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Modelling of Water Droplet Wettability on Anti-wetting Sheet of Sand/HDPE

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***Abstract* — High-density polyethene (HDPE)has unique mechanical and physical properties and is implemented in personal protective equipment. One of its precious hydrophobicity applications is in medical applications such as protective surgical gloves and aprons. The material has the ability of this hydrophobic to repel fluids by ensuring cleanliness. HDPE's performance can be improved further by adding fillers to enhance mechanical and surface characteristics. The wettability, or the way natural fluids of a particular system interact with its surface. Contact angles were measured in computational simulations performed on HDPE to study its wettability in this research work. These findings were validated using published experimental data. The results demonstrated that the contact angles obtained from the simulations and those of the experimental ones agreed, confirming that the proposed computational method could reliably estimate the wettability of both HDPE and HDPE with sand fillers, avoiding lengthy and tedious experimental work.**

Keywords—Wettability, Anti-wetting, Contact angle, Sand/HDPE composite.

I. INTRODUCTION

During pandemic situations, personal protective equipment (PPE) is vital for the safety of healthcare workers. An example is a coverall and apron commonly produced from high-density polyethene (HDPE), which exhibits excellent mechanical properties, is hydrophobic (i.e., has a water-repelling surface), and can repel fluids. However, the challenge is that HDPE material must protect without sacrificing skin breathability, comfort, and durability during extended wear. Besides that, safety and usability considerations are critically important in the medical environment.

HDPE is one of the most widely used polymers in various industrial, medical, and biomedical applications. It is a widely used substitute material because of its unique mechanical, physical, and functional attributes, including stability, durability, and compatibility [1, 2]. Compared to other polymers, HDPE has disadvantages such as low toughness, low weather resistance, and environmental stress cracking. Its partially hydrophobic surface also happens due to the low energy state and absence of functional groups, which results in low adhesion and chemical reactivity [3]. HDPE can be filled with fillers to overcome these drawbacks and improve its performance and characteristics [4, 5].

The hydrophobicity of a material is an important consideration in determining wettability and evaluating polymer characteristics in various related applications. Wettability is the tendency of a fluid to spread on or adhere to a material's surface. Polymers with poor wettability (hydrophobic) have a low adhesive interaction with the fluids in contact with the surface; therefore, they are easily removed from the surface during cleaning, which can reduce contamination [6, 7]. This characteristic is advantageous in applications requiring desired fluid repellency, such as medical or protective apparel [7].

Wettability, often described through the surface contact angle, is a mechanism to evaluate the interaction of a fluid with a polymer surface [2]. The contact angle is a meaningful parameter for characterising a liquid droplet on a polymer surface, among polymers, or in terms of droplet geometry such as droplet shape, adhesion energy, or material surface energy [8, 9]. The surface properties in the hydrophilic or hydrophobic can be determined from the liquid contact angle, which enables estimation of the surface energy of polymers [10].

The contact angle is between the tangent and the liquid droplet at the contact point on the solid surface. This indicates that the hydrophobicity or hydrophilicity of the polymer material is measured directly. A contact angle of 0° represents complete wetting (fully hydrophilic), where the liquid spreads entirely across the surface. When the contact angle ranges from 0° to 90°, the surface is considered hydrophilic, which attracts and interacts well with the fluid. Conversely, if the contact angle exceeds 90°, the material is classified as hydrophobic, where the liquid forms beads and does not spread, indicating poor wetting. In extreme cases, an angle approaching 180° signifies a superhydrophobic surface, where liquid droplets maintain a nearly spherical shape and exhibit minimal interaction with the surface.

Polymeric surfaces generally exhibit nonpolar characteristics and low surface energy, which limits their compatibility with certain compounds, such as water-based or polar adhesives [10, 11]. This low surface energy contributes to the hydrophobic nature of polymers, as seen in materials like HDPE, which affects their wettability and fluid interaction. This characteristic suggests that polymeric surfaces are unsuitable for various compounds, mainly water-based and polar nature, such as adhesives. Therefore, reliable and efficient computational approaches are needed to evaluate the wettability of HDPE and its composites so that advanced materials with enhanced performance can be developed efficiently.

