Final Report for "Sources and Turnover Times of Dissolved, Colloidal and Particulate Organic Carbon in the Middle Atlantic Bight and Chesapeake Bay" (PIs J. Bauer, VIMS, Grant no. DE-FGO~94ER61833 AO02 and E. Druffel, UCI, Grant no. DE-FG03-95ER62063)

Radiocarbon (14C) and stable carbon (lSC) isotopic natural abundances have been measured in over 307 samples of dissolved organic carbon (DOC), suspended particulate organic carbon (POC), colloidal organic carbon (COC), and dissolved inorganic carbon (DIC) in seawater collected from Mid-Atlantic Bight (MAB) shelf and slope waters between Long Island and Cape Hatteras in April-May 1994 (R/V Columbus Iselin cruise) and March 1996 (R/V Endeavor cruise), and August 1996 (R/V Seward Johnson cruise). This dataset represents the largest spatial and temporal assemblage of natural radiocarbon measurements of marine organic matter ever conducted in a single research program (i.e., DOFS Ocean Margins Program). Results to date areas follows:

a. Carbon isotopic evidence suggests that ocean margins are sources of both 14C-enriched and 14C-deleted DOC and of 14C-depleted POC to this region of the interior ocean.

b. Young, 14C-enriched DOC of shelf and shallow slope waters contains a terrestrial component (i.e., low 31SC) that persists throughout the entire MAB.

c. Deep (300-1000 m) slope waters contain old, 14C-depleted marine DOC and POC (i.e., higher 31SC), possibly the result of lateral advection of eroded, 14C-depleted slope sediments and pore waters.

d. Carbon isotopic values indicate that the northwest Atlantic margin can introduce relic (14C-depleted) DOC and POC to the interior ocean basin. The origin of this relic material is likely derived from resuspended sediment from shelf and slope regions.

e. Relatively 14C-depleted DIC confirms that an older source of DIC exists in some MAB slope waters, and possibly arises from a component of older upwelled waters originating in Antarctic Intermediate Water (AAIW) or Antarctic Bottom Water (ABW) or Labrador Sea Water (LSW) as has been previously observed by other workers.

The final geochemistry cruise of this program was conducted aboard the R/V Seward Johnson in August 1996, during which the same transects and stations were occupied as during the March 1996 geochemistry cruise. Taken in total, these three cruises will evaluate the temporal variability (seasonal and intra-annual) in DOC and POC pool sizes and isotopic signatures, their radiocarbon ages and residence times, and, using general mass-balance models, the relative fluxes of these forms of organic matter along and across the MAB to open ocean waters. In addition, vertical profiles of colloidal organic carbon (COC) were also collected at all of the deepest MAB shelf stations to evaluate the role of colloids in carbon partitioning.

Work has also been conducted in the York River estuary, a major subestuary of the Chesapeake Bay. Samples have been collected along the York River estuary salinity gradient on a seasonal basis for 14C and 31SC analyses in order to identify the major sources (terrestrial vs. marine, young vs. old) and radiocarbon ages of DOC and POC being transported to the Chesapeake and subsequently to the MAB. Microbial incubations have also revealed the proportion and radiocarbon ages of this estuarine DOC that is labile and the isotopic signatures of the highly labile and relatively refractory forms of DOC in this system that are both utilized within the York and available for export to the MAB.

Products of the Research

This work has resulted in the publication of one Nature paper, with three other manuscripts being submitted and prepared for publication. Fifteen abstracts presented the results of this component of the Ocean Margins Program for dissemination of this material.
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A Simulator for Copper Ore Leaching

