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CFD Study on Effects of Geometric Shape and Surface Hydrophilicity and Hydrophobicity on the Drainage Capacity of Plant Leaves

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Abstract. The photosynthesis process of plant requires fast removal of surface contaminant of leaves. The removal of surface contaminants is highly related to the drainage capacity of the leaf. This paper conducted a comprehensive study on the drainage capacity of plant leaves. The effects of both leaf shape and leaf hydrophilicity/hydrophobicity are investigated. This paper uses Computational Fluid Dynamics (CFD) technology to simulate the drainage process of plant leaves. The numerical simulation results indicate that hydrophilic leaves requires the sharp parts on the edges to remove the water. On the other hand, the drainage capacity of hydrophobic leaves is independent of the shape of the leaves.

Keywords: CFD; Drainage capacity; Leaf; Geometry; Hydrophilicity; Hydrophobicity

1 Introduction

The fundamental function of leaves is to convert solar energy and inorganic carbon dioxide into chemical energy and organic nutrients for plants. Therefore, any foreign matter on the leave surface, including water, is undesirable[1]. This is because water will accumulate dusts and make the surface of the leaf dirty, which has a negative effect on the photosynthetic synthesis. Therefore the plant leaves need to quickly remove the water on their surface. The factors affecting the drainage capacity of plant leaves mainly include the following two parts:

1.1 Geometric shape of plant leaves

There are various geometric shapes of plant leaves in nature such as polygons, ellipses, etc. In most cases, there are sharp triangular portions on the edge of the plant leaves. This paper firstly studies the effect of geometric shape on the drainage capacity of the leaf. According to the geometric shape of the leaves, the most representative triangle and ellipse shapes were selected in this study, as shown in Fig. 1. The ellipse shape represents the overall profile of the leaf, while the triangle represents the sharp portions on the edge and at the tip of the leaf. At the same time, the combined shape with the ellipse and the triangle (Fig. 1c) was also studied and compared with the triangle and the ellipse shapes to understand the drainage capacity of the natural leaf geometry. For the three geometric shapes in Fig 1, the comparative analysis was carried out in two conditions. In the first condition, the drainage capacity of the three shapes was compared when their length and width were the same. In the second condition, the three shapes kept the same area when their drainage capacity was compared. Through the comparative analysis of these two conditions, the effects of the length, width and area of the leaf on its drainage capacity can be understood.

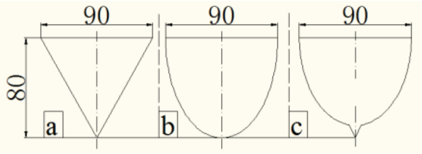

Fig.1. Calculation model (Height and width is the same:height -80mm,width-90mm) a: Triangle model ; b: Elliptical model; c: Mixed shape model(Ell + Tri)

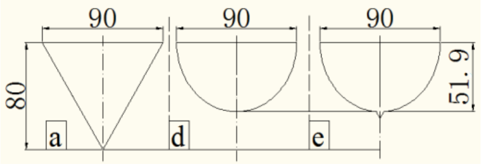

Fig.2. Calculation model (Surface area is the same:area-3600 mm^2,a-model is the basic model) d: Elliptical model; e: Mixed shape model(Ell + Tri)

1.2 Surface hydrophilicity and hydrophobicity

In nature, the surface of the leaf can be either hydrophobic or hydrophilic. The hydrophobicity and hydrophilicity of the surface of the leaf directly affects the drainage mechanism. The hydrophobicity/hydrophilicity of the leaf can be determined using the surface contact angle θ

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(Fig. 3). θ is the angle between the solid-liquid-gas three -phase junctions, from the solid-liquid interface to the gas-liquid interface, in other words, the most direct indicator of hydrophobicity and hydrophilicity.

The contact angle θ of the droplet on a perfectly smooth and flat solid surface is given by Young's equation (1).

$$\cos\theta = \frac{\gamma_{SV}-\gamma_{SL}}{\gamma_{LV}}$$

(1)

where $\gamma_{SL}, \gamma_{SV}, \gamma_{LV}$ stand for the interface free energy (J/m^2) of the solid-liquid, solid-gas and liquid-gas interface and are also called the interface tensile force (N/m).