This study aimed to investigate the wettability properties of HDPE reinforced with fillers using the computational method. The results were analysed and validated using the experiment results from previous literature presented by Siraj *et al.* (2020)[12].

II. METHOD

A. Experimental Study

For validation, the experiment was performed using coloured water. As shown in Fig. 1, a plunger was under very controlled conditions to form a droplet, and a defined volume of water flowed through the needle. After 5 sec of wetting period, a camera recorded the wetting behaviour of the droplet on the tested paper. The wetted droplet was subsequently analysed with angle measurement software to obtain the contact angle. An experimental measurement was made to validate the numerical simulation results.

Table I. Measured contact angles from Siraj *et al.* (2020) [12] which was used as the input to computational study.

Sheet Material	Contact Angle (Degree)
0 wt%	97.96 ± 9.2
35 wt%	89.60 ± 0.89
35 wt%+C	92.0 ± 5.74
Regular A4	83.34 ± 7.75

In a paper published previously by Siraj *et al.* (2020), the contact angle was also used to assess the wettability of the HDPE composites reinforced by powdered sand fillers. The contact angle was obtained by drawing an angle between a tangent to the water droplet and the surface of the HDPE composite. A similar test was conducted on 35% of the filler composition of the composite sheet. Besides that, the same test was also performed on a test paper as a reference. The reported results are shown in Table I below [12]. 0 wt% sheet material is HDPE without filler, 35 wt% sheet material was the composition of HDPE with 35 wt% filler of powdered sand, where 35 wt%+C composition of HDPE with powdered sand and polyethene grafted maleic anhydride (PE-g-MA) the compatibiliser, C.

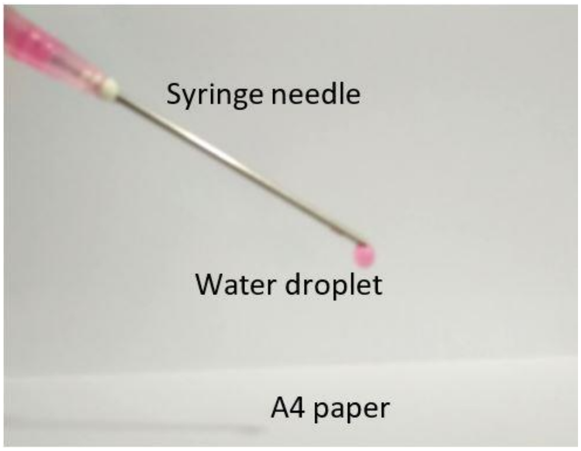

Fig. 1. Wettability test of a water droplet on the tested paper.

The result of the computational study was validated using experimental results and other results published previously, as in Table I [12].

B. Computational Study

The computational study was carried out using Surface Evolver software version 2.70, 32-bit. Surface Evolver is a freeware license software whose input file is written in C. The initial surface of a water droplet was defined as a simplicial complex containing a set of points in three-dimensional space connected using a line to form a closed volume.

The study was conducted to simulate the wettability condition of the water droplet in the aspect of droplet geometry and contact angle. The properties of water were included in the input file as listed in Table II. Since the droplet of the water was considered microfluid, the effect of the surface tension force is higher than its weight; thus, surface tension, density, and volume were considered.

According to Young's Equation (As in Eq. (1)), the contact angle is the key to the droplet's wettability, which can be related to its energy content. The contact angle of the liquid is formed at the three-phase boundary where liquid, gas and solid intersect, where γ_{SV} is solid surface free energy, γ_{Sl} is solid/liquid interfacial free energy, and γ_{lV} is liquid free surface energy.

$$\gamma_{sv} = \gamma_{sl} + \gamma_{lv} cos\theta \quad (1)$$

The formation of water droplet shape was based on the energy-based approach as Eq. (2) [13], which Surface Evolver software used to solve geometrical droplet formation. Total Energy, E_T of the water droplet was the sum of surface tension energy, E_S and the gravitational energy, E_G.

$$E_T = E_S + E_G \quad (2)$$

Total energy was resolved by integration of the surface tension, γ at the specific contact angle, θ, Eq. (3).

$$E_T = y \int -\gamma cos\theta dx \quad (3)$$

The surface tension energy was calculated at the interfacial surface tension, γ, on the contact line of the droplet as in Eq. (4).

$$E_s = \iint \gamma dA \quad (4)$$

The gravitational energy due to the droplet's weight was calculated as Eq. (5), where ρ is the density of the liquid and g gravity acceleration.

$$E_G = \iiint \rho gzdV \quad (5)$$

Table II. Material properties of water as input to the simulation study using surface evolver.

