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# Simulation of meniscus stability in superhydrophobic granular surfaces under hydrostatic pressures

#### B. Emami, T.M. Bucher, H. Vahedi Tafreshi\*, D. Pestov, M. Gad-el-Hak, G.C. Tepper

Department of Mechanical and Nuclear Engineering, Virginia Commonwealth University, Richmond, VA 23284-3015, United States

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#### ABSTRACT

In this work, a series of numerical simulations has been devised to study the performance of granular superhydrophobic surfaces under elevated hydrostatic pressures. Using balance of forces, an analytical expression has also been developed to predict the critical pressure at which a submersed idealized granular superhydrophobic surface comprised of spherical particles, orderly packed next to one another, departs from the Cassie state. Predictions of our analytical expression have been compared with those of a series of 3-D full-morphology numerical simulations, and reasonable agreement has been observed between the two methods. Full-morphology simulations were then used, for the first time, to compute the critical pressure of superhydrophobic surfaces comprised of randomly distributed spherical particles (e.g., superhydrophobic coatings developed by depositing of hydrophobic aerogel particles), where no analytical method is applicable due to the complexity of the coatings' morphology. Results of our numerical simulations indicate that for coatings made up of mono-disperse hydrophobic particles, critical pressure increases with increasing the solid volume fraction. However, increasing particle diameter results in lower critical pressures when the coating's solid volume fraction is held constant.

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#### 1. Introduction

It is known that a combination of hydrophobicity and micro- or nanoscale surface roughness can result in a phenomenon known as superhydrophobicity. Research has shown that liquid flow slips on a superhydrophobic surface. This is because a rough hydrophobic surface can entrap the air in its pores, resulting in a reduced contact between water and the frictional solid walls. From a macroscale viewpoint, this causes a reduction in the overall drag force exerted on the surface. From an engineering standpoint, superhydrophobic surfaces can be exploited to reduce the drag force exerted on submerged moving objects such as ships, submarines, or torpedoes.

When the pores in a superhydrophobic surface are filled with air, the system is considered to be at the Cassie state [1]. If the pressure is high, water may penetrate into the pores of the surface and displace the air. This results in the elimination of the superhydrophobicity, and transition to the so-called Wenzel state [2]. The pressure at which a superhydrophobic surface departs from the Cassie state is hereon referred to as the critical pressure [3].

Superhydrophobic surfaces are usually manufactured by the microfabrication of grooves or posts on a hydrophobic surface. Hence, most of the theoretical [4–9] and experimental [10–14]

studies in the literature correspond to microfabricated surfaces. Microfabrication, however, is a costly process and cannot be easily applied to large surfaces with arbitrary shapes. An alternative approach to produce a superhydrophobic surface is by depositing hydrophobic fibers or particles on a substrate. Our group, among many others [15–21], is currently active in producing and characterizing fibrous and granular superhydrophobic coatings. As will be discussed in the next section, such coatings can be produced at a much lower cost and can better conform to the surface of objects with arbitrary shapes. Coatings produced by randomly deposited fibers or particles do not, however, provide a precise control over the surface microstructure, and are more susceptible to elevated pressures [22].

As mentioned earlier, the major problem in utilizing superhydrophobic surfaces for submersible applications is that the slip effect diminishes under elevated hydrostatic pressures (i.e., depths). The objective of the study presented here, therefore, is to better our understanding of the importance of microstructural parameters such as particle size or porosity on the superhydrophobic performance of such coatings under elevated hydrostatic pressures. In the current study, we only consider surfaces made up of granular materials. Surfaces obtained by fiber deposition will be studied in a future work.

In the next section, we present a superhydrophobic surface made up of ground aerogel particles as an example of granular superhydrophobic surfaces. In Section 3, we present an analytical

<sup>\*</sup> Corresponding author. Tel.: +1 804 828 9936; fax: +1 804 827 7030. *E-mail address:* htafreshi@vcu.edu (H.V. Tafreshi).

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Nomenclature	
d <sub>c</sub>	diameter of posts
$d_s$	diameter of spheres
$F_{\sigma}, F'_{\sigma}$	surface tension force
L <sub>c</sub>	center to center distance between two adjacent
	posts
Ls	center to center distance between two adjacent
	spheres
Р	the net pressure exerted on a meniscus
$P_c$	capillary pressure
Pcr	critical pressure of a superhydrophobic surface
$P_{\infty}$	ambient pressure
r	radial coordinates in an axisymmetric system
$r_c$	capillary radius
S	water saturation
$S_{cr}^{o}$	critical water saturation of a superhydrophobic sur-
	face with ordered spheres
$S_{cr}^r$	critical water saturation of a superhydrophobic sur-
	face with random spheres
Ζ	axial coordinates in an axisymmetric system
α	angle determining the solid-meniscus contact loca-
	tion on a sphere
ε	solid volume fraction
$\theta$	liquid-solid contact angle
σ	surface tension
$\phi_g$	gas fraction ratio of a superhydrophobic surface

formula that we have derived for predicting the critical pressure of superhydrophobic surfaces. In Section 4, we describe the numerical scheme that we have considered for conducting our 3-D simulations. This section also contains a series of simulations that has been performed to ensure that our results are not affected by statistical errors or simulation artifacts. Our results and discussions are given in Section 5, where we compare the predictions of our analytical formula with the results of 3-D simulations. In this section we also present a parameter study to compare the performance of coatings with different microstructural parameters. This discussion is followed by our conclusions presented in Section 6.

#### 2. Superhydrophobic surfaces made up of aerogel particles

As mentioned in Section 1, a superhydrophobic surface can simply be produced by depositing randomly distributed hydrophobic particles on a sticky solid surface. For demonstration purposes here, we have produced a granular superhydrophobic surface by grinding trimethylsilylated aerogel (consisting of  $(CH_3)_3Si$ – groups) particles and depositing them onto an adhesive surface. The average diameter of the ground aerogel particles was measured using an optical microscope and was about 20–100  $\mu$ m. To test the hydrophobicity of our aerogel coating, a water droplet was placed on the surface and its contact angle was measured using an optical microscope. Fig. 1a is an optical-microscope image of our aerogel coating, and Fig. 1b is a photograph of a water droplet placed on the aerogel coated surface.

The objective of the current paper is to provide a better understanding of the performance of superhydrophobic granular surfaces under hydrostatic pressures. The aerogel coating explored in this work is only an example of such surfaces. As will be discussed later in this paper, our numerical simulations are also aimed at providing guidelines for design and optimization of the coating microstructure in terms of particles size and thickness of the coating, as well as its porosity and randomness.



**Fig. 1.** (a) Optical-microscope image of our aerogel superhydrophobic coating. (b) Contact angle between a water droplet and the coating.

#### 3. Analytical formula

By applying balance of forces, an analytical relationship was proposed for predicting the stability of the meniscus formed between the cylindrical posts on a microfabricated superhydrophobic surface [23,24]. In this work, we extend this analytical relationship to superhydrophobic surfaces with ordered spherical particles. In the following subsections, the above method is briefly described for the case of cylindrical posts arranged in aligned configurations.

#### 3.1. Surfaces with ordered posts

An ordered array of vertical cylinders representing the posts on a microfabricated superhydrophobic surface, is shown in Fig. 2. The



**Fig. 2.** Schematic of an array of ordered posts and the force balance on the gas-liquid meniscus. Note that only half of the meniscus is shown, as the geometry is symmetrical.

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