9th International Conference on Computational and Mathematical Biomedical Engineering – CMBE2026
22-24 June 2026, Kobe, Japan
P. Nithiarasu, M. Oshima, M. Ohta, and M. Tsubokura (Eds.)

REPELLING PLATELETS FROM THE WALL: A PROSPECTIVE STUDY

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SUMMARY

This prospective study investigates the feasibility of repelling rigid particles with sizes comparable to those of platelets away from a solid surface equipped with microstructures. Simulations agree with the kinematic reversibility theorem in the Stokes flow regime, which states that fore-aft symmetric roughness cannot induce drift. In contrast, sawtooth asymmetric patterns are demonstrated to produce a drift angle on the order of 10^{-3}, theoretically sufficient to prevent biochemical binding after less than $100\ \mu m$ of particle motion over the surface.

Key words: *Platelets dynamics, Microscopic roughness, Lift force*

1 INTRODUCTION

Cardiovascular diseases remain the leading cause of death globally, driving a critical need for effective medical devices. Given their direct contact with blood, ensuring the hemocompatibility of these devices is paramount yet remains a significant challenge. Surface structuring at the micrometer scale has been shown to influence thrombogenicity, although this effect is not yet fully characterized or understood. Experimental evidence suggests that surface topography can either promote [1] or inhibit [2] platelet adhesion, highlighting the complexity of this interaction. Existing research primarily focuses on how microstructures reduce the blood-material contact area, thereby limiting the surface available for protein adsorption, blood cell adhesion, and platelet activation [3]. This prospective study explores how microstructures can modulate hydrodynamic forces to enhance the separation of platelets from surfaces, thereby limiting adhesion.

2 METHODOLOGY

To repel platelets away from the surface and prevent adhesion, which occurs when platelets are within tens of nanometers of a surface for an extended period, surface roughness must be carefully designed. It should be small enough, less than a few platelet diameters, to avoid trapping platelets and increasing contact area, yet large enough to influence platelet trajectories through microscale flow features, being at least a significant fraction of a platelet diameter. Given the near-zero particle Reynolds number for platelets ($Re = \frac{\dot{\gamma} a^2}{\nu}$ is of the order 10^{-3} when a particle of typical radius $a = 1\ \mu m$ flows in a fluid of kinematic viscosity $\nu = 10^{-6}\ m^2/s$ under (arterial) shear rate $\dot{\gamma}$ of the order $1000\ s^{-1}$), any inertial lift mechanism like the Segré-Silberberg [4] effect should be marginal. Moreover, due to the kinematic reversibility property of the Stokes flows, only asymmetric roughness patterns can potentially generate drifted particle trajectories in absence of inertia.

To test these ideas, numerical simulations of a single platelet, represented by a rigid ellipsoid, flowing over surfaces with different roughnesses were performed with the in-house YALES2BIO solver developed at IMAG (https://imag.umontpellier.fr/~yales2bio/) and dedicated to the simulation of blood flows [5]. The surrounding plasma movement is described by the incompressible Navier-Stokes equations:

$$\nabla \cdot \mathbf{u} = 0 \tag{1}$$

$$\rho\frac{d\mathbf{u}}{dt} = -\nabla p + \mu\Delta\mathbf{u} + \mathbf{f}(\mathbf{x}, t) \tag{2}$$

The presence of a rigid particle in the flow is accounted for by the force $\mathbf{f}(\mathbf{x}, t)$ derived following the Force Coupling Method (FCM) [6], a Lagrangian tracking method over an Eulerian fluid grid that does not require conformal mesh of the particles. The i^{th} component of $\mathbf{f}(\mathbf{x}, t)$ for a single particle which center of mass is in $\mathbf{Y}$ is detailed in equation 3, where $\mathbf{F}$ and $\mathbf{G}$ denote the monopole and dipole amplitude, respectively.

$$f_i(\mathbf{x}, t) = F_i\Delta(\mathbf{x} - \mathbf{Y}) + G_{ij}\frac{\partial}{\partial x_j}\Delta_d(\mathbf{x} - \mathbf{Y}) \tag{3}$$

$\mathbf{F}$ is related to the external forces acting on the particle, the skew-symmetric part of $\mathbf{G}$ models the external torques and the symmetric part of $\mathbf{G}$ is a stresslet ensuring the rigidity of the particle. These quantities are transmitted from the particle to the fluid by spreading over the Gaussian supports Δ and Δ_d, respectively. See [6] for more details about the size of these supports, comparable to the particle size.

