Simulation of droplet impact on super hydrophobic surface

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Abstract
Super hydrophobic surfaces find uses in many applications; therefore proper design of super hydrophobic surfaces is very crucial. A lot of work has already been done for static droplets and super hydrophobic surface interactions. There have also been some significant experiments carried out for dynamic droplet impact on super hydrophobic surfaces. The present work focuses on the super hydrophobic surface under dynamic conditions, with the study predominantly carried out through numerical simulation. Various parameters during impact and time variance after impact (typically up to 10 µs) were considered. The transition from water hammer pressure (order of ρCV) to flow pressure (order of $\frac{1}{2}\rho V^2$) is taken as the main parameter of analysis. During water hammer pressure domain, a strong tendency to cause wetting (Wenzel state) is seen. During flow pressure domain, wetting tendency is significantly reduced (Cassie-Baxter state). These states and the transition from one to the other are very crucial to the design of super hydrophobic surfaces. Hence analyses of pressure regimes are important in designing super hydrophobic surfaces for dynamic conditions. Furthermore, the transition from water hammer pressure regime to normal flow regime is studied. A parametric study is done on this transition of regime.

1. INTRODUCTION

Super hydrophobic surfaces are bio-mimic materials based on the lotus leaf. In nature, the lotus leaf is famous for its hydrophobic nature. When a drop of water is placed on it, it rolls off the surface. A super hydrophobic surface exhibits such water repellent properties. However, liquids like oils do wet the lotus leaf and thus superhydrophobic structures need not essentially be oleophobic by nature and super hydrophobic surfaces need to be designed for non wetting behaviour even under such situations. The non wetting property of super hydrophobic surface results in very applications. One popular usage is in self cleaning of the surface [1]. As the liquid rolls off the surface, it can clean the surface without requiring any active assistance. The super hydrophobic surfaces have strong potential in boilers and other large industrial appliances where manual cleaning or active cleaning is very costly and time consuming [2]. Another application is in separation of mixtures [3] wherein, the difference in wetting properties of different liquids is exploited to achieve this feature. De-icing is another problem which can be solved by potential super hydrophobic surfaces [2]. The super hydrophobic property inhibits accumulation of liquid which leads to reduced ice formation. There are many other varied features possible by utilizing super hydrophobic surfaces. All these benefits have lead to exhaustive research being carried out on super hydrophobic surfaces.

Extensive research has been carried out on super hydrophobic surfaces with the liquid droplet in static condition. In the study carried out by Tuteja et. al. [3], a static droplet on a super hydrophobic surface has been found to exhibit the transition between two states of wetting (the meta-stable Cassie-Baxter and Wenzel state). This finding has been used to analyze the various important parameters associated with super hydrophobic surfaces leading directly to more robust designs corresponding to a static droplet on a super hydrophobic surface. In the present work we aim to describe parameters which will lead to a more robust design corresponding to dynamic impact by a droplet on such surfaces.

Modelling and simulation of droplet impact on a flat surface by Šikalo et. al. [4] has been considered for understanding the dynamics associated with droplet impact surfaces. Various parameters, which are crucial for simulating the behaviour of the liquid during and after impact, have been studied. These results have been used to model the impact of a liquid droplet on a super hydrophobic surface. To study the dynamic impact of droplets, the water hammer pressure phenomenon, which varies in the order of ρCV [8] is studied. The results by Haller et. al. [5] are used to study the magnitude and variation of water hammer pressure. Subsequently the results of Toivakka [6] are used for validation of the numerical simulation. There are very few literature on analysis of impact of liquid droplets on super hydrophobic surfaces. Semi analytical methods for describing super hydrophobic surfaces in dynamic conditions have been described by Bartolo et al [7]. Therefore the present study puts forward a detailed analysis on the behaviour of the liquid during dynamic conditions.

In this study a numerical simulation of droplet impact on super hydrophobic surfaces using the volume of fluid (VOF) formulation has been carried out. For this purpose, a quantitative validation of droplet impact on a flat surface has been carried out as a precursor study. Also validating the droplet impact results by comparing with the few experimental results available in literature have been performed. Subsequently important parameters like pressure and velocity field needs have been analysed to reveal the physics of such impacts.

