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Molecular Dynamics Simulation and Mechanical Property Analysis of Unsaturated Polyester/Glass Fiber Composites

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Abstract

Composite materials are essential for engineering applications due to their superior mechanical properties. Unsaturated polyester reinforced with glass fiber is widely used but optimizing its mechanical performance remains challenging. This study combines experimental testing and molecular dynamics (MD) simulations to investigate the mechanical properties of unsaturated polyester/glass fiber composites. Composites were fabricated with varying glass fiber volume fractions. The impact strength and density of each variation were tested. The results showed an optimal glass fiber fraction at 12.5%v, achieving the highest impact strength (142.80 kJ/m^2) and increased density (1.4408 g/cm^3). MD simulations validated these findings, highlighting the role of van der Waals forces in molecular aggregation and interfacial bonding. This study bridges experimental and MD computational insights, recommending the simulation of treated glass fiber in the future to explore the potential of treated glass fibers in enhancing the interfacial bonding and overall mechanical performance of unsaturated polyester/glass fiber composites.

Keywords: *unsaturated polyester, glass fiber, molecular dynamics*

Abstrak

Material komposit memiliki peran yang sangat signifikan dalam berbagai aplikasi teknik karena keunggulan sifat mekanik. Unsaturated polyester yang diperkuat dengan glass fiber sering digunakan, namun mengoptimalkan kinerja mekaniknya tetap menjadi tantangan. Penelitian ini menggabungkan pengujian eksperimental dan simulasi dinamika molekul (MD) untuk menyelidiki sifat mekanik komposit unsaturated polyester/glass fiber. Komposit dibuat dengan variasi fraksi volume glass fiber. Kekuatan impak serta densitas masing-masing variasi diuji. Hasil penelitian menunjukkan fraksi glass fiber optimal pada 12,5%v, dengan kekuatan impak tertinggi (142,80 kJ/m^2) dan terjadi peningkatan densitas (1,4408 g/cm^3). Simulasi MD memvalidasi temuan ini, menyoroti peran gaya van der Waals dalam agregasi molekuler dan ikatan antar muka. Penelitian ini menjembatani hasil eksperimental sifat mekanik komposit dan komputasional MD. Rekomendasi dikemudian hari adalah dilakukan simulasi glass fiber yang telah diberi perlakuan untuk mengeksplorasi potensinya dalam meningkatkan ikatan antar muka dan kinerja mekanik keseluruhan dari komposit unsaturated polyester/glass fiber.

Kata Kunci: *polyester tak jenuh, glass fiber, simulasi molekul*

1. Introduction

Composite materials have become a cornerstone in the development of advanced engineering applications, owing to their superior mechanical properties and design flexibility. Unsaturated polyester resins reinforced with glass fiber have emerged as a widely used composite system in industries such as automotive, aerospace, and construction, primarily due to their lightweight characteristics, high strength, and cost-effectiveness [1]. However, optimizing the mechanical performance of these composites, especially their impact resistance and density, remains a critical challenge.

Numerous studies over the past decade have explored the mechanical properties of unsaturated polyester/glass fiber composites. The tensile and flexural strength of glass fiber-reinforced polyester composites, demonstrate that increasing the fiber volume fraction improves tensile properties but may compromise impact resistance [2]. Previous studies also investigated the impact of the toughness on unsaturated polyester composites reinforced with pineapple leaf fibers, highlighting the importance of fiber orientation and composition on mechanical performance [3]. The influence of glass fiber volume variation on mechanical properties using compression molding increases tensile strength but can introduce voids, leading to reduced impact strength [4]. Despite these advances, there remains a lack of comprehensive studies that integrate both experimental and molecular-level insights into the behavior of unsaturated polyester/glass fiber composites.