In the case of a rigid and non-inertial particle moving freely, external forces must cancel out according to Newton's law. Thus, in this situation, both the monopole and the skew-symmetric part of the dipole are zero. These values are used to calculate the trajectories of the solid object, updating the position and orientation of the particle over time using the (angular) velocity of the object, following the force coupling method approach:

$$\mathbf{u}_p = \iiint \mathbf{u}\,\Delta(\mathbf{x} - \mathbf{Y})dv \quad ; \qquad \boldsymbol{\omega}_p = \iiint \boldsymbol{\nabla}\times\ \mathbf{u}\,\Delta_\mathrm{d}(\mathbf{x} - \mathbf{Y})dv \tag{4}$$

In the present study, drift angles corresponding to different surface patterns were computed by following this methodology for $Re = 10^{-3}$, typical of platelets in a $1000\ s^{-1}$ shear flow. However, due to time stepping constraint, this way of proceeding is not tractable in the zero Reynolds number limit, where the simulations can be analyzed in terms of reversibility. In the $Re = 0$ case, the assessment of the trajectory relies on the linearity of the Stokes equations, which induces a linear relationship between the particle's velocity and the forces acting on it. This writes:

$$[\mathbf{U}] - [\mathbf{U}]_\mathbf{0} = [\mathbf{M}][\mathbf{F}] \tag{5}$$

where $[\mathbf{U}]$ contains the translational and rotational velocity components of the particle submitted to the external forces and torques $[\mathbf{F}]$, $[\mathbf{U}]_\mathbf{0}$ is the velocity of the freely evolving particle, and $[\mathbf{M}]$ is the mobility matrix. The latter can be computed accurately at a Reynolds number close to zero by performing a series of simulations where the particle is successively submitted to one single component of $[\mathbf{F}]$. An additional computation is performed in which the external force $[\mathbf{F}]_\mathbf{0}$ required to achieve $[\mathbf{U}] = 0$ is found iteratively. Then, the velocity of the freely evolving particle at the position of interest can be obtained as follows:

$$[\mathbf{U}]_\mathbf{0} = -[\mathbf{M}][\mathbf{F}]_\mathbf{0} \tag{6}$$

The drift angle is then obtained as the ratio between the normal and longitudinal components of velocity. Further details on the implementation and the validation of the methodologies to compute particle trajectory drift are available in [7].

3 RESULTS

3.1 Zero Reynolds number simulation of spherical particle

Simulations with zero Reynolds number and spherical particles were first performed for comparison with theoretical results. In addition to the flat plate configuration, three surface structures were investigated: square grooves, right-sided sawtooth grooves (green) and left-sided sawtooth grooves (red), as illustrated in Figure 1. At zero Reynolds number, due to the kinematic reversibility property, the flat plate and square grooves pattern should not induce any drift motion, while left-sided and right-sided sawtooth patterns should have opposite effects. The results obtained from the mobility matrix methodology are in good agreement with these expectations, as shown in Table 1 (first row).

They were obtained by averaging the drift angle for eight positions evenly distributed over each roughness pattern at a distance $2.5a$ above the surface tip.

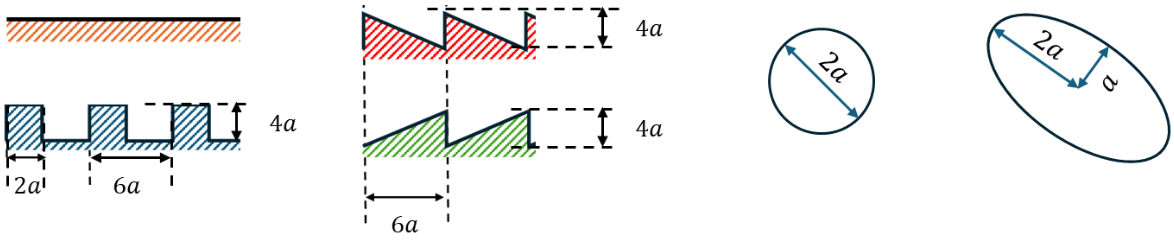

Figure 1: Roughness patterns used for simulations where a particle (either spherical or oblate ellipsoidal) is transported by a pure shear flow from left to right. Not to scale for more clarity.

Reynolds number $\frac{\dot{\gamma}a^2}{\nu}$	Particle	Flat plate	Squared groove	Right-sided sawtooth	Left-sided sawtooth
~0	Sphere	$< 10^{-6}$	$< 10^{-6}$	4.6×10^{-4}	-4.6×10^{-4}
10^{-3}	Sphere	4.2×10^{-5}	4.2×10^{-5}	4.2×10^{-4}	-3.6×10^{-4}
	Ellipsoid	1.5×10^{-4}	2.5×10^{-4}	1.4×10^{-3}	-1.2×10^{-3}

Table 1: Averaged drift angles $\bar{\theta}$ obtained from the various simulations (a positive value corresponds to a particle repelled away from the surface). The initial distance between the particle center and the tip of the roughness is $2.5a$

