

Hypothetical Modeling of Redox Conditions Within a Complex Ground-Water-Flow Field in a Glacial Setting

ABSTRACT

This poster describes a modeling approach for studying how redox conditions evolve under the influence of a complex ground-water-flow field in a glacial valley-fill dual-aquifer system. The MODFLOW-MT3D-RT3D suite of codes has been applied to a glacial valley-fill setting to test the interplay of flow patterns, sources of reactive organic carbon or pyrite, and availability of electron acceptors in controlling redox processes. Modeling results indicate that local sources of electron donors such as wetlands, lacustrine deposits, and pyrite-rich horizons can influence the chemistry of aquifer systems at a regional scale, and, thereby, give rise to relatively widespread reduced water conditions. The distribution of redox conditions within a flow system affects the susceptibility of an aquifer to contaminants such as arsenic.

MODFLOW

Ground-water flow solution

MT3D

Transport solution

RT3D

Predominant redox reaction zones

MODEL SETUP

HYDROGEOLOGICAL MODEL: Complicated 3-facies model of glacial deposition in bedrock valleys is incorporated in a heterogeneous 3-D ground-water flow model of the Susquehanna River Valley, NY (Randall, 1986).

MODEL GRID: 61 rows and 157 columns for each layer of the three layers, with variable cell spacing averaging 250 feet on a side.

Distribution of geological deposits defined in MODFLOW

Cross-section view

Plan view

GEOCHEMICAL MODEL: Posits that reducing conditions occur in ground water when, due to microbial respiration, redox reactions involving electron donors and electron acceptors occur and reactions are approximately first-order with respect to the electron donor and sequential with respect to electron acceptors. Geochemical model assumes that redox reactions occur not only within but also downgradient of electron donor source areas.

REACTION MODEL: Sequential first-order decay reactions between a single electron donor (natural organic carbon or pyrite) and five electron acceptors, via five different pathways: aerobic respiration, denitrification, iron reduction, sulfate reduction, and methanogenesis.

Selected parameters input to the RT3D reaction code

Parameter	Source concentration (mg/L)	Stoichiometry
E-Donor	100/1	1
DO ₂	6	1.07
NO ₃	0.2	1.65
Fe ₂	0.005	7.44
SO ₄	10	1.60
CH ₄	0	0.267

Maximum build-up of dissolved Fe₂ = 40 mg/L, dissolved CH₄ = 10 mg/L.

Single 1st order kinetic rate = 0.001 (1/day)

→ moderate rate of reaction

Small dispersivities:
α_L = 1 ft (Longitudinal dispersivity)
α_{TH} = 0.1 ft (Transverse horizontal dispersivity)
α_{TV} = 0.01 ft (Transverse vertical dispersivity)
→ mixing controlled by mapped heterogeneity

RT3D SIMULATIONS

The three images below correspond to three various scenarios which show the configuration of the electron-donor source areas.

LACUSTRINE SOURCES
in layer 2 (green)
concentration = 1 mg/L

WETLAND SOURCES
in layer 1 (blue)
concentration = 100 mg/L

RANDOM SOURCES
in layer 1 (blue)
concentration = 100 mg/L

RT3D OUTPUT

These six images show the simulated redox conditions for ground water in the layer containing the electron-donor source areas and the underlying lower aquifer—that is, it shows the spread of reduced water to the lower aquifer from the source areas.

Layer 2

REDOX ZONES

Layer 3

REDOX ZONES

Layer 1

REDOX ZONES

Layer 3

REDOX ZONES

Layer 1

REDOX ZONES

Layer 3

REDOX ZONES

Inactive

DO₂

NO₃

Fe₂

SO₄

CH₄

Layer missing or cell inactive

No redox reaction (DONOR < 0.01 mg/L)

EXERCISING THE MODEL

EFFECT OF PUMPING WELLS FOR THE MODELED “RANDOM” SCENARIO
Runtime = 20 years
Contour interval = 10 feet
Pumping well locations are in red

Layer 3

DRAWDOWN (ft)

EFFECT OF PUMPING ON REDOX CONDITIONS FOR THE THREE SCENARIOS
The table shows how the median and range of dissolved electron donor concentration is correlated with the redox condition of the water. The lowest simulated electron donor concentration is seen in aerobic conditions, while the highest simulated concentration occurs in methanogenic conditions.

