Examining the uniqueness of biogeochemical models developed for ion-bacteria adsorption.

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Accurate models describing metal-bacteria adsorption are necessary to understand the availability and cycling of metals in the environment, predict the fate of heavy metal contaminants, and develop bioremediation techniques. Surface complexation models (SCMs) are a specific type of chemical equilibrium approach that have been used to successfully quantify the extent of ion adsorption. SCMs of any metal-bacterium system require determination of the concentrations and deprotonation constants of the proton active functional groups on and/or within the cell wall [1,2], obtained via modeling potentiometric titrations.

Acid-base titrations were conducted using the thermophilic bacterium *Anoxybacillus flavithermus*. The titration data indicate that *A. flavithermus* displays similar protonation behaviour as previously studied mesophilic bacteria, but with a lower total concentration of titratable sites per unit weight of biomass. MathCad was used to develop a a non-electrostatic model (by curve fitting) to characterize proton adsorption by the thermophile. To investigate whether the problem posed is non-unique, prediction error surface plots were examined and multiple numerical simulations performed. The fit of each minimization was compared to the experimental data and uncertainty analyses were conducted to estimate correlation coefficients between the parameters and errors associated with the optimised values.

Results indicate that the SCM parameters are non-unique. This indeterminacy in SCMs may be resolved by incorporation of prior information – additional information about the parameters generated from collecting other data (e.g. electrophoretic mobility). These findings have profound implications for the predictive ability of SCMs constructed for proton (and metal) adsorption. Our results do not, necessarily, invalidate previous models published, but rather, emphasize the importance of constraining SCMs with data from several different complimentary experimental methods.

References

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