A key gap in the current literature is the limited use of molecular dynamics (MD) simulations to model the atomic-level interactions in polymer composites. MD simulations provide a powerful tool to analyze the interfacial bonding and stress distribution within composites, offering insights that are difficult to achieve through experimental methods alone [5]. Although previous research has extensively focused on macroscale mechanical testing, few studies have combined these results with molecular simulations to achieve a holistic understanding of composite behavior [6], [7]. This study addresses this gap by employing both experimental and simulation methods to analyze the mechanical properties of unsaturated polyester/glass fiber composites. Specifically, composites with varying glass fiber volume fractions were fabricated using the hand lay-up method and tested for impact strength and density. Concurrently, molecular dynamics simulations using LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator) were conducted to model the atomic interactions and stress distributions within the composite.

This research integrates experimental testing with molecular simulations, to provide a comprehensive analysis of the mechanical properties of unsaturated polyester/ glass fiber composites. This approach not only validates the simulation model against experimental data but also offers valuable insights into the atomic-scale interactions that influence composite performance. By bridging the gap between experimental and computational methods, this study may contributes to the optimization of composite materials for advanced engineering applications. The objective of this research is to investigate glass fiber’s influence on the mechanical properties of unsaturated polyester/glass fiber composites, leveraging both experimental data and molecular dynamics simulations to enhance the understanding and design of high-performance composites.

2. Material and Methods

This study executes both experimental and simulation methods. The first stage involves the fabrication of unsaturated polyester/glass fiber composites using the hand lay-up method, with glass fiber volume fractions set at 8.9%v, 10.7%v, 12.5%v, and 14.3%v. The second stage utilizes LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator) to model bonding and atomic interactions within the Unsaturated Polyester/glass fiber composite. Simultaneously, mechanical properties were tested using Zwick Roell for impact testing and a Density Determination Kit for density testing. Each volume percentage variation of glass fiber will be tested using 10 specimens. These tests were conducted at the Polymer Chemical Engineering Instrumentation Laboratories at Politeknik STMI Jakarta. The primary materials used in this study include liquid unsaturated polyester resin YUKALAC 157® BQTN-EX, glass fiber as a reinforcing material, and MEKP catalyst with cobalt for the resin curing process. Figure 1 presents the flowchart illustrating the methodology steps in this research, with each box representing a stage in the process: composite fabrication, mechanical testing, simulation in LAMMPS, data comparison, and data analysis.

Experimental and simulation data were analyzed to investigate glass fiber's influence on the mechanical properties of the composite. The Molecular Dynamic (MD) simulation results were validated by comparison of experimental data, confirming the model's reliability. The study imposed several limitations to simplify the analysis. The molecular structure of unsaturated polyester was represented by a simplified polymer chain without considering crosslinking, focusing solely on interactions between short polymeric chains and the SiO_2 surface. The SiO_2 component was modeled as pure, non-functionalized silicon dioxide, excluding the effects of metal oxides such as MgO, Al_2O_3, or Na_2O. This isolation ensured that the influence of non-bonded interactions, including van der Waals and electrostatic forces, could be thoroughly analyzed.