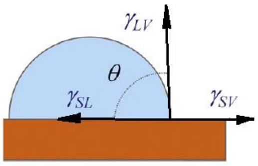


Fig.3. The states of water droplets on smooth surface

However, the surface that is absolutely smooth and flat does not exist in nature. Wenzel, R.N and Cassie, A.B.D modified the Young's equation, and proposed a theoretical model describing the relationship between the contact angle and the roughness of the solid surface [错误!未找到引用源。-5].

Wenzel equation:

$$\cos\theta_w = r\frac{\gamma_{SV}-\gamma_{SL}}{\gamma_{LV}} = r\cos\theta$$

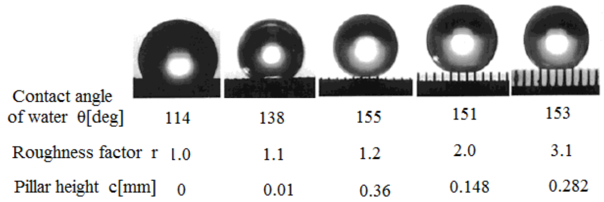
(2)

Cassie equation:

$$\cos\theta_c = f\cos\theta + f - 1$$

(3)

In equation (2), θ_w is the surface contact angle of the rough surface (also known as the Wenzel contact angle); r is the surface roughness factor, which is a ratio of the actual area of the surface and its geometric projection. It is always greater than one. In the Wenzel equation, the surface free energy of the solid part of the rough surface is r times larger than the surface free energy of the perfectly smooth surface, so the hydrophobicity of the rough surface can be enhanced by increasing the solid-liquid contact area. In equation (3), θ_c it is also the surface contact angle of the rough surface (also called Cassie contact angle); f is the area fraction of the solid-liquid interface, and (1-f) is the area fraction of the solid-gas interface. In the Cassie equation, the reduction in solid-liquid contact area emphasizes the hydrophobicity of the rough surface. Yoshimitsu experimentally observed the relationship between contact angle, roughness factor and rough surface morphology as shown in Fig. 4 [4].



Contact angle of water θ[deg]	114	138	155	151	153
Roughness factor r	1.0	1.1	1.2	2.0	3.1
Pillar height c[mm]	0	0.01	0.36	0.148	0.282

Fig.4. Shapes of 1 mg water droplets on prepared pillar structures, and corresponding water contact angles θ, roughness factors r, and pillar heights c.

Fig. 4 shows that when the roughness is small (1.00 < r < 1.10), the liquid will saturate the entire surface, including all the surfaces of the groove. Under this condition, the relationship between surface roughness and contact angle can be described by the Wenzel mode. On the other hand, when the roughness continues to increase (1.23 < r), the contact angle remains almost constant. It is observed that the liquid dose not cover all the solid surfaces and some air exists at the interface between the liquid and the solid, in which case the contact angle is described by the Cassie mode. In general, when the contact angle $\theta > 130^\circ$, the solid surface is considered to be a hydrophobic surface. On the hydrophobic surface, the liquid will form droplets, while on the hydrophilic surface, the liquid will spread over the surface to form a water film. Therefore, the drainage performance of the hydrophobic surface is superior to that of the hydrophilic surface. It can be seen from the above discussions that the hydrophilicity and hydrophobicity of the surface of the leaf is closely related to its surface roughness. The relationship between the roughness factor r and the surface topography can be expressed by the following formula [4]:

$$r = \frac{(a+b)^2+4ac}{(a+b)^2}$$

(4)

In equation (4), a is the width of the pillar column, b is the groove width, and c is the height of the pillar column. As the surface roughness increases, the contact angle also increases, and the surface hydrophobicity also increases. Therefore, this paper explores the effect of leaf surface hydrophobicity and hydrophilicity on the drainage capacity of leaves by studying the surface roughness of the leaves.

