flexural strengths, as well as reduced water absorption and higher density.

iii. Finite Element Analysis (FEA) confirmed experimental findings, with maximum stress and deformations peaking at 10% MK replacement. While FEM predicted slightly higher stress values than laboratory results, the overall agreement validated its reliability as a complementary predictive tool.

iv. The combined experimental and numerical outcomes confirm that MK is an effective supplementary cementitious material, with an optimum replacement level of about 10% for balancing mechanical performance, durability, and structural response.

Data availability

The datasets used and/or analysed during the current study are available from the corresponding author on reasonable request.

Ethics Declaration

- Ethical approval:

This is a TETFund project and approval was duly for the conduct of this research

- Consent to participate

This research had the consent of all participating members prior its commencement. This was achieved through a joint inauguration of all members chaired by some of the principal officers of the Ladoke Akintola University of Technology, Ogbomoso.

- Consent to publish

There is not any constraint to publishing this work is reputable journal outlet(s). In fact, it serves as a mandatory task to be fulfilled in ensuring the successful completion of the research work.

Acknowledgements

The authors acknowledge the following:

i. The Tertiary Education Trust Fund (TETFund) for the grant award through the National Research Fund (NRF) 2021 for this research, with research grant award reference number: **TETF/DRandD/CE/NRF2021/SETI/III/00030/VOL.1** without which this research would not have been possible of which part of the research works is hereby published.
ii. Also worthy of acknowledgement is the leader of LAUTECH Cement and Concrete Research (CEMCON) Group in person of Prof. Akeem Ayinde Raheem for his contribution to ensure the successful completion of the research and through whom the research team was encouraged to develop the concept note which eventually earned us the award of the research grant by the NRF.
iii. The technical support rendered by Mr. L. O. Abogunde, all of Civil Engineering Department, LAUTECH Ogbomoso.

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