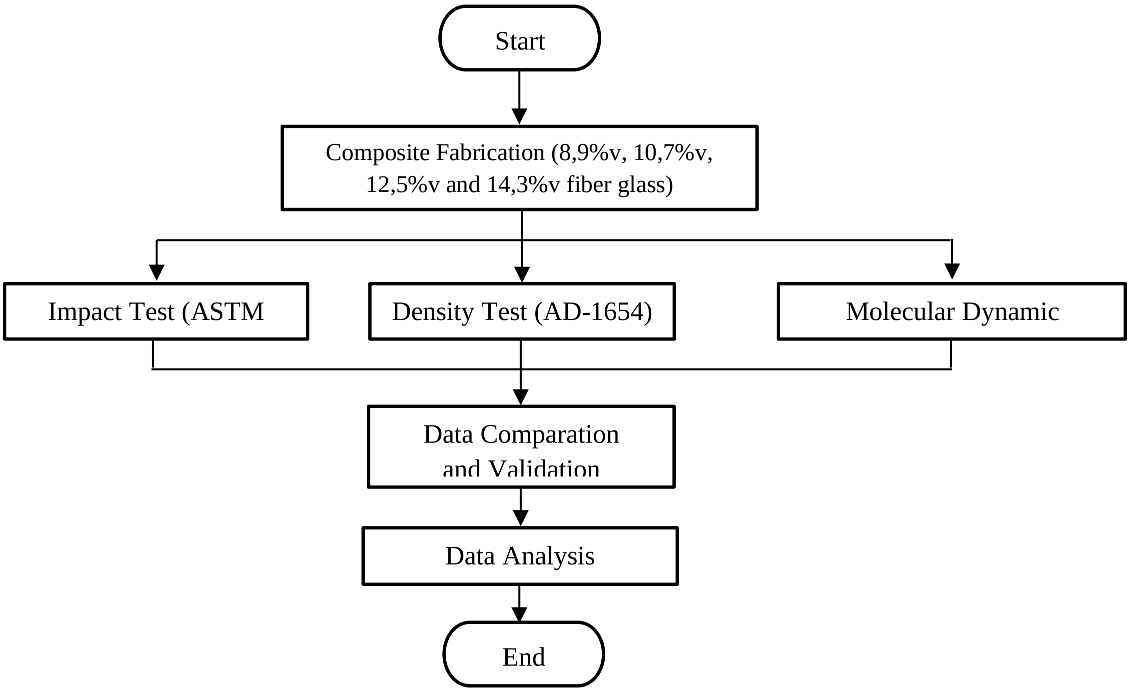


Fig. 1: Flowchart of Experimental and Simulation Methodology for Unsaturated Polyester/Glass Fiber Composites

Unsaturated Polyester Molecular Structure

Figure 2 illustrates the molecular structure of unsaturated polyester, a thermosetting polymer synthesized through the polycondensation of unsaturated anhydrides and glycols. The resulting oligomers are dissolved in a vinyl monomer such as styrene, which acts as a reactive diluent and facilitates crosslinking during curing. That polymer is combined with styrene monomer to create the unsaturated polyester [8].

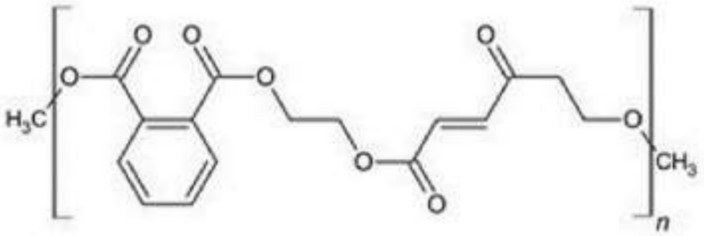


Fig. 2: Unsaturated Polyester Molecule Structure [9]
Source: Grimalt J, et. al, 2023

Unsaturated Polyester contains polar functional groups such as ester linkages, making it capable of forming hydrogen bonds or Van der Waals interactions with other polar surfaces, such as glass fiber [10]. Ester linkages exhibit polarity due to the significant electronegativity difference between oxygen and carbon atoms within the functional group. This polarity enables ester linkages to interact effectively with other polar molecules or functional groups. Notably, the ester group possesses a permanent dipole moment of approximately 1.7 Debye, highlighting its intrinsic polar nature [10], [11]. The carbonyl (C=O) groups within the ester linkages are highly polar due to the oxygen atom's strong electronegativity, creating a partial negative charge on oxygen and a partial positive charge on carbon [12]. This polarity can contribute to transient charge distributions that, in turn, facilitate van der Waals interactions, as these weak intermolecular forces arise from temporary positive and negative charges caused by electron movement. Van der Waals interactions are Weak intermolecular bonds between regions of different molecules bearing transient positive and negative charges which are caused by the movement of electrons. The molecular structure of Unsaturated Polyester enables van der Waals interactions, particularly through the polar region and non-polar regions (hydrocarbon chains) [13]. Polar molecules experience stronger van der Waals interactions due to dipole-dipole forces compared to nonpolar molecules, where dispersion forces dominate. Van der Waals forces, including dipole interactions, are fundamental for both polar and nonpolar molecular systems, but their strength and type differ based on the presence of permanent dipoles (polar molecules) or induced dipoles (nonpolar molecules) [12], [14]. These intermolecular forces make unsaturated polyester, an adaptable material for various composite applications, as it bridges polar and nonpolar systems with relative ease.

