

## Influence of surface chemical heterogeneity on attachment and detachment of microparticles



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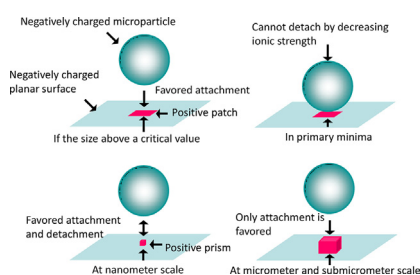
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### HIGHLIGHTS

- We examine effect of chemical heterogeneity on colloid attachment and detachment.
- A critical size of a positive patch on a negative plane is needed to attach a colloid.
- The colloid attached on chemical heterogeneity is irreversible to reducing ionic strength.
- The presence of chemical heterogeneity increases irreversible attachment in primary minima.

### GRAPHICAL ABSTRACT



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### ABSTRACT

This study theoretically examined attachment/detachment of negatively charged microparticles onto/from a negative planar surface carrying a positively charged square patch of different sizes. The surface element integration technique was used to calculate Derjaguin–Landau–Verwey–Overbeek (DLVO) interaction energies at different ionic strengths. Results show that a critical patch size is needed to attach a particle at a given ionic strength. The critical size decreases with increasing ionic strength and decreasing particle size. Colloid attachment on the patch via primary-minimum association is irreversible to reduction of ionic strength, in contrast to the experimental observations in the literature. We attributed the discrepancy to the fact that chemical heterogeneity is commonly accompanied with topographical variation. To account for the coupled effects on colloid detachment, the collector surface was modeled as a negative planar surface carrying a square prism. If the size of the prism is  $\leq 5 \text{ nm} \times 5 \text{ nm} \times 5 \text{ nm}$ , whether the prism surface is positively or negatively charged does not have significant influence on the interaction energy curves at  $\leq 0.01 \text{ M}$ . These tiny asperities mainly play a role in eliminating the primary minima of interaction energy curves at the low ionic strengths, causing detachment of colloids from primary minima. For larger prisms, the primary-minimum depths can be increased significantly if the prism surfaces are positively charged, resulting in more irreversible attachments in primary minima. Findings from this study have implications to understanding particle–surface interactions that involve only one ligand–receptor bond (e.g., cell–biomaterial interactions via a single contact).

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## 1. Introduction

Knowledge of the mechanisms governing colloid transport in porous media is of importance to understanding diverse natural and engineered processes such as riverbank filtration, chromatographic separation, and transport and fate of biocolloids (e.g.,

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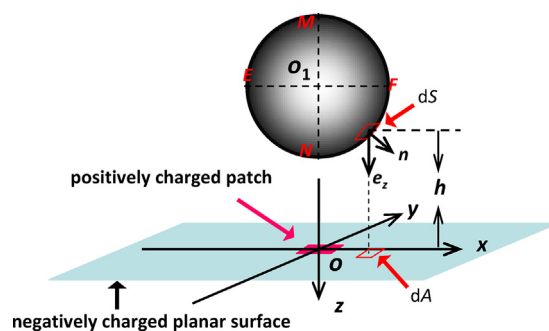
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viruses and bacteria) and colloid-associated contaminants in subsurface environments [1–5]. Surface chemical heterogeneity has been frequently regarded as an important factor influencing colloid transport in porous media [6–8]. Surface chemical heterogeneity is ubiquitous in subsurface aquatic environments, due to geochemical, biological, and structural variability associated with surfaces of aquifer materials [9]. The aluminum, iron, and manganese oxides represent the most common sources of surface chemical heterogeneity in subsurface environments [10]. These compounds can exist as discrete crystals, as coating on mineral grains and humic substances, or as mixed gels [9,10].

Various experimental studies have been performed to investigate effects of surface chemical heterogeneity on colloid transport at both macroscopic and microscopic scales [9,11–20]. When macroscopic chemical heterogeneity is present on collector surfaces, the attachment rate is directly related to the favorable surface fraction of the collectors, which can be predicted by the patchwise model developed by Johnson et al. [9]. If the chemical heterogeneity is micro-sized, the experimental attachment rates were observed to deviate from predictions by the patchwise model [12]. Elimelech et al. [12] attributed the discrepancy to the interplay between hydrodynamic and double layer interactions (i.e., the so-called “hydrodynamic bump” effect). Santore and Kozlova [18] and Kozlova and Santore [19] showed that, if the size of chemical heterogeneity is further decreased to nanometers, a critical density of positively charged patches is needed to successfully capture negatively charged colloids on negative surfaces and the spatial fluctuations in the nanoscale patch arrangement control adhesion of colloids. The aforementioned experimental results indicate that the size of chemical heterogeneity plays a critical role in colloid attachment.