2. NUMERICAL METHODOLOGY

Numerical simulation has been carried out using the VOF formulation. The governing equations of continuity and momentum (Eqn 1.1 and 1.2) are solved simultaneously with the transport equation for an indication function (Eqn 1.3), representing the volume fraction of one phase [2];

$$\nabla . u = 0 \tag{1.1}$$

$$\frac{\partial(\rho V)}{\partial t} + \nabla .\left(\rho V V\right) = -\nabla p + \nabla . T + \rho f_b \tag{1.2}$$

$$\frac{\partial \alpha}{\partial t} + \nabla .\left(V \alpha\right) = 0 \tag{1.3}$$

The governing equations have been modified for working with VOF formulation. Air is taken as the primary phase and the liquid as the secondary phase. The secondary phase is defined in terms of a volume fraction 'α_s' in each computational cell; such that,

$\alpha_s = 0$ the cell does not contain the secondary phase

$\alpha_s = 1$ the cell contains only the secondary phase

$0 < \alpha_s < 1$ the cell contains the interface between the primary and secondary phases

The value of α_s is obtained by solving the convection equation, Equation (1.3). The volume fraction of the primary phase is then given by

$$\alpha_p = 1 - \alpha_s \tag{1.4}$$

To ensure bounded form and conservation, a modified convection equation is solved

$$\frac{\partial \alpha_s}{\partial t} + \nabla .\left(V_r \alpha_s\right) + \nabla .[\alpha_s (1 - \alpha_s)] = 0 \tag{1.5}$$

Where, V_r represents the relative velocity between the two phases [8].

The velocity V_r is usually dependent on the interaction of the fluid with the surface and thereby dependent on parameters like contact angle. The contact angle significantly changes during flow [4]. While the motion of a liquid on the a hydrophilic surface strongly depends on the contact angle and its variation; variation of contact angle does not significantly affect the flow over hydrophobic and super hydrophobic surfaces [2]. Hence a simplified approach, wherein the maximum advancing contact angle on a flat surface is used for the simulation input, has been used.

For the simulation, non-iterative time advancement is used and the velocity formulation used is absolute. The unsteady formulation used is 1^{st}-order implicit. The gradient option used is Green-Gauss cell based. The discretization for pressure has been done using the PRESTO algorithm, momentum through First order upwind algorithm and volume fraction was discretized through Geo-reconstruct. Coupling between pressure and velocity is done using PISO algorithm. The residuals are not directly observed. They are monitored indirectly through the courant number. The courant number is given as

$$\text{Courant number} = u * \Delta t / \Delta x \quad (1.6)$$

where, Δx corresponds to grid spacing and u is the instantaneous velocity at the current flow time. The courant number is monitored and kept under a certain value by varying Δt. The maximum allowed courant number is set as 0.2. A fixed wall is set as the boundary condition for the surface on which the impact takes place. All other sides are kept as pressure outlet. These conditions have been utilized for all simulations.

3. RESULTS AND DISCUSSION

a) Flat plate quantitative validation

Results published by Toivakka [6] are used to show quantitative validation for a flat plate. The computational domain dimensions are 0.1 mm x 0.4mm with axis symmetry. The impact velocity is set as 20 m/s. The diameter of droplet is set as 0.1 mm. The contact angle between the liquid ink and air interface is set as 90°. The ink has the material properties same as that of water, except it is more viscous. It has a viscosity of 50 mPas at the computational temperature. The computational domain is illustrated in Fig. 1.

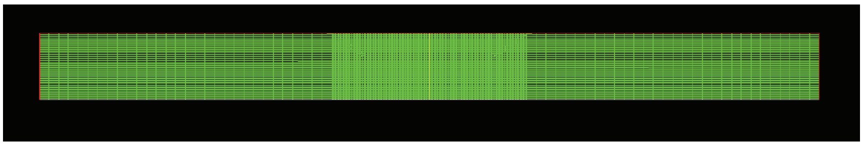


Figure 1. Computational domain used for quantitative validation

The plot showing the comparison of results obtained from numerical simulation and from the result published by M.Toivakka [6] is shown below.