Glass Fiber Molecular Structure

Glass fiber-reinforced composites are among the most widely utilized materials in the fiber-reinforced polymer composite industry for both commercial and industrial applications [15]. This popularity stems from the exceptional tensile and compressive strength achieved by combining resin with glass fibers. Glass fibers are amorphous materials predominantly composed of a silica (SiO_2) network, with additional oxides such as sodium, boron, calcium, and aluminum contributing to their properties [16]. These fibers are produced from extremely fine, non-crystalline glass fibers characterized by a short-range network structure, as illustrated in **Fig. 3**.

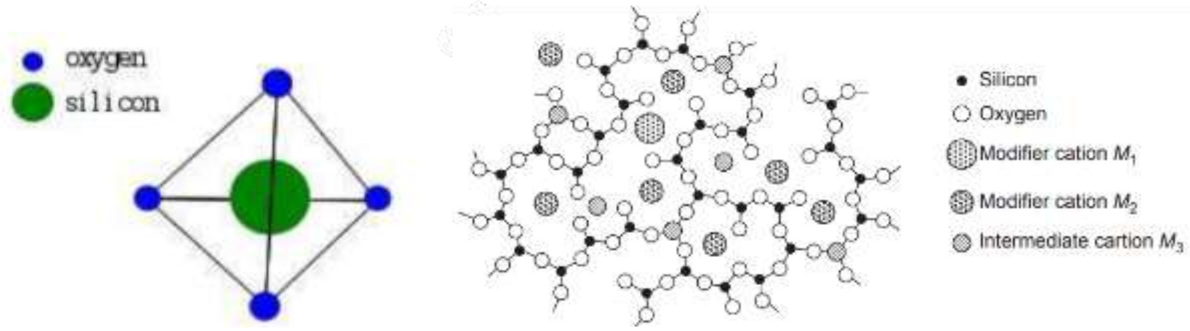


Fig. 3: Three-Dimensional and Two-Dimensional Glass Fiber Molecule Structure [17], [18]
Source: Hasan, K. et. al, 2016 & Jones, F. et. al., 2018

The structural framework of glass fiber consists of an amorphous silica matrix, where interconnected SiO_4 tetrahedral units form Si-O-Si bonds [18]. This molecular configuration underpins the material's remarkable stiffness, thermal stability, and mechanical strength. Optimizing the glass fiber composition is crucial to achieving a balanced and effective composite design.

3. Results and Discussion

The Mechanical Properties of Unsaturated Polyester/Glass Fiber

The data presented in Table 1 highlights the mechanical behavior of unsaturated polyester/glass fiber composites, specifically in terms of impact strength and density, as a function of varying glass fiber volume fractions. The trends observed can be scientifically explained by considering the interactions between the unsaturated polyester matrix and the glass fiber reinforcement.

Table 1. Experimental Data on Impact Strength and Density of Unsaturated Polyester/Glass Fiber Composites at Various Glass Fiber Volume Fractions

Percentage of Glass Fiber	Impact Strength (kJ/m^2)	Density (g/cm^3)
8,9 %v	78,41	1,3831
10,7%v	111,78	1,3872
12,5%v	142,80	1,4408
14,3%v	97,74	1,4755