	Average concentration in lower aquifer		Average concentration in well discharge	
	Before pumping	Under pumping conditions	Before pumping	Under pumping conditions
LACUSTRINE SCENARIO (Layer 2, E-DONOR = 1 mg/L)				
DO ₂	5.3	5.0	5.4	5.3
Fe ₂	0.3	0.3	0.3	0.1
CH ₄	0.0	0.0	0.0	0.0
WETLANDS SCENARIO (Layer 1, E-DONOR = 100 mg/L)				
DO ₂	5.1	4.8	3.9	3.7
Fe ₂	1.7	2.1	10.2	7.3
CH ₄	0.3	0.2	1.2	0.6
RANDOM SCENARIO (Layer 1, E-DONOR = 100 mg/L)				
DO ₂	3.1	3.1	1.0	2.8
Fe ₂	12.0	9.5	25.2	10.7
CH ₄	0.6	0.6	1.6	0.3

Bold values: lower aquifer in communication with oxygenated parts of the system.

SENSITIVITY ANALYSIS OF THE MODFLOW-MT3D-RT3D MODEL
Many simulations were conducted to better understand the influence of key assumptions on modeling results. Assumptions tested include:

- Background electron-acceptor concentrations (NAWQA regions)
- First-order rate constant for reactions assumed (between “deep sea deposits” and “deep aquifer deposits”)
- Lacustrine dominated horizon represented by three layers
- Electron-donor strength in source areas (lacustrine, wetlands, and random)
- Dispersivity values (i.e., degree of heterogeneity below model scale)
- Transport solver (effect of numerical dispersion)
- Sorption of electron donor
- Redox reactions restricted to electron-donor source areas
- Monod kinetics substituted for first-order reaction rate
- Change of maximum Fe₂ concentration from 40 mg/L to 10 mg/L
- Nitrate addition at the water table

AGE MASS ANALYSIS was performed to determine distribution of young and old water in aquifers and the confining bed.

- Pure advection
- Advection-dispersion

Ground-water age in aquifers on the order of 1 to 100 years; ground-water age in lacustrine material on the order of 100 to over 1,000 years.

RELATION BETWEEN CONCENTRATION OF ELECTRON DONOR AND REDOX CONDITION IN LOWER AQUIFER FOR RANDOM SOURCE CASE → link to ARSENIC occurrence

Redox condition	Percent present in lower aquifer	Median E-DONOR, in mg/L	Q10 E-DONOR, in mg/L	Q90 E-DONOR, in mg/L
Aerobic	75%	0.54	0.12	3.21
Iron-reducing	11%	2.55	0.47	12.01
Sulfate-reducing	8%	4.53	1.55	20.89
Methanogenic	6%	6.45	0.85	29.23

80% of the lower aquifer volume falls between the Q10 and Q90 concentrations.

CONCLUSIONS

- Different distributions of electron donor sources have been simulated, showing how a complicated flow field typical of the bedrock valley glacial setting can yield reducing conditions in areas not immediately adjacent to source areas, such as an underlying aquifer, due to mixing of water along 3D flow paths.
- Discharge from wells increases mixing which, when the pumped aquifer is in good connection with shallow oxygenated waters, can reverse reduced conditions in ground water.
- The spread of reduced ground water, particularly iron-reducing and methanogenic waters, partially explains where higher than average arsenic concentrations occur in natural glacial aquifer systems and in well discharge from those aquifers.

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REFERENCE: Randall, A.,D., 1986, Aquifer model of the Susquehanna River Valley in Southwestern Broome County, New York: U.S. Geological Survey Water-Resources Investigations Report 85-4099, 38 p.

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