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Abstract

This is the final report of a one-year, Laboratory Directed Research and Development (LDRD) project at Los Alamos National Laboratory (LANL). Copper is a strategic metal and the nation needs a secure supply both for industrial use and military needs. However, demand is growing worldwide and is outstripping the ability of the mining industry to keep up. Improved recovery methods are critically needed to maintain the balance of supply and demand. The goal of any process design should be to increase the amount of copper recovered, control movement of acid and other environmentally harmful chemicals, and reduce energy requirements. To achieve these ends, several improvements in current technology are required, the most important of which is a better understanding of, and the ability to quantify, how fluids move through heterogeneous materials in a complex chemical environment. The goal of this project is create a new modeling capability that couples hydrology with copper leaching chemistry. Once the model has been verified and validated, we can apply the model to specific problems associated with heap leaching (flow channeling due to non-uniformities in heap structure, precipitation/dissolution reactions, and bacterial action), to understand the causes of inefficiencies, and to design better recovery systems. We also intend to work with representatives of the copper mining industry to write a coordinated plan for further model development and application that will provide economic benefits to the industry and the nation.

Background and Research Objectives

Extraction of copper from the earth is an energy and pollution intensive operation. Typically, ore is mined and transferred to a large heap leach pile, where a highly acidic chemical mixture is applied to release copper metal, which is recovered at the toe of the heap. Alternatively, in situ leaching of ore deposits is being considered; in this case, the process of injecting acids and extracting copper is done through well-to-well solution recovery. The goals of copper ore process design are to increase the amount of copper recovered, control movement of acid and other environmentally harmful chemicals, and reduce energy requirements. To achieve these, several improvements in current technology are required. The most important of these is a better understanding of, and the ability to

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quantify, how fluids move through heterogeneous materials in a complex chemical environment. For in situ processing, what is sought is improved characterization and quantitative resolution of the subsurface distribution of ore and flow paths.

There is a strong conviction among industry scientists that copper extraction technology can be improved through better modeling capability. Models provide a mechanism for collecting what we know about a site and the processes involved into a single dynamic consistent system, whose interactions are constrained by fundamental laws of physics and chemistry. Models can be used in various ways: (1) to provide sensitivities of a process to the various parameters, data, forces and constraints; (2) to aid in interpretation of laboratory experiments, field tests and field data; and (3) for design and forecasting of in situ operations and post-closure remediation. To be an effective interpretation and design tool, a model must capture at least approximately the primary forces and interactions. Sensitivity analysis indicates which data are most crucial, it reveals the impact of parameter uncertainty on predictions, and it is a first step towards parameter estimation. Further, full benefit of modeling requires coupling with optimization methodologies, as currently optimization of field operations is either not considered or is done in a trial-and-error manner.

The goal of this project is to create a new modeling capability that couples hydrology with copper leaching chemistry, and that can be used to improve the percentage of copper extracted, provide better control on the movement of environmentally harmful chemicals during operation and post-closure, and reduce energy use.

**Importance to LANL’s Science and Technology Base and National R&D Needs**

The National Mining Association (NMA) Technology Committee in their meeting at LANL in April, 1996, identified underground communications and *copper leaching simulation* as their priority projects for development. The NMA Technology Committee was also excited by the presentation given by the principal investigator for this LDRD project that applied new simulation tools to the copper leaching process. There is a strong conviction in the mining industry that copper extraction technology can be improved through better modeling capability. As copper extraction is energy and pollution intensive, this project should interest the DOE Office of Industrial Technologies, which is considering adding 'Mining' as an 8th industry for collaboration. This project has a major "science from Yucca Mountain" component. Another area of interest to the NMA Technology Committee is the application of simulation tools to mine safety issues. Some of the same developments in model simulation can be used, particularly for rock failure and fracture.
This research effort addresses one of the five major areas identified by the Environmental Management (EM) Program Office as best matching primary, near-term customer needs and LANL’s capabilities and interests: The Removal of Solvents and Heavy Metals from Groundwater. Our work brings together LANL’s capabilities in modeling and advanced computing, environmental science, chemistry, and microbiology to help develop and implement solutions to a very real and important national problem. This project supports LANL’s tactical goals in High Performance Computing and Industry and its missions in Environmental Stewardship and Energy and Environment.