Theoretical studies [21–33] have also been conducted to investigate the effects of surface chemical heterogeneity on colloid attachment and transport. For example, Duffadar and Davis [29], based on surface element integration technique [1,2,34], developed grid-surface integration to calculate Derjaguin–Landau–Verwey–Overbeek (DLVO) interaction energy between a colloid and chemically heterogeneous surface. By using the grid-surface integration technique, it was shown that the presence of chemical heterogeneity increases colloid attachment in primary minima by decreasing interaction energy barrier, and the attachment behavior cannot be predicted by a mean field approach [29–31]. The grid-surface integration technique and patchwise model have been combined with Lagrangian/Eulerian method to investigate transport behavior of colloids in various flow systems (e.g., porous media and radial impinging jet) in the presence of microscopic and macroscopic chemical heterogeneities, respectively [22–24,28,32]. The results from these studies consistently illustrate that it is the degree of surface chemical heterogeneity that controls colloid attachment kinetics in flow under unfavorable conditions (i.e., in the presence of repulsive DLVO interaction energies). However, because the number of chemical heterogeneities is commonly limited on a solid phase in natural and engineering systems, the attachment rate decreases with time elapsed (i.e., as a result of blocking) [15,16,21,25].

Whereas various mechanisms governing colloid attachment in the presence of surface chemical heterogeneity have been elucidated as indicated above, understanding of the influence of surface chemical heterogeneity on colloid attachment is not complete. For example, the theoretical research to systematically examine the observed size effect of chemical heterogeneity on colloid attachment has not been reported. In addition, the influence of surface chemical heterogeneity on colloid detachment is unclear to date. Specifically, while a number of experiments [15,25] showed that attachment of colloids onto chemically heterogeneous surfaces is irreversible, other experimental studies [19,35–40] observed



**Fig. 1.** Illustration of a spherical particle interacting with a chemically heterogeneous flat surface. The origin of the coordinate system ( $O$ ) is the center of the projection of the particle on the flat surface. The  $xy$  plane of the coordinate system is oriented superposing the flat surface. The  $z$  axis passes through the particle center and faces away from the particle.  $dS$  is a differential area element on the particle surface,  $e_z$  is the unit vector directed towards the positive  $z$  axis,  $n$  is the outward unit normal to the particle surface,  $dA$  is the projected area of  $dS$  on the planar surface.

detachment of colloids from chemically heterogeneous surfaces during transients in solution chemistry. The mechanisms governing the detachment behaviors under different experimental conditions are not clear and require theoretical investigation.

This study theoretically examined attachment/detachment of microparticles onto/from a negative planar surface carrying a patch or a square prism of positive charge. Special attention was paid to the effect of patch/prism size on the attachment and detachment. The surface element integration technique was used to calculate DLVO interaction energies at different solution ionic strengths. We demonstrated that a critical size of the positive patch is necessary for attachment of a colloid at a given ionic strength, and the critical size decreases with increasing ionic strength. We additionally showed that while nanoscale physical heterogeneities favor both attachment in and detachment from primary minima, the coexistence of physical and chemical heterogeneities increases irreversible attachment in primary minima. Findings from this study improve understanding of the mechanisms governing (i) the interactions of particles (e.g., cell and bacteria) with biomaterials via single-point contact and (ii) colloid transport in natural environments and engineering systems where physical and chemical heterogeneities are commonly coupled.

## 2. Theory

**Fig. 1** schematically depicts the model system of a spherical colloid interacting with a chemically heterogeneous flat surface. The heterogeneous substrate was represented by an elementary model, i.e., a negative planar surface covered by one square patch of positive charge. In **Fig. 1**, the Cartesian coordinate system was employed for the model system. The  $xy$  plane of the coordinate system is oriented superposing the flat surface and the  $z$  axis passes through the colloid center and faces away from the colloid. The surface element integration was modified to calculate the interaction energy between the colloid and substrate. Specifically, the heterogeneous flat surface was discretized into small area elements by taking chemical heterogeneity into account, similar to the grid-surface integration [29–31]. Each surface element  $dA$  on the flat surface interacts with both hemispherical surfaces  $EMF$  and  $ENF$ . The interaction of  $dA$  with hemispherical surface  $EMF$  was not considered in this study because it is minimum compared to that between  $dA$  and hemispherical surface  $ENF$  for microparticles. Similar to the Derjaguin approximation or surface element integration used for treating the interaction between two curved surfaces, the interaction of  $dA$  with the hemispherical surface  $ENF$  was taken as that

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