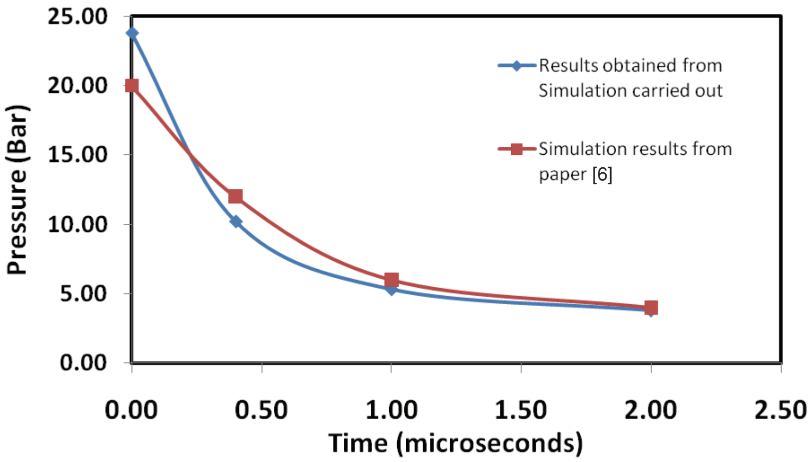


Figure 2. Comparison of results (Flat plate quantitative validation.)

Different sizes of meshes were used. The configuration shown has 100 grid points on the vertical side, 100 grid points for the first 0.1 mm on the horizontal and 30 grid point for the rest 0.3 mm. The second configuration has 50 grid points on the vertical side, 50 grid points for the first 0.1 mm on the horizontal and 15 grid point for the rest 0.3 mm. It has been observed that the variation in result from using different size of mesh is very small. This shows that the dependence on the grid spacing is low at the current level of spacing. Hence it can be established that quantitative validation on a flat plate is satisfactory.

b) Qualitative validation on superhydrophobic surface

Experimental results obtained by Deng et al [1] have been used to show a qualitative validation of the numerical simulation on super hydrophobic surface. For validation on super hydrophobic surfaces, two configurations are considered. For each configuration, simulation is carried out in 2D as well as 3D computational domain. In all cases, water is the liquid which is impacting the surface. The speed of impact of the droplet on the super hydrophobic surface is 3 m/s. The first configuration has a post width of 15 µm, post spacing of 150 µm and post height of 20 µm. The advancing contact angle as measured on the flat surface of this material is 128°. The second configuration has an average pore size of 38 nm and pore to pore spacing of 10nm. The advancing contact angle as measured on the flat surface of this material is 120°. As per the published experimental results by Deng et al [1], it is expected that in the first configuration, the super hydrophobic surface will be wetted by the liquid which impacts the surface. In the second configuration, the super hydrophobic surface is not expected to be wetted by the liquid which impacts the surface. It has been conclusively shown that the simulation results agree with the published experimental results.