Scientific Approach and Accomplishments

Copper is a strategic metal and the nation needs a secure supply both for industrial use and military needs. However, demand is growing worldwide, and is outstripping the ability of the mining industry to keep up. Copper consumption grew about 2.4% per year throughout the 1980s and early 1990s. Despite occasional market fluctuations, the rate of production is expected to increase through the remainder of this decade (an additional 2.5-3.0 million tons of copper per year). Current data indicates that supply lags demand and a deficit of several million tons is already projected by the first decade of the next century (Graybeal, 1994). Improved recovery methods are critically needed to maintain the balance of supply and demand.

Most of the world’s copper is produced from open pit mines. Large volumes of overburden rock are stripped away to gain access to the higher-grade ore (see Figure 1). In the past, the overburden rock, although it also contained copper, was discarded. However, the accumulated overburden rock contains as much total copper as in the higher-grade ore that is processed and sent to mills (R.W. Bartlett, 1992). As high-grade ore deposits have dwindled in numbers, the ore-bearing overburden rock is no longer discarded. Alternative recovery processes, primarily heap leaching, are applied to the overburden rock, providing a significant portion of our copper supplies. In heap leaching, ore is mined and transferred to a large heap leach pile, where a highly acidic chemical mixture (primarily sulfuric acid) is applied to release copper metal, which is recovered at the toe of the heap. Alternatively, in situ leaching of ore deposits is being considered (see Figure 2), but the process of injecting acids and extracting copper is done through well-to-well solution recovery (Burt, Wiley & Rex, 1994). The goal of copper ore process designs is to increase the amount of copper recovered, control movement of acid and other environmentally harmful chemicals, and reduce energy requirements. To achieve this goal, several improvements in current technology are required, the most important of which is a better understanding of, and the
ability to quantify, how fluids move through heterogeneous materials in a complex chemical environment.

Copper ores are primarily copper oxides (chrysocolla = CuSiO$_3$·2H$_2$O; malachite = CuCO$_3$) and copper sulfides (chalcopyrite = CuFeS$_2$; chalcocite = Cu$_2$S, covellite = CuS). Typical concentrations are on the order of 1/4 to 1/2 %. In the Western Hemisphere, the most common form of deposit is called porphyry, originating from plutonic material rising from great depth in the earth to the near-surface environment. Copper oxide minerals leach rapidly in acid, whereas primary copper sulfides leach at a considerably slower rate. Bacterial action is important for leaching copper and iron sulfides. Iron sulfide (pyrite) is usually present with chalcopyrite, complicating the leaching process.

The stoichiometric equation for leaching of chrysocolla, the primary copper oxide, is:

\[
\text{CuSiO}_3 \cdot 2\text{H}_2\text{O} + \text{H}_2\text{SO}_4 = \text{CuSO}_4 + 3\text{H}_2\text{O} + \text{SiO}_2
\]

SiO$_2$, amorphous silica, is solubility limited, and can clog pores. Carbonate rock will consume additional acid:

\[
\text{CaCO}_3 + \text{H}_2\text{SO}_4 + \text{H}_2\text{O} = \text{CaSO}_4 \cdot 2\text{H}_2\text{O} + \text{CO}_2
\]

CaSO$_4$·2H$_2$O is gypsum, which can precipitate and clog pores, reducing permeability which changes the flow field and can reduce the recovery of copper. If acidic conditions are not maintained in the oxidized zone, copper carbonate may also precipitate. Secondary copper sulfides are fairly easily leached:

\[
\text{Cu}_2\text{S} + 2\text{Fe}_2(\text{SO}_4)_3 = 2\text{CuSO}_4 + \text{CuS} + 2\text{FeSO}_4
\]

\[
\text{CuS} + 2\text{Fe}_2(\text{SO}_4)_3 = \text{CuSO}_4 + \text{S} + 2\text{FeSO}_4
\]

\[
3\text{Fe}_2(\text{SO}_4)_3 + 4\text{H}_2\text{O} + \text{S} = 4\text{H}_2\text{SO}_4 + 6\text{FeSO}_4
\]

