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Biofilm initiation: A modeling approach

C. J. DAUGHNEY¹, S. KRACK² AND D. FORTIN²

¹Institute of Geological & Nuclear Sciences, PO Box 30368, Lower Hutt, New Zealand (c.daughney@gns.cri.nz)

²Department of Earth Sciences, University of Ottawa, 140 Louis Pasteur, Ottawa, Ontario, Canada (skrac049@science.uottawa.ca; dfortin@science.uottawa.ca)

Surface Complexation Models (SCMs) have been extensively employed to predict metal adsorption by bacterial and mineral surfaces. Implicit in these SCMs is a quantitative model of electric potential distribution in the near-surface region. It stands to reason that SCMs for bacterial and mineral surfaces could be applied to predict the initial stages of biofilm formation, through bacteria-mineral adhesion. However, this requires that the model of electric potential is realistic. For mineral surfaces, measurement of zeta potential provides an additional constraint on the SCM, and measured and predicted surface electric potentials are often in reasonable agreement. In contrast, for bacterial surfaces, zeta potential measurements and SCM predictions of surface electric potential are generally not in agreement. Here, zeta potential measurements are combined with titration and metal adsorption data to produce a single integrated bacterial SCM capable of describing all forms of the input data. The approach requires assumption of non-specific electrolyte ion adsorption, which can be built into a modified form of the computer program FITEQL 2.0. The predictions of the new bacterial SCMs can be combined with mineral SCMs to predict the early stages of biofilm formation, as shown using experimental adhesion data.

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Shewanella's surface physicochemistry and adhesiveness to Fe-oxides

A.A. KORENEVSKY¹, Y.A. GORBY² AND T.J. BEVERIDGE¹

¹Department of Microbiology, University of Guelph, Ontario, Canada

²Pacific Northwest National laboratories, Richland, Washington, USA

Bacterial adhesion is a prerequisite of surface colonization and biofilm formation. In case of dissimilatory iron reducing bacteria (DIRB), it is an important factor controlling the reduction efficiency of iron minerals. It is generally recognized that initial adhesion of bacteria to surfaces is a complex interplay of Lifshitz-van der Waals, electrostatic, Lewis acid-base, and steric interactions which is greatly influenced by cell surface macromolecules such as lipopolysaccharides (LPS) or capsular polysaccharides.

Strains of the DIRB *Shewanella* with previously established cell surface ultrastructure, LPS composition [1], and adhesive properties (ability to adhere to hematite) were further characterized with respect to their physicochemical properties. By combining the results of hydrophobic interaction chromatography (HIC), electrostatic interaction chromatography, and iron oxide adsorption experiments, we demonstrated that electrostatic interactions predominate over hydrophobic interactions at the cell-iron oxide interface. However, since HIC provides only relative hydrophobicity, quantitative data was obtained using contact angle measurements [2] to assess apolar, Lifshitz-van der Waals (LW) and polar (Lewis acid-base) surface properties.

Advancing contact angles (Θ_w) of *Shewanella* strains in water were in the range of 22-41°. This suggested that the overall cell surface character of all strains is predominantly hydrophilic (assuming a threshold of ~70°). Contact angles in glycerol, formamide, and diiodomethane were used to calculate the apolar (γ^{LW}) and polar (γ^+ , γ^-) components of surface tension. All strains displayed low (~0 mJ/m²) values of γ^+ and high (more than 50 mJ/m²) values of γ^- . Considering that $\gamma^- = 28$ mJ/m² is the threshold point that separates hydrophilic from hydrophobic surfaces, we conclude that *Shewanella* cell surfaces are quite hydrophilic. Because of this, adhesion of *Shewanella* cells to hydrophilic iron oxides must be mostly via electrostatic factors.

References

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- [2] van Oss C.J. (1994) Interfacial forces in aqueous media. Marcell Dekker, NY, 440 pp.