2 Numerical simulation: Overview

In this paper, computational fluid dynamics (CFD) simulation was used to establish the hydrodynamic model of plant leaf. Through parametric analysis, the effects of leaf geometric shape and surface hydrophilicity and hydrophobicity on the drainage capacity of the leaves was studied. The numerical analysis in this paper was divided into two parts. Firstly, the effects of the three geometric shapes shown in Fig 1 on the drainage capacity of the leaves were studied. In this part, the other physical parameters of the leaf such as interfacial tension force, contact angle and roughness are not considered. The second part is to use different surface roughness to explore the effect of surface hydrophilicity and hydrophobicity on the drainage capacity of the leaf. The simulation of CFD is carried out by using the commercial software Fluent. The numerical model is shown in Fig. 5.

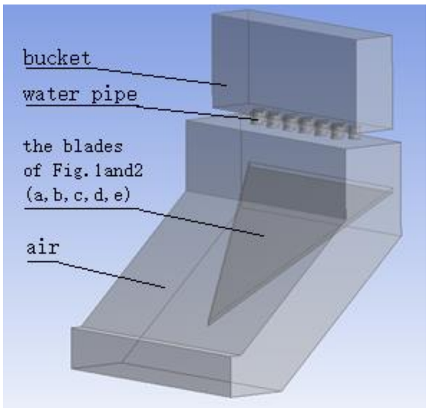


Fig.5. CFD model, The blades in the blade area are replaced by the a, b, c, d, e models of Fig. 1 and Fig.2.

In Fig. 5 taking a triangular leaf as an example, the leaf has an inclination angle of 45 ° from the ground, and the leaf thickness is 1mm. The water was supplied using the top bucket, and a row of 13 water pipes is placed under the bucket for the flow of the water. The diameter of the water pipe is 5 mm. The flow of water on the leaves involves the influence of the surrounding air. The surface tension of the solid, liquid and gas three-phase boundary was considered, so the surrounding air is also modeled in the model.

3. Numerical model

3.1 Meshing and control equation

One of the key issues in CFD numerical simulation is meshing. Although the size of the model to be simulated in this paper is large, but the geometric shape is not complicated. Considering the factors such as structure size, calculation time, model accuracy and analysis stability, the CFD model of this paper adopts the structure grid division mesh method. In addition, the CFD model in this paper used the Finite Volume Method to discretize the governing equations in the spatial and temporal domains. The numerical interpretation used the SIMPLE (SemiImplicit Method for Pressure-Linked Equation) method, which is based on the Finite Volume Method (one of dispersion methods). It guarantees calculation stability, so it is widely used in many CFD practices. The Laminar model was used to study the influence of geometric shape on the drainage capacity of the leaves. When analyzing the surface hydrophilicity and hydrophobicity of the leaf surface, the tempering model (Realizable k-ε model) was used. Considering the influence of leaf surface roughness, it is more reasonable to use the tempering model (Realizable k-ε model). This paper uses the multiphase flow model, VOF (Volume of Fluid, VOF).

3.2 Initial conditions

Under gravity, the air in the model is the same as the outside atmosphere, and the air flow is static and the pressure is higher than atmospheric pressure. When the viscosity of air is 1.7894×10^{-5}kg/(m·s), the liquid is water, and its density and viscosity are respectively 998.2kg/m^3, and 1.003×10^{-3} kg/(m·s). The surface tension coefficient of water is 72.5×10^{-3} N/m, and the working pressure of the inlet and outlet of the water pipes is the same as the atmospheric pressure.

3.3 Boundary conditions

The water pipe wall is set to no slip. When analyzing the influence of geometric shape on drainage capacity, it is assumed that the leaf surface is perfectly flat (no roughness). When the hydrophilicity and hydrophobicity of the simulated leaf affects the drainage performance, the pillar height of the leaf is the values used in the literature of Fig. 4, as shown in Table 1.