Secondary copper sulfide minerals can generate some of the acid needed to leach oxide copper minerals when mixed oxide/sulfide ore is being leached, which is often the case. However, acid must be present in sufficient concentration (low pH, i.e., about 2.0 to 2.8) to prevent hydrolysis of ferric ions to insoluble forms. The major problems occur with
leaching of primary sulfide, chalcopyrite, which is a relatively slow process. However, when bacteria are present, this reaction can be enhanced. Usually pyrite (FeS₂) is present at higher concentrations than chalcopyrite and complicates the operations. Oxidation of pyrite is expressed as:

$$\text{FeS}_2 + 7/2 \text{O}_2 + \text{H}_2\text{O} = \text{FeSO}_4 + \text{H}_2\text{SO}_4$$

Pyrite oxidation generates ferrous sulfate and sulfuric acid. Acid generation is very important to sulfide heap leaching; if it can be generated in the heap leach pile it saves the costs of being added as a purchased material. The oxidation of pyrite actually occurs through several distinct reactions:

outside rock (aerobic)

$$14\text{FeSO}_4 + 7\text{H}_2\text{SO}_4 + 7/2 \text{O}_2 = 7\text{Fe}_2(\text{SO}_4)_3 + 7\text{H}_2\text{O}$$

inside rock (anaerobic)

$$7\text{Fe}_2(\text{SO}_4)_3 + \text{FeS}_2 + 8\text{H}_2\text{O} = 15\text{FeSO}_4 + 8\text{H}_2\text{SO}_4$$

Next, the large quantity of ferrous sulfate generated by oxidation of pyrite is oxidized to ferric sulfate. This generally occurs outside the rock pores under aerobic conditions:

$$2\text{FeSO}_4 + \text{H}_2\text{SO}_4 + 1/2 \text{O}_2 = \text{Fe}_2(\text{SO}_4)_3 + \text{H}_2\text{O}$$

The ferric sulfate is further hydrolyzed to various insoluble forms, such as jarosite. Oxidation of the dominant copper sulfide, chalcopyrite, is actually a relatively minor reaction:

$$\text{CuFeS}_2 + 4\text{O}_2 = \text{CuSO}_4 + \text{FeSO}_4$$

The iron reactions are controlling, along with reactions between gangue minerals and acid. Copper leaching requires a supply of ferric ions to oxidize the sulfides and acid to dissolve copper oxides and to keep dissolved material from precipitating. Continuous copper sulfide leaching at economically profitable rates requires oxygen and the presence of certain Thiobacillus bacteria (iron-oxidizing bacteria, Thiobacillus ferrooxidans, and sulfur-
oxidizing bacteria, Thiobacillus thiooxidans) that convert ferrous ion to ferric ion much more rapidly than will occur abiotically. In addition, thermophilic bacteria, which can function at 55°C to 80°C, have been shown useful in accelerating the leaching of chalcopyrite. There are several other reactions, mostly involving carbonate minerals that can affect the pH during leaching operations.

There are several factors that affect efficiency of heap leach processing. In addition to the amount of acid added and the grade of ore, probably the most important factor is the uniformity of the flow achieved through the leach pile. Many observations show that channeling of flow is quite common. There are several causes: (1) Heterogeneity in heap pile permeability. The ore fragmentation process will generally create a distribution of particle sizes, which will preferentially settle out during dumping of the rock onto the leach pile, creating a non-uniform bed. (2) Precipitation/dissolution reactions, primarily of gypsum, amorphous silica, and ferric hydroxides. These minerals have limited solubility in water and acid solutions; they can precipitate out, clogging pores, reducing permeability, and changing flow paths. Gangue minerals in the host rock usually compose the vast majority of material present in a copper deposit. Problematic gangue minerals include carbonates and feldspars which react strongly with acid, and clay minerals which can absorb dissolved copper or clog fluid channels (Schmidt, Earley & Friedel, 1994). (3) Pore clogging from bacterial action. If bacteria grow to sufficiently large numbers, they can greatly accelerate the conversion of ferrous iron to ferric, but they can also clog pores, reducing access to unoxidized ore.