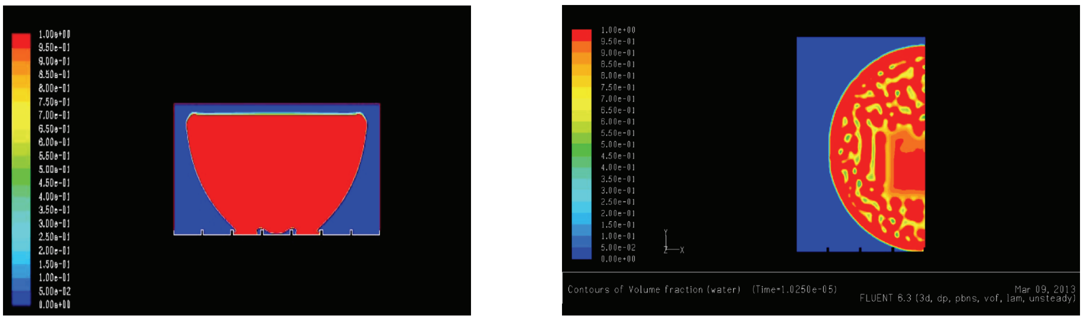


Figure 3. (a) Configuration 1, 2D domain (b) Configuration 1, 3D domain

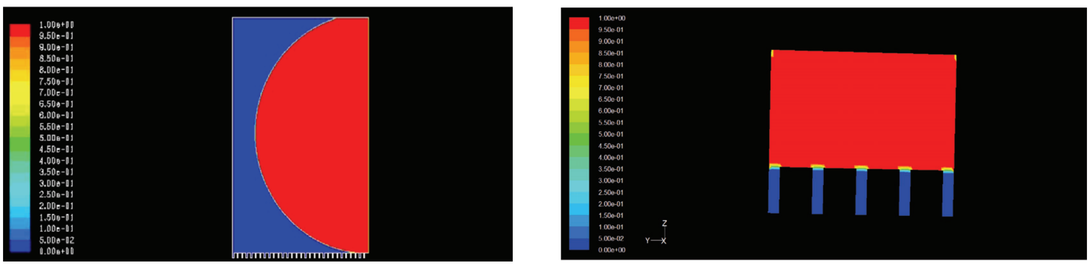


Figure 4. (a) Configuration 2, 2D domain (b) Configuration 2, 3D domain

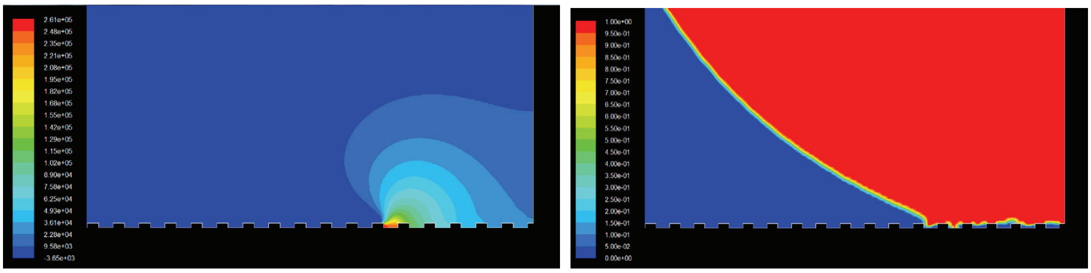
Table1: Qualitative comparison on super hydrophobic surface

Sl. No	Surface parameter	Published experimental result	Simulation Result
1	Post width : 15 m Spacing : 150 m Height : 20 m Advancing contact angle for flat a surface : 128° Impact velocity: 3m/s	Fully wetting	Fully wetting
2	Average pore size : 38 nm Pore to pore spacing : 10nm Advancing contact angle for flat a surface : 120° Impact velocity: 3m/s	Fully non wetting	Fully non wetting

c) Variation of water hammer pressure

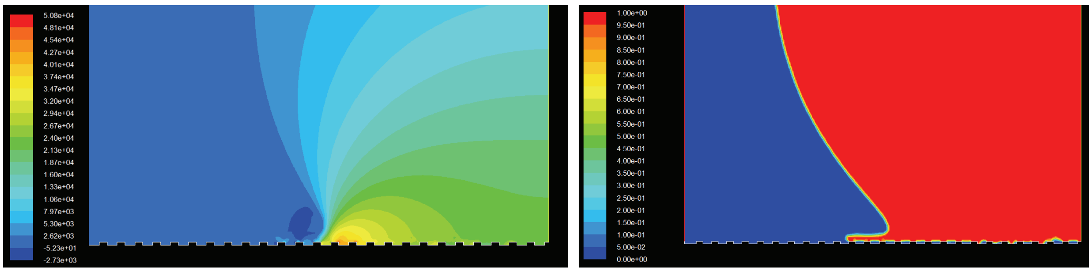
Some parameters like instantaneous pressure, velocity field are hard to accurately estimate. The analytical solutions are often too complex. It is almost impossible to measure some of these parameters experimentally. Hence numerical simulations are used to study these parameters. It was determined to pursue studying pressure and it's variation with time. Two types of pressure are observed. One is the normal flow pressure and the other is the water hammer pressure. Normal flow pressure scales as ½ ρV^2, while water hammer pressure scales as ρCV [1]. Water hammer pressure is significantly higher than normal flow pressure. This high pressure is seen at the time of impact and for a short time after impact. It dies down very quickly. It is also observed that presence of water hammer pressure significantly increases the wetting tendency of the liquid. When the pressure dies down wetting tendency is significantly reduced. In super hydrophobic surface there are two states, one in the fully wetting state (Wenzel state), the other is the fully non wetting (Cassie-Baxter state). This change of state is crucial to the design of super hydrophobic surfaces [3]. Thus, these two pressure regimes of water hammer pressure and flow pressure is similar to the two wetting state. Hence it is easy to see that information about the pressure variation will be a very significant factor in the design of super hydrophobic surfaces in dynamic conditions. Thus, results obtained from simulation regarding variation in pressure will be discussed in subsequent sections. Various configurations of super hydrophobic surfaces were considered. One sample analysis has been elaborated. This configuration of super hydrophobic surface has a post width of 22 µm, a post spacing of 38 µm and post height of 11 µm. The fraction of solid in contact is 0.37. The advancing contact angle as measured on the flat surface of this material is 110°. A 2D symmetry is used for the computational domain.