Material Property	Detail
Surface tension (dynes/cm) [16]	72.0
Density (gm/cc)	1.0
Volume (mm^3)	1.8

The experimental results of Siraj *et al.* (2020) [12] were used to select three contact angles corresponding to different sand-reinforced HDPE sheet composite compositions (Table III). These measurements show that the filler content affects the wettability of the composites. The differences in surface properties, especially hydrophobicity and adhesion of the composite, were confirmed by measuring the contact angles on surfaces with different sand fillers in the HDPE matrix. This data establishes a baseline for the computationally simulated results in this study, serving as a means of comparison.

Table III. Polymer material properties.

Composition	Contact Angle (Degree)
0 wt% sheet	97.96
35 wt% sheet	89.60
35 wt% + C	92.00

The model was set up using the following boundary conditions based on the collected data. Droplet volume remained in contact during the simulation to ensure no change in volume. The surface was evolved to minimise the surface energy while maintaining the initial volume. The contact line intersection between liquid, gas and solid is free to move horizontally to achieve minimal surface energy; the contact angle at the contact line was fixed to the assigned value in Table III. Heigh of the droplet was free to be adjusted to ensure that the fluid's weight in the vertical direction was equivalence to the surface tension and contact angle.

III. RESULTS

Figure 2 shows the wettability condition of the water droplet on A4 paper. The contact angle obtained from the experimental test was 83.74 degrees, while the modelling result showed the contact angle was 84.61 degrees. There was only a 1.0% disparity between the two results, which is strongly accepted for further study. Besides that, the results from the current study also strongly agree with the previous study by Siraj *et al.* (2020) [12], which averaged 83.34 ± 7.75 degrees.

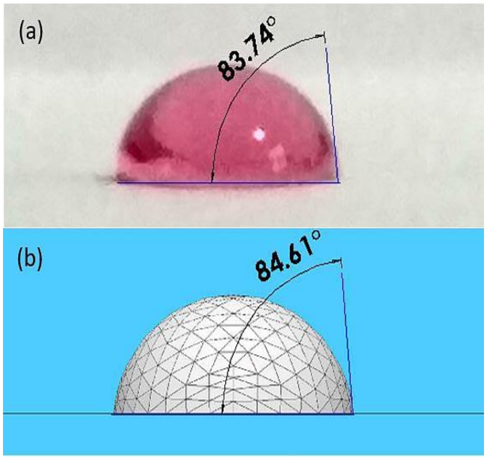

Fig. 2. (a) Contact angle of droplet on the tested paper obtained from the current experimental study (b) Contact angle from the current modelling result on the tested paper using Surface Evolver.

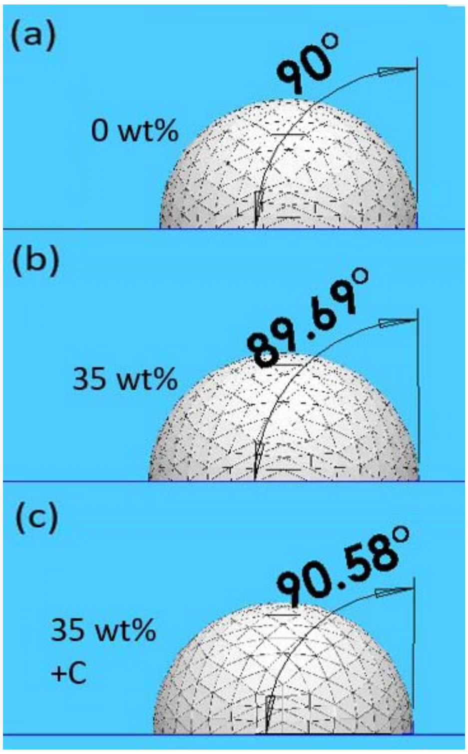

Fig. 3. Wettability condition of water droplet on Sand/HDPE sheet (a) 0 wt% composite (b) 35 wt% composite (c) 35 wt% + C composite.