The primary goal of this research was to create a new modeling capability that couples hydrology with copper leaching chemistry. Secondary goals, contingent on funding being available, were (1) to apply the model to specific problems associated with heap leaching (flow channeling due to non-uniformities in heap structure, precipitation/dissolution reactions, and bacterial action) to understand the causes of inefficiencies and design better recovery systems and (2) to work with representatives of the copper mining industry to write a coordinated plan for further model development and application that will provide economic benefits to the industry and the nation. These goals were scaled back because of the reduced financial support provided. Nevertheless, a measure of success was achieved, which is summarized below.

Model Development

Coupling Chemistry and Flow

A coupled flow/transport/chemistry model must be able to simulate both saturated and unsaturated multiphase flow, with heat transport in 2-D and in 3-D geometries. It must
also allow for heterogeneity in properties such as mineralogical composition, porosity and anisotropic permeability, have a rock fragment size distribution capability, and handle permeability that changes in response to precipitation and dissolution. In addition, concentration-dependent density variations are expected to be important. On the chemistry side, a comprehensive ability is needed for aqueous reactions based on the law of mass action and stoichiometric balance for copper compounds, pH, and a full suite of mineral phase reactions including ion exchange, adsorption, volume changes, precipitation and dissolution under kinetic as well as equilibrium conditions. In addition, it must include a bacterial model since microbial action mediates some chemical transformations, especially those involving sulfates.

Until recently, much of the hydrochemical model components existed in separate codes. There are fairly comprehensive chemical packages such as EQ3/EQ6 and PHREEQE, but these do not have a mass and heat transport capability. There are other computer codes that have most of the flow and heat transport requirements, but either have no or only limited chemistry. A part of the modeling community has focused on comprehensive chemistry modules but using only simple flow and transport capabilities, while another group has concentrated on comprehensive flow and transport models while slowly increasing the chemistry capability. A recent model, TRANQUI, is one of the most advanced of the first type; it is a marked improvement over previous coupled models as it relies on the EQ3/EQ6 database but is still restricted to 2-D and does not incorporate important flow features such as transient precipitation/dissolution-porosity-permeability interactions. The Los Alamos TRACR3D model is among the most advanced of the second type, having considerable flow and transport capability coupled with limited but growing chemical reaction capability. For example, a version of TRACR3D (Bridwell and Travis, 1995) can simulate pyrite (iron sulfide) oxidation with kinetic mineral phase reactions and precipitation and dissolution in a transient, saturated/unsaturated environment. A total of 15 reactions are currently tracked, but the model is not limited in the number of species that can be carried (except by available computer power). Coupling of permeability to precipitation/dissolution and concentration-dependent density are included. Both equilibrium and rate equations for chemical reactions are allowed. In addition, microbial kinetics is included (Travis and Rosenberg, 1995). A shrinking core model is included (see Figures 3 and 4). Further, adjoint versions of TRACR3D exist that are prerequisite for sensitivity analysis and optimization. A nested-grid option is also under consideration to provide TRACR3D with most of the advantages of finite-element models. In recent years, there has been a proliferation of models coupling porous flow and transport with chemical reactions. The reader is referred to Lichtner,
Steefel and Oelkers (1996) for a recent review of the state-of-the-art in modeling reactive transport.

The FEHM code (Zyvoloski, Dash and Kelkar, 1991), a finite-element model of multiphase mass and heat transport in heterogeneous media, forms the basis of our new coupled porous flow and reactive transport model. It allows for 2-D and 3-D geometries, has a dual permeability model for fractured rock, and has chemical species transport capability. It is fully integrated with an advanced grid generation package (GEOMESH, Gable et al. 1995) to allow modeling of highly complex geology. Two important improvements have been made in FEHM in its flow and transport physics: (a) concentration-dependent density, and (b) changes in permeability and porosity in response to precipitation/dissolution reactions. FEHM has an additional important feature in that it allows energy transport, so that temperature changes due to chemical and microbial activity, as well as seasonal temperature variations, can be accounted for. The biological kinetics package of TRACR3D has been modularized for easy inclusion in FEHM. Finally, FEHM has been upgraded with aqueous chemistry and mineral reaction models, yielding the most advanced flow+transport+reaction model available. The isothermal, structured-grid code TRACR3D is now used as a support tool for FEHM for studies in which geology is not complicated and temperature variations are not important.