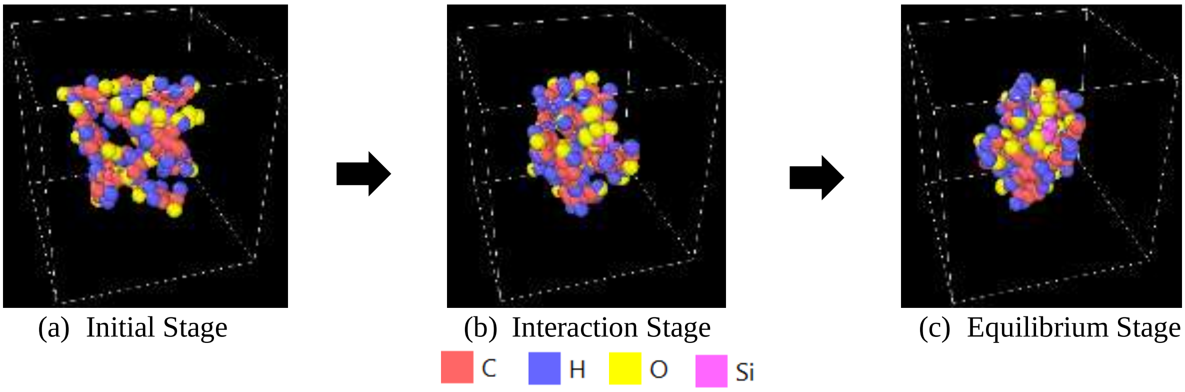
Impact strength, a measure of a material's ability to absorb energy during sudden loading, is heavily influenced by the fraction of glass fiber in the composite. The initial increase in impact strength is observed as the glass fiber volume fraction rises from 8.9%v to 12.5%v, with values increasing from 78.41 kJ/m^2 to 142.80 kJ/m^2. This improvement is attributed to the uniform dispersion of fibers at moderate volume fractions, facilitating efficient energy transfer between the matrix and the fibers [19]. The matrix binds the fibers cohesively, preventing crack propagation and enhancing the composite's toughness [20]. Previous studies on glass fiber reinforcement in polyurea have also demonstrated that increasing fiber volume fraction and fiber length significantly enhances the elastic modulus and absorbed energy, with improvements of approximately 103% and 137.5%, respectively [21].

The observed decline in impact strength of unsaturated polyester/glass fiber composites beyond 12.5% volume fraction (to 97.74 kJ/m^2 at 14.3%v) can be influenced by the effects of excessive fiber volume fraction. Excessive glass fiber leads to poor matrix encapsulation, which compromises the matrix-fiber bonding and promotes delamination. At higher glass fiber content, the interlaminar shear strength decreases, as observed in other composite systems, leading to easier propagation of cracks through the composite structure and a reduction in energy absorption capability [22]. These factors collectively result in reduced impact strength and toughness at higher glass fiber volume fractions. Thus, optimizing the fiber volume fraction is crucial to avoid such adverse effects while maintaining mechanical performance in composite design.

The density of the composite increases steadily with the fiberglass content, ranging from 1.3831 g/cm³ at 8.9%v to 1.4755 g/cm³ at 14.3%v. This trend is attributed to the higher intrinsic density of fiberglass compared to unsaturated polyester resin. The increase in density observed with the addition of glass fiber to the unsaturated polyester composites is primarily attributed to the higher intrinsic density of glass fiber compared to that of the unsaturated polyester matrix. Glass fibers typically have a density of approximately 2.56 g/cm³ [23], which is significantly higher than the density of unsaturated polyester resin, which ranges between 1.025 g/cm³ [24]. As the proportion of fiberglass increases, the overall composite density rises proportionally, consistent with the principle of volumetric averaging of composite constituents.

Molecular Dynamics Simulation with LAMMPS

Molecular dynamics (MD) simulations offer an in-depth view of atomic-level interactions within composite materials. This study visualizes the interaction and aggregation process between Unsaturated Polyester and Glass Fiber using the LAMMPS software. By employing MD methods, the compatibility of Unsaturated Polyester and Glass Fiber was evaluated, highlighting the role of intermolecular forces, including van der Waals interactions, in forming composite structures. The simulation, depicted in **Fig. 4**, is divided into three distinct stages:

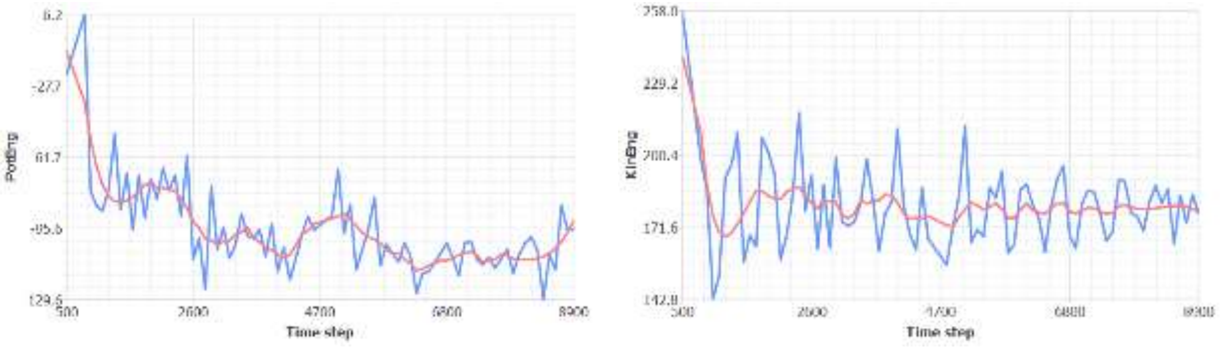


(a) Initial Stage (b) Interaction Stage (c) Equilibrium Stage

Fig. 4: Visualization of Interaction between Unsaturated Polyester and Glass Fiber in Molecular Dynamics (MD) Simulation

At the beginning of the simulation shown in **Fig. 4**(a), Unsaturated Polyester and Glass Fiber molecules are distributed randomly within the simulation box. Glass fiber molecules, represented by silicon (Si) and oxygen (O) atoms, are positioned in specific regions, while Unsaturated Polyester molecules, consisting of carbon (C), hydrogen (H), and oxygen (O) atoms, occupy other areas. There is no significant interaction between the two components at the initial stage, reflecting their separate initial configuration. The intermolecular forces at this point are minimal, and no structural integration is observed. At the initial phase of the simulation, the potential energy exhibits a decline from a positive value to a significantly negative range. This rapid drop reflects the system's transition toward a more stable configuration, driven by the intermolecular forces. In this case, molecules rearrange themselves to minimize the overall energy, primarily facilitated by van der Waals interactions [25]. The progression of potential energy changes during the molecular interactions over time is illustrated in **Fig. 5** (a). At the onset of the simulation, the kinetic energy experiences a sharp decrease from an initially high value. This initial drop reflects the system's relaxation process as atomic interactions commence, redistributing energy and adjusting the atomic positions and velocities to achieve more stable configurations [26]. During this phase, excess energy is dissipated as atoms respond to intermolecular forces and reorganize into energetically favorable arrangements. The changes in kinetic energy can be observed in Fig. 5(b).

The internal energy—comprising both kinetic and potential energy—plays a pivotal role in molecular behavior. Internal energy represents the sum of all kinetic energies from molecular motion and potential energies arising from intermolecular interactions within the system. The decline in potential energy observed in Fig. 5(a) indicates a shift toward a stable configuration driven by van der Waals interactions, minimizing the system's energy. Meanwhile, the sharp drop and subsequent stabilization in kinetic energy, as shown in Fig. 5(b), reflect the system's attainment of thermal equilibrium. The internal energy embodies these transformations, with energy redistribution enabling structural organization and molecular interactions [26], [27]. This synergy between potential and kinetic energy illustrates the dynamic interplay governing molecular behavior and composite performance.



(a) *(b)*

Fig. 5: The Profiles of (a) The Potential Energy and (b) The Kinetic Energy of the Unsaturated Polyester and Glass Fiber System Obtained from Molecular Dynamics Simulation

During the interaction stage shown in **Figure 4** (b), the intermolecular forces begin to act, pulling unsaturated polyester and glass fiber molecules closer together. The dominant force driving this interaction is the van der Waals force, which arises from nonpolar-nonpolar and polar-polar atomic interactions [28], [29]. The polar interactions between oxygen atoms in glass fiber and unsaturated polyester contribute to additional attraction, expediting the formation of a compact structure. The decreasing potential energy observed during this stage confirms the stabilization of the molecular structure as a result of van der Waals interactions. Van der Waals forces, although weak, are essential for molecular interactions, particularly in maintaining structural stability and material properties [14]. These forces facilitate the interaction between Unsaturated Polyester polymer chains and the Glass Fiber surface. Additionally, the interaction of polar groups enhances molecular compatibility between the components, as reflected in the compact molecular arrangement achieved during this phase.