3.2 Finite Reynolds number simulation

When the Reynolds number is typical of a platelet in arterial flow (Re of the order of 10^{-3}), the mobility matrix methodology (see Section 2) is not fully justified, and the drift angle can be computed directly from the trajectory. The drift angle θ was measured over each of the structures for different initial particle positions x_c^0 and constant initial altitude z_c^0, after a 180° rotation of the particle induced by the ambient shear flow (see Figure 2). Since the shape of the trajectory depends on the initial position of the particle, the relevant drift angle $\bar{\theta}$ is an average over the initial positions, as in Section 3.1. The same procedure was used for spherical and oblate particles, and the results are displayed in Table 1. For a spherical particle, the square grooves produce a mean drift angle comparable to that observed on a flat surface, of the order of 4×10^{-5}. This higher value compared to the $Re = 0$ case is caused by the small yet non-zero inertial forces that induce lift on the particle. It reaches an even larger value for the ellipsoidal particle, of the order of 2×10^{-4}.

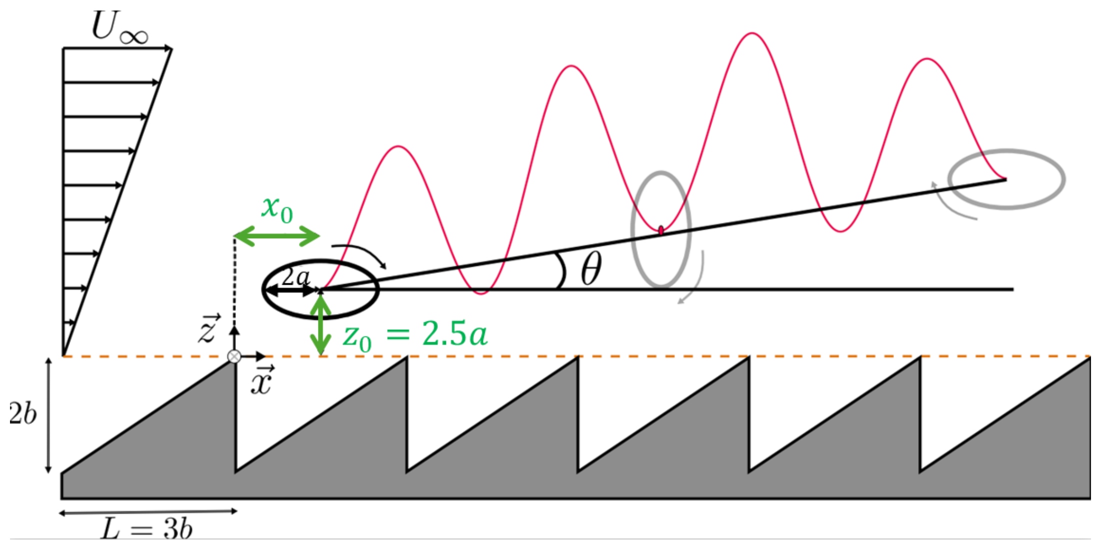

Figure 2: Drift angle θ over right-sided sawtooth grooves after a 180° rotation (scaled for clarity).

In contrast, sawtooth structures generate an average drift whose sign depends on the orientation of the sawteeth, and whose amplitude is significantly greater, on the order of 4×10^{-4} and 10^{-3} for the sphere and the ellipsoid, respectively. Although a 10^{-3} drift angle remains at a low value, it could have a very beneficial effect on the platelet adhesion mechanism. Indeed, it corresponds to a situation where the particle only has to travel $100\ \mu m$ to drift 100 nm away from the surface, which is greater than the typical length of adhesive bonds [8]. Moreover, it is anticipated that the lifting effect will be stronger for actual platelets, for two reasons. First, the FCM simulations were conducted with a relatively large particle-surface distance $1.5a$ to ensure accuracy. However, in real conditions, platelets can approach much closer to the surface (down to $100\ \mu m = 0.1a$) where the surface-induced lift effect is expected to be significantly stronger. Second, the enhanced drift for the ellipsoid of aspect ratio 2 compared to the sphere suggests that the drift increases with the aspect ratio of the particle. Additional simulations at higher aspect ratio (4 is the typical value for a platelet) are needed to confirm this hypothesis.

4 CONCLUSIONS

A numerical model has been used to study the effect of an artificial microstructured surface on the dynamics of platelet-like particles. In a flow going from left to right, right-sided sawtooth grooves appear to be particularly effective at repelling particles away from a solid surface through a non-inertial mechanism, thereby reducing interaction with the surface and, ultimately, platelet adhesion.

Acknowledgements

This work has been initiated during the Extreme CFD Workshop & Hackathon (https://ecfd.coria-cfd.fr). It is part of the THROMBOSURF project co-funded by Agence Nationale de la Recherche (ANR-21-CE45-0035-02) and DFG. CFD simulations were performed using HPC resources from GENCI-TGCC and GENCI-CINES (Grants No. A0140307194 to A0180307194) and from the Institut de Sciences des Données de Montpellier (ISDM).

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