It is important to test the coupled model against a variety of data sets, both at the laboratory scale and full field (heap) scale. There are numerous reports (usually through the Bureau of Mines) on results of heap leaching experiments and production operations that contain sufficient data for testing the model. In addition, a copper-producing company has provided us with additional data for model validation/testing, as well as their expertise in interpreting model results. Based on these simulations, 2-D models of field scale leaching with 20,000 cells in the numerical grid will require roughly 18-20 hours on an IBM RISC-level machine, which is certainly feasible. A full 3-D simulation with approximately a million grid cells would require about a month of workstation run time, which is at the upper limit of feasibility with current hardware. However, these time estimates will shrink dramatically within a few years as hardware performance increases, or if the model is moved to a massively parallel supercomputer. The Delphi system (tens of teraflops, which is thousands of times faster than a single high-performance workstation) is scheduled to be online at LANL within five to six years. Model development now will position the mining industry to be able to take full advantage of the next generation of supercomputers as soon as they come online.
Modeling Complex Geology

Los Alamos has developed a highly sophisticated grid-generation software package called GEOMESH. GEOMESH can generate well-conditioned finite-element and integrated finite-difference grids for very complex geology in 2-D and in 3-D. Although this capability was originally developed for high pressure-temperature-strain rate applications, it has been transformed by the Los Alamos team into a highly versatile geophysics tool. This software generates grids for both FEHM and TRACR3D. In addition, GEOMESH is compatible with STRATAMODEL. The structured grid output of STRATAMODEL can be used directly in GEOMESH so that interfaces, wells, etc., are preserved, but the STRATAMODEL structured mesh is converted to an unstructured grid to provide more flexibility in treating pinchouts, smoother changes in grid elements and better conditioning of the finite-element solution. We have worked with NMA member companies to apply GEOMESH to create discretizations of sites of their choosing suitable for use in the coupled copper-leaching model (as well as other flow and non-reactive transport simulation studies), and to adapt it to another geologic/mining model—MEDSystem (MEDS).

Coupling the Process Model with Sensitivity, Inverse and Optimization Methods

The mathematics of optimization and control theory can be used in conjunction with our coupled flow and transport model to design a leaching operation that provides maximum containment of the process fluid, thereby limiting the hazard to the environment. The same methods can also be applied to recover as much of the fluids as possible in the post-leaching phase. Further, the most efficient copper leaching operation can be determined, within the copper leaching model assumptions, through rigorous application of optimization theory. The control variables in the optimization process are limited to locations and numbers of wells, the injection/extraction schedule for each well, and the mix of chemicals injected. There are several algorithms that can be used. However, an adjoint/gradient search algorithm would likely be best, based on past experience; evolutionary algorithms require an enormous number of simulations, which is not feasible with present computer hardware. Numerical experimentation will be required to determine the computational burden of a full optimization of an in situ and a heap leach operation.

We have developed an adjoint/gradient search version of FEHM to provide efficient computation of model derivatives. This code provides the basis for sensitivity analysis, parameter estimation, and optimization. We have used it, e.g., to determine permeability distributions given well pressure data. Sensitivity analyses of the leaching operations can be conducted with the adjoint version of FEHM to quantify and rank the various parameters in terms of importance. The optimization phase will only be attempted if the sensitivity
analysis indicates sufficient sensitivity to warrant use of optimization methodology, and then optimization can be limited to the most important variables.