The simulation is run for a sufficient amount of flow time (around 10 µs) to ensure transition from water hammer pressure to normal flow pressure is captured. The velocities used in the simulation are in the region where most experiments or analysis available in literature have been carried out [1] [7]. The pressure contour and phase movement at a certain time is given below in Fig. 5. The contours in Fig. 5 are at a flow time corresponding to a regime when the water hammer pressure in dominant. The contours in Fig.6 show the pressure contour and phase contour at a flow time when the water hammer pressure is not dominant.



(a) (b)

Figure 5. Contour corresponding to early regime, dominated by water hammer pressure, for an impact velocity of 3 m/s (a) Pressure contour (Pressure in Pa) (b) Phase contour



(a) (b)

Figure 6: Contour corresponding to late regime, water hammer pressure is not dominant, for an impact velocity of 3 m/s. (a) Pressure contour (Pressure in Pa) (b) Phase contour

A clear difference can be observed between the two regimes. In the first case, there is a strong tendency for wetting. In the second, the tendency for wetting is very weak. Also the pressures have a significantly higher magnitude in the first case. Fig. 7 shows the variation of pressure at an impact velocity of 3m/s on the configuration of super hydrophobic surface.

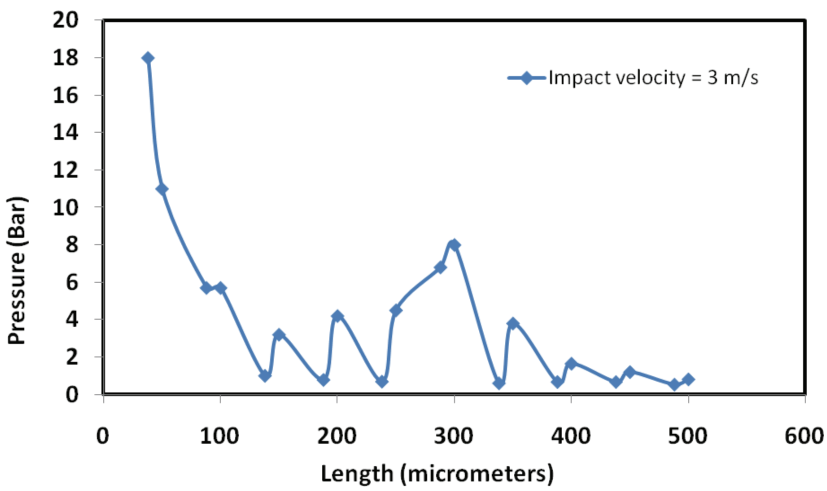


Figure 7. Variation of pressure with distance from point of impact. The fraction of solid in contact =0.37

In this plot the local peaks are due to the secondary phase (water) hitting the post. After a certain distance this pressure variation dies off. This can be seen as the transition from water hammer pressure regime to normal flow pressure regime. This length, from this point on, will be referred as cut-off length. Simulation is carried out other velocities as well. Fig. 8(a) and (b) illustrates the results obtained. The same plot (Figure 8a) is shown with only the water hammer pressure in Fig. 8(b).

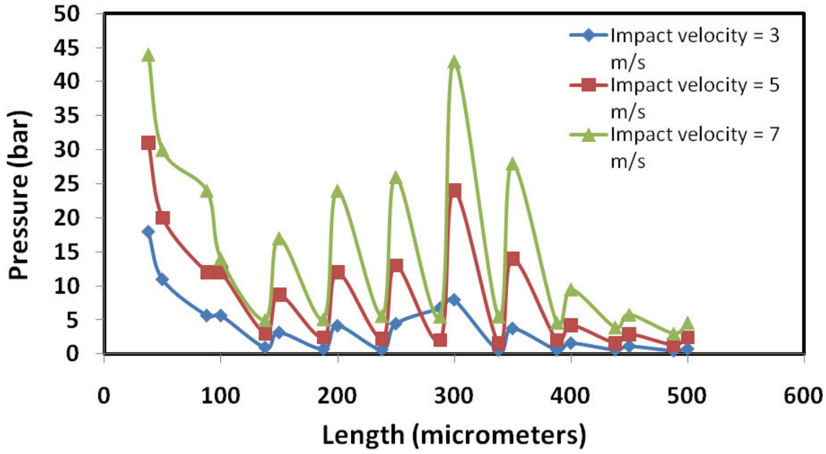


Figure 8(a): Variation of pressure with distance from point of impact, with multiple velocities. The fraction of solid in contact =0.37