Figure 3 shows the wettability condition of the water droplet on three samples with different HDPE filler compositions. The simulation results showed that when the filler concentration increased, the contact angle decreased from 90 degrees for 0 wt% to 89.69 degrees for 35 wt% [12]. This decreasing pattern might be caused by the composite's surface property (i.e., roughness) [14]. Badgayan *et al.* (2020) also mentioned that the decrease in contact angle might be caused by the micro asperities on the sample surface [7]. The higher roughness of the HDPE sheet increased the interfacial surface tension, subsequently decreasing the contact angle and causing the proper wetting of the HDPE sheet [15].

The wettability behaviour of the droplet on the composite sheet is illustrated in Fig. 4(a)-(e). Initially, the droplet was modelled as a simplified square shape to represent the falling water (Fig. 4(a)). Upon contact with the composite surface, the droplet spread out due to the influence of gravity (Fig. 4(b)). This process involves three phases: 1) the fluid phase of the water droplet, 2) the solid phase of the composite surface, and 3) the gas phase of the surrounding air. Each phase works toward achieving equilibrium by minimising the exposed surface area of the droplet. Figures 4(c), 4(d) and 4(e) show that the droplet gradually reduces its surface area. Once equilibrium is reached, no further changes in the droplet's geometry occur, signifying the stabilisation of the system.

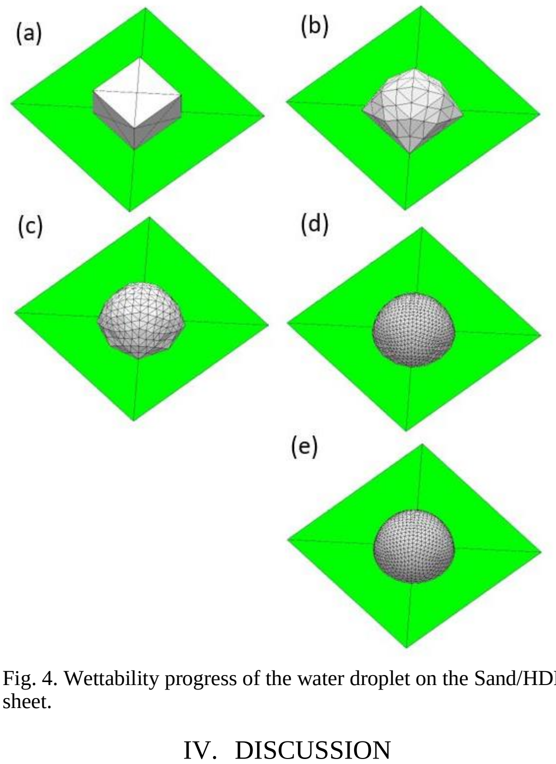

Fig. 4. Wettability progress of the water droplet on the Sand/HDPE sheet.

IV. DISCUSSION

A lower error percentage at a 1% difference, as in Figure 2, was achieved in the modelling due to several precautions taken during the experiment and simulation. First, a wetting time of 5 seconds was observed before capturing the droplet's wet condition. Second, the model's geometry was carefully evolved, starting with small steps and re-meshing to enhance geometric features, particularly at the edges.

Wettability occurs when a water droplet adheres to a surface and spreads out, governed by the balance of forces between the three involved phases: water, the composite sheet, and the surrounding air. According to Young's Equation, force equilibrium is achieved when the liquid minimises its energy through surface tension and contact angle [16]. A contact angle less than 90 degrees indicates a wetting condition, while a contact angle greater than 90 degrees suggests a non-wetting surface. A higher contact angle (> 90 degrees) of water droplets will be formed on a hydrophobic surface due to its high interfacial tension.