In situ leaching of copper is attractive because it avoids the expense of digging out the ore and transporting it to a heap leach pile. However, the tradeoff is that there is more uncertainty about the ability to extract copper because of the importance and uncertainty about the distribution of fracture-controlled flow paths. It is critical to extract as much information as possible from wells, cores, and flow and tracer tests regarding the subsurface conditions. Methods of data and model inversion can be used to determine the most likely situation. In addition, information on and simulations of the evolution of ore body geology, such as cooling and tectonic fracture patterns, can be used as constraints on the inversion, providing a possible improvement in resolution.

There is an associated problem both for in situ leaching and for heap leaching and that is the uncertainty in the distribution of copper ore. This is a more challenging inversion problem; simple flow and tracer tests will not be sufficient to resolve the distribution of ore. Either tests using tracers that adsorb preferentially (see, e.g., Hagelberg & Travis, 1997) on copper-bearing minerals or a more reactive process, such as the leaching process itself, may be useful in improving the resolution of the spatial distribution of copper ore. These are issues that should be studied now that the computational tools are available.

Developing a Plan for Future Model Development and Applications in Conjunction with Representatives of the Copper Mining Industry

It is important to establish good communications with the mining industry so they are aware of the computational tools we have developed and can help direct further model development and define applications that will be of most benefit. Staff at several copper mining companies are working with us to define applications of the copper-leaching simulator that will have the greatest economic impact on their operations. The initial applications have been to heap leaching. (In situ leaching is also being considered by a number of companies, but there are additional technical complexities that should be addressed in a future effort.) In particular, simulations have been carried out to quantify the non-uniformity of flow in a heap leach pile under different fluid application rates. Although some of the details of particular sites and applications may be proprietary, our simulator system is of a generic nature and so can be shared easily among the companies involved.

Prevention of environmental contamination from the highly acidic and toxic lixiviant fluids involved in copper (and gold) heap leaching is of great concern to copper mining companies. Large heap leach piles can be hundreds of feet high and run for several
thousands of feet in length. In a few cases, these are located near national parks, and so there is heightened concern about possible environmental contamination. Our model can be used to compute the movement of these fluids through the leach pile, and track their dispersal into the surrounding environment. The model can also be used to evaluate the effectiveness of strategies to prevent environmental contamination at these sites.

**Summary**

We have accomplished the primary goals of this research project:

1. Created a comprehensive, fully coupled flow + transport + copper chemistry and bacterial action model.
2. Integrated this reactive transport model with state-of-the-art software for capturing complex geology, as might occur in a heap leach pad, and especially at an in situ leaching operation.
3. Calibrated the leaching model against laboratory data provided by a copper mining company.
4. Applied the coupled simulator to current problems in heap leaching, specifically to flow channeling and to contaminant transport in a heap leach pile.
5. Explored future model development and applications in conjunction with representatives of the copper mining industry.
References


Figure 1. Typical mineral zoning of upper part of porphyry copper-ore deposit. Above the water table, an oxidized and a naturally leached zone predominate, with low copper concentrations (1/4 - 1/2 % wt). Below the water table, the highest copper concentration is found in the enriched zone (about 3 %), with a smaller fraction (1 %) in the primary sulfide zone below that. Vertical depth shown is approximately 1 km. After Bartlett (1992).
Figure 2. Cross-section schematic of in situ leaching of oxide zone of copper-ore deposits. Injection wells penetrate to about 300-m depth. Copper-rich solution drains through sulfide region to a rubblized zone, where it is collected in mined areas. After Burt et al. (1994).
Multiple Particle Size Distribution

Figure 3. Numerical grid encompasses two process length scales: that of the ore deposit zone and that of the individual particles and blocks in which leaching reactions occur. A distribution of particle sizes in each grid cell, with several spherical shells in each particle, is provided. After Travis et al (1983).
Shrinking Core Model
Copper Sulfide Ore

Mixed Kinetics
Pyrite & Copper ores

Oxidant

Oxidation Products

Trickle Leaching

Partially Reacted Sulfides

Oxidant Conc.

Copper Ore %

Figure 4. The shrinking core particle is a necessary part of the leaching model since important reactions occur within grains and blocks, and the rates of reaction depend on the diffusion of chemicals through pores and fractures. After Bartlett (1992).