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Roughness Versus Charge Contributions to Representative Discrete Heterogeneity Underlying Mechanistic Prediction of Colloid Attachment, Detachment and Breakthrough-Elution Behavior Under Environmental Conditions.

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The key element of a mechanistic theory to predict colloid attachment in porous media under environmental conditions where colloid-collector repulsion exists (unfavorable conditions for attachment) is representation of the nanoscale surface heterogeneity (herein called discrete heterogeneity) that drives colloid attachment under unfavorable conditions. The observed modes of colloid attachment under unfavorable conditions emerge from simulations that incorporate discrete heterogeneity. Quantitative prediction of attachment (and detachment) requires capturing the sizes, spatial frequencies, and other properties of roughness asperities and charge heterodomains in discrete heterogeneity representations of different surfaces. The fact that a given discrete heterogeneity representation will interact differently with different-sized colloids as well as different ionic strengths for a given sized colloid allows backing out representative discrete heterogeneity via comparison of simulations to experiments performed across a range of colloid size, solution IS, and fluid velocity. This has been achieved on unfavorable smooth surfaces yielding quantitative prediction of attachment, and qualitative prediction of detachment in response to ionic strength or flow perturbations. Extending this treatment to rough surfaces, and representing the contributions of nanoscale roughness as well as charge heterogeneity is a focus of this talk. Another focus of this talk is the upscaling the pore scale simulations to produce contrasting breakthrough-elution behaviors at the continuum (column) scale that are observed, for example, for different-sized colloids, or same-sized colloids under different ionic strength conditions. The outcome of mechanistic pore scale simulations incorporating discrete heterogeneity and subsequent upscaling is that temporal processes such as blocking and ripening will emerge organically from these simulations, since these processes fundamentally stem from the limited sites available for attachment as represented in discrete heterogeneity.