In this study, the Sand/HDPE sheet composite demonstrated a non-wetting condition with an average contact angle of 90 degrees. Even though the contact angle is less than 90 degrees at a composition of 35wt%, it can increase the contact angle by more than 90 degrees with the addition of C Composite. C composite had a higher impact on the water absorption rate as it altered the surface roughness [17].

As noted in previous studies, the Sand/HDPE sheet composite has demonstrated excellent mechanical properties [15, 18]. Combined with its anti-wetting characteristics, these properties offer cost-reduction potential and broaden the material's application scope. While HDPE is typically known for its stiffness and susceptibility to stress cracking, adding sand as a filler enhances ductility by reducing stiffness. Despite varying filler percentages, the wettability of the composite sheet remains consistent, maintaining stable contact angle values. The mentioned properties make sand/HDPE composites attractive for use in various conditions and environments.

Comparing sand/HDPE composite with other composite materials, it can be said that the hydrophobicity of sand/HDPE is low. For example, using silica as the filler for composite decreases the capability of water absorption and increases the water contact angle by more than 140 degrees [19]. Other than that, the addition of graphene oxide (GO) to epoxy resin to produce the GO composite also gave higher hydrophobicity effects when the water contact angle is more than 100 degrees [20], and X. Zhang e*t al.* [21] also found that composition of composite that combines with natural fibre also increases the hydrophobicity effects where the water contact angle reaching as high as 138 degrees. However, some of the mentioned composite materials above its benefits and usability are overshadowed by its disadvantages. One of the critical disadvantages is that silica is easily hydrolysed in an alkaline environment, and it has low interaction (low binding force) with ionic species [21]. Meanwhile, complicated synthesis is time-consuming and time-consuming to produce GO [21]. Therefore, sand/HDPE does show a unique combination of moderate hydrophobicity, ductility, and application versatility, which makes it suited for cost-effective applications that require better mechanical properties and non-wetting characteristics.

Figures 2, 3 and 4 provide an understanding related to the wettability condition of the droplet under selected conditions based on difference filler and how the droplet interacts with the composite sheet, which droplet spreading and stabilises, driven by the minimising energy and driven by equilibrium between water, air and composite sheet surface. Adding filler to HDPE is expected to reduce the contact angle in some instances, indicating faster wetting time and reducing interfacial surface tension. In this study, a significant improvement in the contact angle was not achieved even though the study could accurately model the droplet of the HDPE composited. It is suggested that improvement can be made, such as improving extruding polyolefin films of the HDPE composite sheet to achieve uniform wetting behaviour through the use of finer power of the sand to ensure homogeneity of fillers and produce consistent surface roughness and better contact angle.

Despite moderate hydrophobicity, sand/HDPE composites remain a better choice for applications such as piping for water supply, medical containers or PPE. One of the reasons is that the surface properties repel the liquid, as extreme water-repellence characteristics are not necessary. Besides that, this material is cost-effective as it can be recycled with enough durability and strength to cope with the suitable application. For specific applications where higher repellence fluid properties are required, mesoporous HDPE was preferred [22]. The hydrophobic properties of the HDPE can be improved via ozonation. The process was reported to increase the contact angle from 90 to 120 degrees due to enhanced surface roughness using nano/microscale surface relief.

V. CONCLUSION

In conclusion, this study successfully modelled the wettability properties of the Sand/HDPE sheet composite, achieving a low error percentage due to several precautions taken during both the experimental and simulation phases. The wetting time and careful evolution of the model's geometry played a key role in accurately simulating the droplet's behaviour on the composite surface. The Sand/HDPE sheet demonstrated a consistent non-wetting condition with an average contact angle of 90 degrees, indicating stable surface properties despite varying filler percentages. Additionally, the composite's excellent mechanical properties and anti-wetting characteristics offer the potential for cost reduction and expanded applications. The approach outlined in this study can accurately predict the wettability of HDPE and its sand-reinforced composites through contact angle measurements, providing a reliable and efficient method for assessing surface properties without extensive experimental procedures.

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