As the simulation progresses, the potential energy stabilizes and fluctuates within a narrower range after several thousand-time steps. This stabilization indicates that the system has reached energetic equilibrium, with molecular configurations achieving a balance between attractive and repulsive forces. The observed fluctuations in potential energy are inherent to molecular dynamics simulations, where atoms and molecules are in constant motion within the simulation box. The magnitude of these fluctuations is influenced by the system's temperature (average 300 K) and the strength of intermolecular interactions. The Lennard-Jones potential, applied through the pair style in LAMMPS, captures the essence of these interactions by modelling Attractive Forces and Repulsive Forces. Van der Waals interactions dominate attractive force at moderate interatomic distances, scaling as r^{-6}, where r represents the distance between atoms. Repulsive Forces arise from core repulsion at shorter distances, scaling as r^{-12} [30], [31].

The atoms from the unsaturated polyester and fiberglass experience these forces, as governed by the Lennard-Jones potential parameters (ε and σ). These interactions facilitate molecular clustering and aggregation, as evidenced by the potential energy profile and molecular visualizations. The substantial drop in potential energy at the start of the simulation underscores the strong intermolecular interactions, particularly van der Waals forces, between Unsaturated Polyester and Glass Fiber molecules. The stabilization of potential energy further suggests that the system has achieved a state of molecular compatibility. This compatibility reflects the binding strength between Unsaturated Polyester and Glass Fiber. In summary, the potential energy profile highlights the attractive and repulsive forces within the system. Van der Waals forces emerge as the primary driver of molecular aggregation and compatibility between Unsaturated Polyester and Glass Fiber molecules, providing valuable insights into their potential as composite materials.

In the final equilibrium stage shown in **Figure 4** (c), Unsaturated Polyester and Glass Fiber molecules form a more integrated aggregate. This compact structure demonstrates that the intermolecular forces, primarily van der Waals forces, and polar interactions, are strong enough to overcome separating forces. The oxygen-silicon interactions significantly contribute to the stability of this aggregation, laying the foundation for superior mechanical properties in composite materials. The dominance of van der Waals forces in stabilizing this composite system emphasizes their role in composite formation. These forces provide structural cohesion, enabling the production of composite materials with enhanced mechanical performance. The fluctuations observed in the kinetic energy after stabilization are a natural consequence of thermal motion within the molecular system. Atoms in the system vibrate and move continuously due to thermal energy, resulting in inherent variations in kinetic energy over time [32]. The magnitude of these fluctuations is determined by the system temperature, the strength of intermolecular forces, and the number of particles included in the simulation. The kinetic energy profile provides critical evidence that the molecular system has attained thermal equilibrium. The steady average value of kinetic energy confirms that the system is dynamically stable and maintains a consistent temperature, aligning with the parameters specified in the simulation.

Validation of Simulation Data Against Experimental Results

The mechanical behavior of unsaturated polyester/glass fiber composites was assessed through a combination of experimental and simulation approaches to elucidate the interplay between molecular interactions and macroscopic properties. The experimental data in Table 1 presents the trends in impact strength and density across various glass fiber volume fractions. These trends were critically analyzed against molecular dynamics (MD) simulation results to validate the findings. MD simulations revealed the insights of the van der Waals interactions between unsaturated polyester and glass fiber molecules, which influence the mechanical behavior of the composite. At the optimal glass fiber volume fraction (12.5%v), simulations showed robust intermolecular interactions leading to strong cohesion between unsaturated polyester and glass fiber molecules. This observation corresponds with the experimental peak impact strength of 142.80 kJ/m², demonstrating effective load transfer and enhanced energy dissipation during mechanical deformation.