Table 1. Leaf surface roughness height

Wall Roughness Height(mm)				
0	0.01	0.036	0.148	0.282

4 Simulation results and analysis

4.1 Effect of geometric shape on leaf drainage capacity

As mentioned earlier, the water on the leaves flowed from the bucket, and a row of 13 water pipes is placed under the bucket. The length of the bucket is 100mm, the width is 10mm, the height is 5mm, and the water volume in the bucket is 5g. Fig. 6 shows the initial state of the triangular leaf model and the drainage. The water flowing rate curve at the leaf tip is shown in Fig. 7.

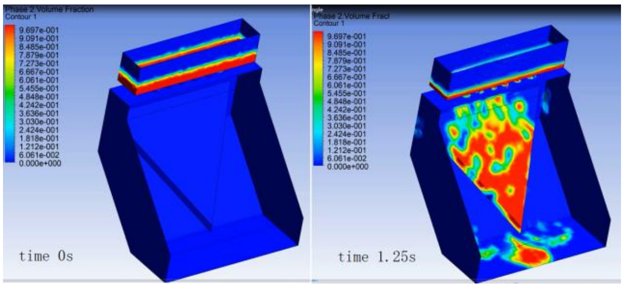


Fig.6. CFD model showing before (left) and after (right) the water is applied

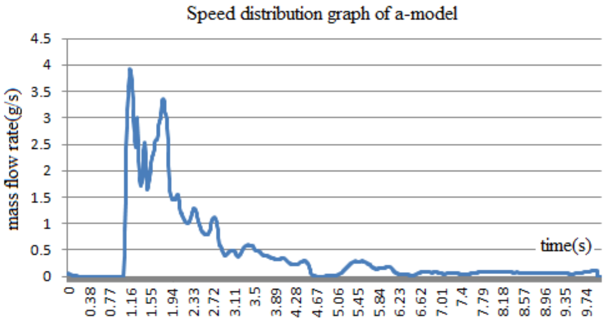


Fig.7. Water flowing rate at leaf tip of a-model

It can be seen from Fig. 7 that most of the water is discharged from the leaf in the range of 0.7s to 5s. The remaining small amount of water is due to the hydrophilicity of the surface, and the discharge speed is slow or even impossible to discharge. To observe this phenomenon more closely, the water flowing rate curve during 0.7s~5s is enlarged and shown in Fig. 8.

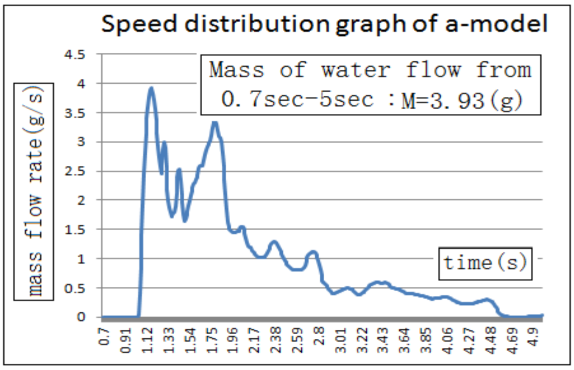


Fig.8. Water flowing rate graph of a-model (0.7sec~5sec)

In order to compare with the drainage capacity of the triangular leaf, this paper also simulated the drainage capacity of the elliptical and hybrid (Fig. 2) leaves with the same width and height as the triangular leaf. A comparison of the drainage speed curves of the leaves of the three geometric shapes is shown in Fig. 9. At the same time, the drainage velocity curve during 0.7s~5s is enlarged and compared as shown in Fig. 10. In Fig. 10 the area under the curve represents the total water that flowed from the correspnding leaf. The comparison results of the areas under the three curves are shown in Fig. 11.

Fig. 11 shows that the triangular leaf (a-model) has the best drainage capacity, and the slowest is the elliptical leaf (b-model). The simulation results explain why the geometric shape of the hydrophilic leaves in nature is generally triangular.

