H11D-1300: Modeling of Reactive Transport of Nitrate in a Heterogeneous Alluvial Fan Aquifer, San Joaquin Valley, California.

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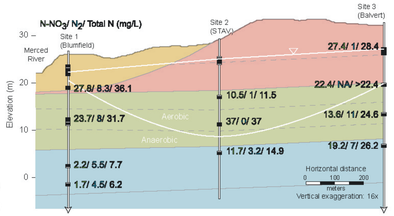
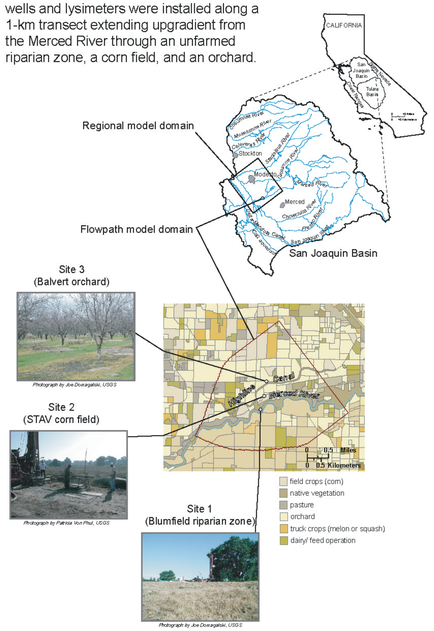
Overview

Fate of nitrate in an alluvial fan aquifer in the San Joaquin Valley, California, was investigated with combined laboratory analyses, field measurements, geostatistics, and flow and transport modeling to address the question: What causes heterogeneity of redox conditions and denitrification at this site?



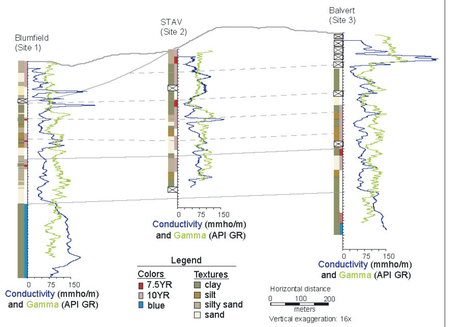
Geographic setting

The study site is located in the Central Valley, California adjacent to the Merced River. In the summer of 2003, groundwater wells and lysimeters were installed along a 1-km transect extending upgradient from the Merced River through an unfarmed riparian zone, a corn field, and an orchard.

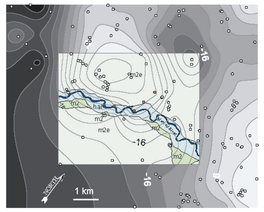


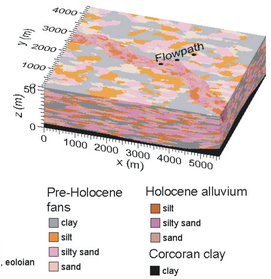
Hydrogeologic setting

Analyses of cores, drillers' logs, and previous interpretations of the local geology were used to generate maps of the boundaries between stratigraphic sequences and transition probability models of hydrofacies distributions within Holocene alluvium and pre-Holocene fans. Multiple 3-D realizations were created and ranked based on lateral and vertical bulk-flow properties.



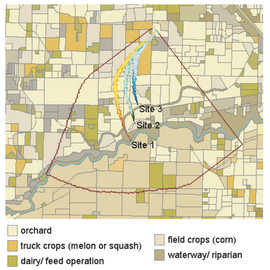
Sediment color, texture, electrical conductivity and gamma reveal likely locations of formation boundaries and paleosols (above), as well as the contours of the upper surface of the Corcoran Clay (below). These data were used to generate conditional transition probability based realizations with downwarping of pre-Holocene fans and incision of Holocene alluvium (below right). Two-hundred 3-D realizations were created and ranked based on lateral and vertical bulk-flow properties.

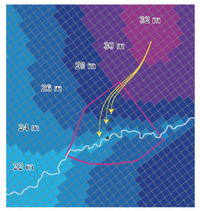




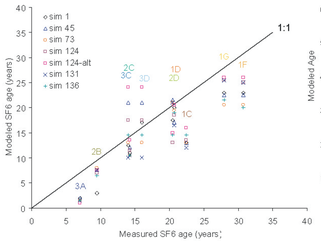
Flow and transport

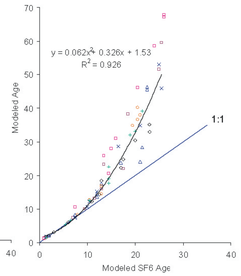
For realizations representing a range of flow conditions, 3-D flow was computed with boundary conditions interpolated from a regional model. A random walk particle tracking algorithm was applied to the flow fields to simulate transport of nitrate. Numerical results show that (1) the vertical strings of wells share more common source areas than wells at similar depths and different horizontal locations, and (2) the the error associated with SF6 age estimates increases with increasing groundwater age.





Results of backwards random walk particle tracking (for realization 124, above left) using RWHet (Labolle et al., 2000) shows that the sites do not share common source areas. Nested wells at each site do have overlapping, elongated source areas. All source areas converge towards the upper right corner of the flowpath-scale model, where strong regional flow controls the head gradients (above right).