The observed decline in impact strength of unsaturated polyester/glass fiber composites beyond 12.5% volume fraction (to 97.74 kJ/m² at 14.3%v) can be attributed to the effects of excessive glass fiber content. At higher fiber volumes, poor matrix encapsulation occurs, compromising the matrix-fiber bonding and promoting delamination within the composite. Additionally, excessive glass fiber content reduces the interlaminar shear strength, facilitating crack propagation through the composite structure and diminishing its energy absorption capability [22]. These factors collectively result in reduced impact strength and toughness at higher glass fiber volume fractions. The findings highlight the importance of maintaining an optimal fiber volume fraction to balance reinforcement benefits with mechanical performance, ensuring the composite's structural integrity and energy dissipation capacity. Furthermore, this decline may also be influenced by void formation and the system's inability to reach equilibrium during the curing process. Unlike molecular dynamics simulations where atoms have sufficient time to achieve a relaxed state, the curing process may introduce defects due to rapid polymerization or uneven distribution of fibers, preventing the composite from achieving an energetically stable configuration. At equilibrium, the displacement energy is significantly lower because all atoms have sufficient time to adjust their positions, and defects only develop when the atomic arrangements and movements coincide in a way that allows a defect to form [26].

Density trends observed experimentally also correlate well with MD simulation results. Experimental data revealed a steady increase in composite density, from 1.3831 g/cm³ at 8.9%v to 1.4755 g/cm³ at 14.3%v. This trend reflects the contribution of the higher-density glass fiber to the overall composite density. Simulations confirmed this behavior, as glass fiber particles exhibited tighter aggregation within the unsaturated polyester matrix at higher glass fiber content, resulting in increased atomic packing and density. The simulation data validate the experimental observations and confirm that MD simulations can effectively predict composite density based on constituent material properties and their interactions.

These results underscore the utility of MD simulations in capturing atomic-scale interactions that help analyze the impact of macroscopic mechanical properties. By simulating van der Waals forces and molecular aggregation, the MD results align with experimental data, validating the simulations as a reliable tool for understanding and optimizing composite material design. The data validation between experimental and simulation demonstrates the critical role of molecular interactions in governing the mechanical behavior of unsaturated polyester/glass fiber composites and highlights the importance of optimizing glass fiber volume fractions for enhanced performance.

4. Conclusion

This study integrates experimental and molecular dynamics (MD) simulation methods to comprehensively analyze the mechanical behavior of unsaturated polyester/glass fiber composites. The experimental data demonstrated trends in impact strength and density as a function of glass fiber volume fraction, with an optimal mechanical performance observed at 12.5%v. At this fraction, the composite exhibited the highest impact strength of 142.80 kJ/m² and a steady increase in density to 1.4408 g/cm³. Beyond this optimal glass fiber content, the impact strength decreased significantly to 97.74 kJ/m² at 14.3%v, primarily due to excessive fiber volume leading to poor matrix encapsulation. This inadequate matrix-fiber bonding promoted delamination and reduced interlaminar shear strength, allowing cracks to propagate more easily and diminishing the composite's energy absorption capacity.

Molecular dynamics simulations corroborated these findings by providing atomic-level insights into the interactions between unsaturated polyester and glass fiber. Van der Waals forces were observed, promoting effective molecular aggregation and enhancing interfacial adhesion. However, excessive glass fiber content resulted in poor matrix encapsulation. Additionally, the density trends derived from simulations closely aligned with experimental results, confirming the higher intrinsic density of glass fiber and its role in contributing to the composite's overall density. This increase in density was further attributed to molecular aggregation driven by attractive forces, which promoted tighter packing within the composite matrix.

By bridging the gap between experimental data and computational insights, this study validated the reliability of MD simulations in predicting composite behavior and highlighted the critical role of molecular interactions in determining composite performance. It is recommended to perform further MD simulations that consider surface treatments or chemical modifications, such as silanization, to enhance the bonding between glass fiber and the unsaturated polyester matrix. MD simulations could be utilized to explore the impact of treated glass fiber surfaces on matrix-fiber interactions, offering deeper insights into their behavior. Investigating the role of crosslinking within the unsaturated polyester matrix is also suggested to better understand its contribution to enhancing toughness and durability and ensuring a balanced and high-performance composite material.

5. Acknowledgment

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