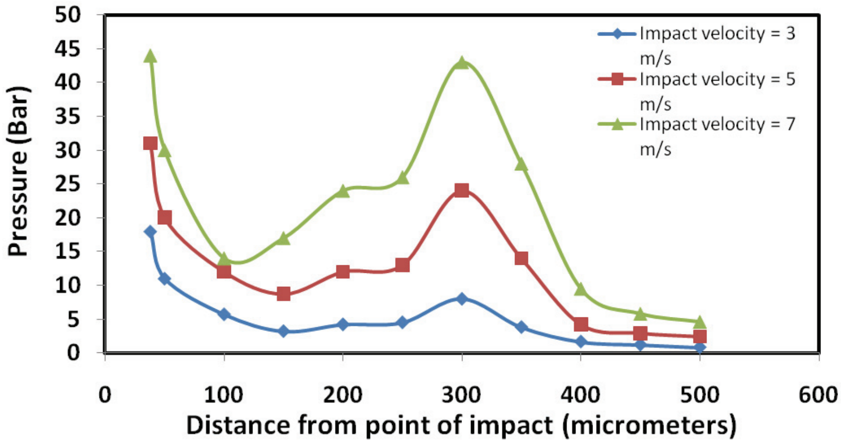


Figure 8(b). Variation of pressure with distance from point of impact with multiple velocities (only water hammer pressure) (The fraction of solid in contact =0.37)

In Fig. 8 the variation of water hammer pressure and the subsequent decay to normal flow pressure is illustrated. It can be observed that the magnitude of the pressure varies with impact velocity as expected. However, the dependence of cut-off length with impact velocity (in this range of velocities) is very low. It can also be seen that the nature of variation of the pressure with distance is also very similar for different impact velocity. It is observed that the cut-off length for this specific case turns out to be around 400 μm irrespective of the impact velocity. Subsequently this exercise is carried for other configuration of super hydrophobic surfaces. Cut-off lengths for few other configurations of super hydrophobic surfaces have been obtained and tabulated in Table 2.

Table 2: Cut-off length for various configurations of super hydrophobic surfaces

Fraction of solid in contact	3m/s	5m/s	7m/s
0.37	400 µm	400 µm	400 µm
0.5	120 µm	120 µm	120 µm
0.6	100 µm	100 µm	100 µm
0.75	80 µm	80 µm	80 µm

It can be seen that the cut-off length is fairly independent of the impact velocity (in this regime) for a given configuration of super hydrophobic surface. The cut-off length is essentially the point where the surface tension of the liquid breaks and the droplet loses the original geometry it possessed and starts to flow. Thus the weak dependence of cut-off length with impact velocity leads to a weak relationship between breaking of surface tension of liquid and the impact velocity. Hence in the regime of impact velocity under consideration, the breaking of the surface tension of the liquid is not governed just by water hammer pressure. If the cut-off length were dependent on just the water hammer pressure (impact pressure) then cut-off length would be related to magnitude of water hammer pressure.

4. CONCLUSION

Super hydrophobic surfaces have immense application in the real world. Hence effective and robust design of these surfaces is crucial. While there is a lot of literature already available for the super hydrophobic surface under static condition, this work focuses on the analysis of these surfaces in dynamic conditions. This present work looks at the variation of pressure with distance from point of impact. The variation of the cut-off length has been studied. We have clearly shown that in the conventional flow regime, the dependence of the cut-off length with impact velocity is not very strong. This shows that the impacting water hammer pressure is not the factor only determining this transition of regime. The magnitude of water hammer pressure is actually a very weak factor in determining the transition of regimes. Other factors need to be considered to get a good understanding of the physics regarding transition of regime.

While the impact velocity is shown to be a weak factor, the present study shows the significant dependence of the transition of regime on the geometry of the super hydrophobic surface. Specifically the fraction of solid in contact is shown to be a strong factor in determining the transition of regimes. It can also be seen that the cut-off length increases slowly at first, then much more rapidly as the fraction of solid in contact decreases (i.e. spacing relative to post size increases).

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