# A Universal Framework for Predicting Deposition and Transport Behavior of Microorganisms in Subsurface Environment

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**Objectives:** This project aims to explore and develop new AFM-enabled techniques for micro-/ nano-scale characterization and quantification of microbe cell surface properties and cell-surface interactions with the aim to correlate the conventional macroscopic deposition-transport measurement with the microscopic single cell characterization. Nano-scale cellular surface properties that govern the macro-scale cell-cell aggregation and cell-surface attachment tendencies for a number of IFRC-relevant microorganisms are obtained and, new theoretical and mathematical framework for microbe transport model in subsurface environments is proposed.

**Material and Methods:** In addition to comprehensive surface characterization of a number of DOE relevant microorganisms, the nature, magnitude and range of intersurface forces and surface potential at cell-cell and cell-substrate interfaces are quantified using Atomic Force Microscopy (AFM) combined with developed computation methods. Recognizing the complexity of factors dictating the cell-surface interactions and subsequent cell attachment behavior, an integrated and dimensionless parameter, Tabor value, $\mu$, was proposed by us with the aim to parameterize the micro-scale cell-surface interactions in order to predict macro-scale cell deposition behavior. An improved theoretical model based on the DLVO theory but incorporating microorganism-specific features is constructed, aiming to generalize the transport behavior of a wide spectrum of microbes in water-saturated porous media. The microbial transport model will ultimately be extended to include other factors influencing microbe deposition to allow the prediction of cell deposition under different fluid condition, ionic strength and relevant sub-surface environments.

**Results and discussion:** The sample microorganisms exhibit distinctive aggregation tendency and attachment efficiency via transport through porous media, indicating microbial bio-originated factors that influence the microbe movement. The attachment efficiency ($\alpha$) ranges widely from 0.93 for strong microbe-substrate attachment to 0.06 for weak attachment, depending on the bacteria strain as well as the ionic strength of the aqueous environment. The electrolyte concentration is found to have significant influence on the cell stiffness and adhesion-detachment kinetics. No consistent correlation is found between $\alpha$ and any individual conventional micro-scale physicochemical properties such as electrophoretic mobility, hydrophobicity and extracellular polymeric substance. Mathematical calculation of interaction energy based on current DLVO formula failed to predict the deposition rates observed, indicating that the current DLVO model is not sufficient for predicting microbial deposition. AFM analysis allowed for quantification of the range and magnitude of the repulsive/attractive surface forces, including both short-ranges forces such as van der Waal and electrostatic and long-range forces such as those due to the presence of cellular surface substances (CSS) with varying thickness and density for each strain. A modified Tabor parameter based on classical colloidal and adhesion science is proposed, which collectively quantify the microscopic cell behavior and interfacial properties. Tabor values determined for the organism studied correlated well with the macroscopic attachment efficiencies measured by flow-through column experiments. This indicates that the rudimentary solid-mechanics model is promising to reliably predict the deposition-transport behavior by the Tabor parameter. For microorganism that have much larger *Ka* (reflect relative particle size to electrostatic layer thickness and density) value than colloids and with soft shell nature, the inevitable elastic deformation couples caused by the presence of both repulsive energy barrier and an attractive secondary minimum in the DLVO surface potential drastically alters the adhesion-detachment mechanism. We derive the theoretical description of distribution of 1st and 2nd minimum force associated to the detachment of a spherical / cylindrical shell of bacteria from an adhering substrate. An experimental verifiable grand theory of microbial deposition will ultimately be constructed to account for static-dynamic behavior of strains in porous media.