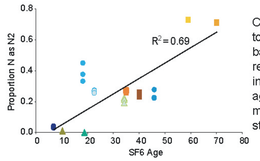




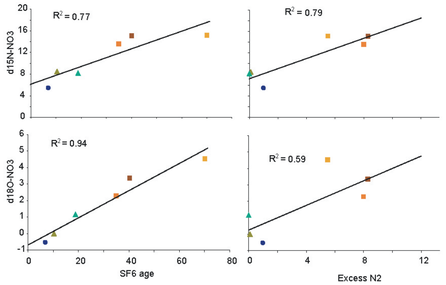
Modeled SF6 ages are comparable to measured values (top right). Shallow wells may be biased by degassing, and deeper wells at Site 1 by exchange with water from below the Corcoran (top left). Actual average groundwater ages are older than SF6 age estimates, a discrepancy which increases with the age of the water (top right).

Chemistry

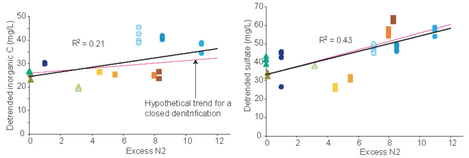
Pore waters were analyzed quarterly for nutrients, anions, and cations. Gases, and isotopes confirm that denitrification is occurring at a slow rate across the entire site. Trends in concentrations of inorganic carbon and sulfate are consistent with use of carbon or sulfide as electron donors. These results will be incorporated in future reactive transport models.



Comparison of excess N gas to the SF6 age (corrected based on transport model results) shows a trend of increasing denitrification with age. Irregularities in the trend may result from different starting nitrate concentrations



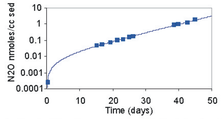
Comparisons of d15N and d18O isotopes to the adjusted SF6 age and excess N2 are consistent with denitrification of a nitrate source with d15N ~ 6 - 7 and d18O ~ -1 - 1, similar to values obtained by Kratzen et al., 2001 for surface waters in the San Joaquin Valley.



Comparisons of detrended inorganic carbon and sulfate with excess N2 are consistent with use of sulfides and carbon as electron donors. Iron may also be used. It remains to be seen which electron donor is most important.

Microbial measurements

Sediment core samples from above and below the water table were analyzed for organic matter, nutrients, inorganic chemistry, particle size distribution, and potential denitrification using denitrification enzyme assays (DEA's) based on the acetylene block technique. These data were used to develop a model of microbial population based on depth and sediment particle size distribution. This information will be used in future reactive transport models.

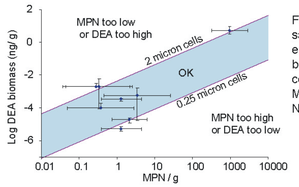


Kinetic model

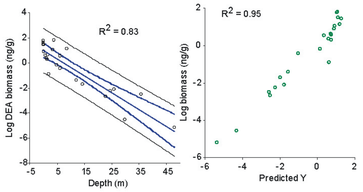
$$\frac{\partial C_{NO_3}}{\partial t} = \frac{-\partial M}{\partial t} Y_1$$

$$M = M_0 \exp(\nu_m t)$$

A simple kinetic model (solid line) typically provided a close fit to experimental data (points). Fitter parameters included microbial population and unlimited growth rate.



For a subset of samples, DEA estimates of biomass were comparable to Most Probable Numbers (MPNs).



Biomass varied by several orders of magnitude. The strongest factor in predicting biomass was the depth of the sample (top left). Multiple regression using grain size data and depth improved the predicted values of biomass relative to use of depth alone (top right and table below).

Term	Coefficient	SE	p	95% CI of Coefficient
Intercept	12.3319	2.8163	0.0005	6.3616 to 18.3022
Clay	-0.0376	0.1207	0.7594	-0.2936 to 0.2183
Silt	-0.1511	0.0361	0.0007	-0.2277 to -0.0745
Very fine sand	-0.0035	0.0389	0.9290	-0.0859 to 0.0789
Fine sand	-0.1763	0.0393	0.0004	-0.2596 to -0.0931
Medium sand	-0.0462	0.0217	0.0486	-0.0922 to -0.0003
Coarse sand	-0.1831	0.0473	0.0013	-0.2834 to -0.0829

References:

Charles R. Kratzer, Peter D. Dileanis, Celia Zamora, Steven R. Silva, Carol Kendall, Brian A. Bergamaschi, and Randy A. Dahlgren, 2001. Sources and Transport of Nutrients, Organic Carbon, and Chlorophyll-a in the San Joaquin River Upstream of Vernalis, California, during Summer and Fall, 2000 and 2001. U.S. Geological Survey Water-Resources Investigations Report 03-4127. Sacramento, California 2004.

LaBolle EM, Quastel J, Fogg GE, Gravner J, 2000. Diffusion processes in composite porous media and their numerical integration by random walks: Generalized stochastic differential equations with discontinuous coefficients. Water Resour Res, 36: 651-662.

Marchand and Allwardt, 1978. Quaternary deposits, northeastern San Joaquin Valley, California. U.S. Geological Survey Mineral Investigations field studies map MF-945.

Well color codes for sites 1, 2, and 3 (lighter colors for deeper wells)

1c 1d 1f 1g 1h 2b 2c 2d 3a 3b 3c 3d