Object-oriented model for metal-bacteria co-transport through porous media

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The object-oriented platform Orchestra [1] is used to develop a model for cadmium co-transport with bacteria through porous media, based on previously published laboratory column break-through curves [2]. The model incorporates: 1) objects describing equilibrium surface complexation, with various electric double layer configurations, to account for cadmium interactions with bacterial and mineral surfaces; 2) a non-equilibrium phase-transfer object to account for bacteria-mineral adhesion; and 3) transport objects to account for advection and dispersion of the dissolved metal and the unattached bacteria. Model calibration to conservative tracer break-through data allows the advective velocity and coefficient of hydrodynamic dispersion to be determined. With the assumption that equilibrium is attained under conditions where bacteria-mineral adhesion is limited, the calibrated model yields a reasonable fit to the cadmium break-through data using previously published stability constants for cadmium adsorption by the bacteria and the mineral surfaces. However, under conditions where bacteria-mineral adhesion is more extensive, a non-equilibrium assumption allows for a better fit to the cadmium break-through data. The results of this study highlight the strength of the object-oriented modeling approach, and also demonstrate the need to account for non-equilibrium when modeling metal-bacteria co-transport through porous media.

References
[1] Yee N. and Fein J.B. (2002) *Chem. Geol.* **185,** 303-319.
[2] Meeussen J.C.L. (2003) *Env. Sci. Tech.* **37,** 1175-1182.