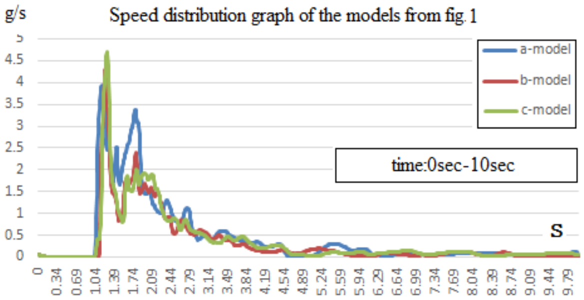


Fig.9. Water flowing rate at leaf tip of the three leaf shapes in Fig.1

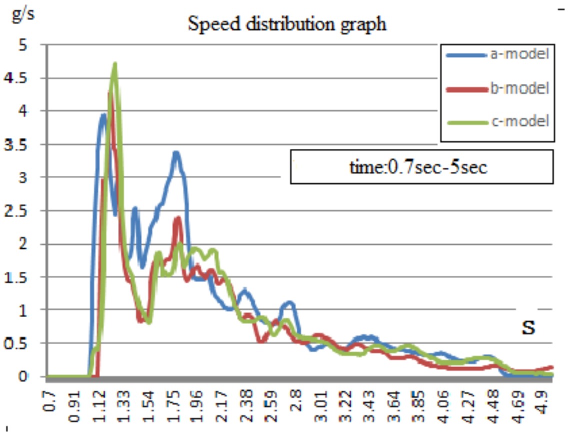


Fig.10. Water flowing rate graph of three shapes (0.7sec~5sec)

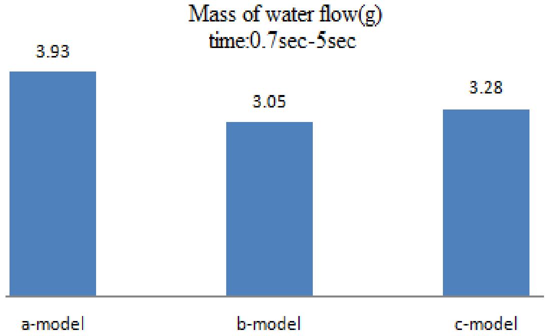


Fig.11. Total amount of water that flowed from the three leaves with different shapes from 0.7 to 5 s. The three shapes have the same width and length

In order to better understand the influence of geometric shape on the drainage capacity of the leaf, the drainage capacity of the triangular, elliptical and hybrid leaves in Fig. 2 was also analyzed when they had the same area. The drainage velocity curves of the three geometrical leafs are shown in Fig. 12. At the same time, the comparison results of the total amount of water flowed over the three leaves in 0.7s~5s are shown in Fig. 13.

Fig. 13 shows that the mixed model (e-model) has the fastest drainage rate. This explains that the geometric shape of the hydrophilic leaf in nature is much similar to that of the hybrid type, especially the reason why the edge of the leaf has small triangular portions.

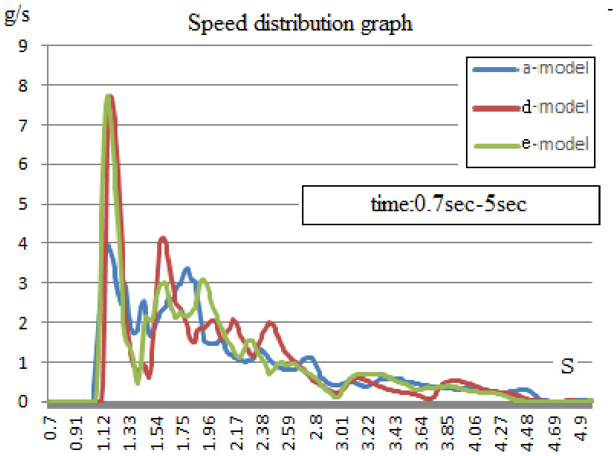


Fig.12. Water flowing rate at leaf tip of the three leaf shapes in Fig.2

Fig. 11 and Fig. 13 show that one of the funcions of the sharp portions (mostly triangles) on the edges of hydrophilic leaves in nature is to remove the surface water more quickly.

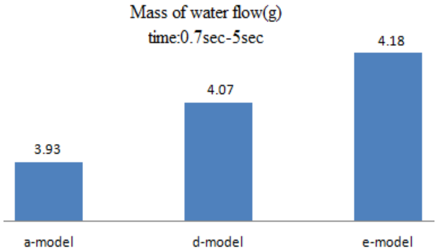


Fig.13. Total amount of water that flowed from the three leaves with different shapes from 0.7 to 5 s. The three shapes have the same area

4.2 Effect of leaf surface hydrophilicity and hydrophobicity on leaf drainage capacity

The literature on the surface hydrophilicity and hydrophobicity has supported the following conclusions:

(1) increasing the surface roughness can improve the surface hydrophobicity;

(2) the liquid will spread on the hydrophilic surface to form a liquid film, and on the hydrophobic surface, droplets will be formed. Therefore, the liquid is more easily discharged on the hydrophobic surface.

(3) the contact angle is an index for evaluating the surface hydrophilicity and hydrophobicity. The contact angle $\theta < 110°$ is a hydrophilic surface, and $\theta > 130°$ is a hydrophobic surface. Increasing the surface roughness increases the contact angle, which increases the surface hydrophobicity.

In order to explore the effect of surface hydrophilicity and hydrophobicity on the drainage capacity of the leaf, a-model leaf was used in this paper to adjust the surface hydrophilicity and hydrophobicity by selecting different pillar heights. In order to compare with the existing results in the literature, the five rough surfaces in Fig. 4 were selected, and the drainage velocity curves of the five rough surfaces were plotted in Fig. 14. The comparison of the total amount of water flowed from various roughness surfaces is shown in Fig. 15.

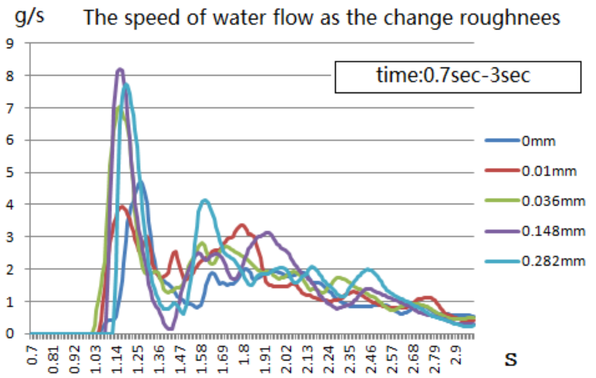
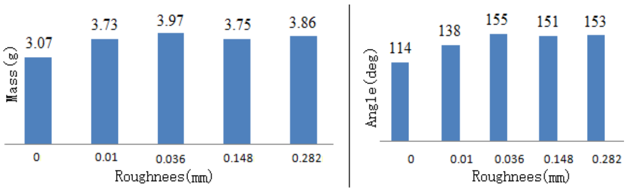


Fig.14. Water flowing rate at leaf tip of triangular leaf with five different surface roughnesses



a: Simulated result b: Literature result

Fig.15. Total amount of water that flowed from the leaves with different roughnesses (left) simulation results of this study ; (b) experimental results from literature

As can be seen from Fig.15, when the surface roughness is higher than 0.01 mm, the drainage capacity of the leaf tends to be stable, which is consistent with the experimental observation in the literature in Fig.4. This is because when the roughness is higher than a certain degree, the surface hydrophobicity tends to be stable, so that the drainage capacity does not change. This analysis shows that when the surface of the leaves is changed from hydrophilic to hydrophobic, the drainage capacity of the leaves does not depend on the geometric shape, but instead the leaf relies on the surface hydrophobicity to enhance its drainage capacity.

5. Summary

1. It is necessary for the leaf to have edges with sharp portions to raplidly remove surface water;
2. It is necessary for the leaf to be hydrophobic to increase the drainage capacity;
3. For hydrophilic leaves, water will form a water film on the surface of the leaf, so the drainage capacity of the leaves depends on the leaf geometric shape; for hydrophobic leaves, the water is formed into droplets on the surface of the leaves and are quickly discharged by the action of wind and gravity, independent of the shape of the leaves.

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