SESSION V: SIMULATIONS AND FORECASTS

Chasing Subsurface Contaminants

Joel G. Burken, University of Missouri

Joel Burken summarized mechanisms that are involved with the phytoremediation of organic compounds. He said that subsurface contaminants can be either bound to soils, mineralized, or taken up by plants. Once inside plants, contaminants can be metabolized, bound in plant materials, or released through phytovolatilization. Burken said that these mechanisms have been documented, but the importance of each is still being debated.

Burken described laboratory studies in which he has been involved, noting that the study results offer interesting insights, but cannot necessarily be extrapolated directly to the field. In the early 1990s, he said, researchers evaluated whether poplars can clean up atrazine. Several interesting findings were recorded. First, investigators learned that poplars do not increase mineralization rates in the subsurface, but they do reduce contaminant concentrations. Also, poplars were shown to take up the atrazine. Once the contaminant was inside the plant, some of it degraded (about eight breakdown products were detected), some became bound, and some transpired. In addition, researchers learned that subsurface soil conditions have a large impact on transpiration rates. Uptake is not as vigorous when components of the subsurface sorb or compete with contaminants. (When poplars were planted in silica sand, all of the atrazine was taken up by plants over a 10-day period. Only 30% was taken up over an 80-day period when a silt-loam soil was used.)

In recent years, Burken said, the University of Missouri has performed several studies to evaluate how poplar cuttings impact a variety of VOCs. In all of the studies, he said, a steady flow of air was injected into a reactor, aerial and subsurface regions were compartmentalized, and significant efforts were made to mimic outdoor conditions. Plants were grown hydroponically in some of the studies, but were rooted in soil in others. When soils were used, investigators were able to create two subsurface zones: a saturated layer (where contaminated water was injected) and a vadose zone. Burken described what was learned when benzene was exposed to poplar cuttings:

- *Subsurface benzene concentrations were reduced.* Benzene was injected into unplanted and planted reactors, and investigators measured the effluent that came out of each. After six days passed, benzene was no longer detected in the planted reactor effluent. It persisted in the unplanted reactor effluent, however, for the entire course of the experiment.

- *Subsurface mineralization processes were enhanced*. Carbon dioxide was measured in the rhizosphere headspace of unplanted and planted reactors. Very little was detected in the former; significant quantities were found in the latter.

- *Very little benzene was stored in plants.* Negligible benzene concentrations were detected in plant tissues.

- *Benzene was transpired, but the amounts recorded differed across experiments.* Significant amounts of benzene were transpired by hydroponically grown plants, but those that were grown in soil released much less benzene. This proves that differences in experimental design have profound impacts on results.

- *Subsurface contaminant migration, water table height, and subsurface oxygen levels were impacted.* Very little benzene migrated to the upper soil layers in unplanted reactors because soil pore spaces were mostly filled with water. In the planted reactors, contaminants moved more freely throughout the subsurface. (Roots removed water, and this opened up pore spaces.) The studies also showed that poplars have a profound effect on rhizosphere oxygen levels. The rhizosphere in planted reactors was aerobic, but soils in the unplanted reactors proved to be oxygen deprived. Aerobic environments attract microbes that help to degrade organics. Thus, it is clear that plants exert a combination of beneficial effects concurrently.

Burken identified areas that require additional research. Efforts should be made to understand plants better, he said, noting that researchers should assess the phytoremedial properties of a wide variety of plants. In addition, he said, researchers should ask: can plant systems be altered to improve their phytoremedial properties? Burken said that some scientists propose using genetically enhanced plants or genetically engineered microbes (GEM) in the rhizosphere. He described some work that has been performed on the latter. Toluene *o* monooxygenase has been incorporated into three different rhizosphere microbes, Burken said, and experiments have been performed to (1) evaluate how well GEM compete in wheat, bean, barley, and poplar rhizospheres; (2) determine the degradation properties of GEM; and (3) determine whether GEM increase TCE reduction rates when they are used in a poplar rhizosphere. The results of the latter, Burken said, suggest that adding GEM to plant systems increase degradation rates dramatically.

Effect of Woody Plants on Groundwater Hydrology and Contaminant Fate
James Landmeyer, U.S. Geological Survey

James Landmeyer said that a study is being performed at a site in Charleston, South Carolina, to evaluate the impact that poplars have on groundwater hydrology. The site is located in an urbanized setting, near a residential area and an aquarium. Groundwater at the site, which is about 2 to 4 feet bgs, is polluted with PAH and BTEX. It is also impacted by a coastal water body; thus portions of the site have saline groundwater and are influenced by the tides. In December 1998, Landmeyer said, 2-foot-tall poplar whips were planted in an effort to address the site's groundwater contamination. Many of the trees prospered even though the site experienced a harsh drought shortly after planting. By September 1999, several of the trees had reached about 14 feet in height. Landmeyer said that excavations were performed to evaluate root

profiles. From this activity, investigators learned that the poplar roots are growing vertically, into the capillary fringe of the shallow water table. Landmeyer said that researchers were relieved to find this, because tree roots typically grow horizontally, rather than vertically, in this part of the country.

Landmeyer said that the Penman equation was used to estimate how much water the poplars extract from the site's groundwater and surrounding soil. A weather station was installed to collect several of the parameters (*e.g.,* wind speed and direction, air temperature, precipitation, solar radiation, relative humidity, barometric pressure) that are required for the equation. In addition, Landmeyer said, information on leaf temperature and wetness was also collected and entered into the equation. The equation's output indicated that the potential evapotranspiration (PET) is about 0.5 inches per day. Extrapolating this over the entire plantation, Landmeyer said, researchers concluded that 2,000 gallons of soil moisture and groundwater would be removed from the site each day. He said that this value exceeds the amount of water (1,500 gallons) that is thought to enter the study area each day. Thus, according to the modeled data, the poplar plantation should cause a depression in the water table. Landmeyer said that extensive groundwater-level sampling would have to be conducted to determine whether depressions are actually resulting.

Landmeyer said that some efforts have been made to measure groundwater fluctuation at the site. He presented a series of graphs, which showed how groundwater levels changed during three different study periods (August 6–11, 1999; August 24–September 2, 1999; and April 5–9, 2000) and at three different locations across the site (in the center of the site, 1,000 feet from the tidal body, and 2,000 feet from the tidal body). These data showed that: (1) rainfall causes the groundwater table to rise, (2) there is no evidence of hydraulic capture yet, (3) fluctuation is more significant in locations that are closer to the tidal body, and (4) groundwater levels dip slightly around noon—the time when evapotranspiration rates are expected to be highest. Using the data obtained, Landmeyer said, investigators determined that each one-year-old poplar at the site is taking up about 0.08 gallons of groundwater and soil moisture each day. This translates to an uptake rate of about 0.0002 gallons per minute. After more data are collected, Landmeyer said, he will use a modeling program to estimate how the trees will perform as they get older.

Landmeyer said that some efforts have been made to determine whether the poplars are impacting subsurface geochemistry. For example, a dissolved oxygen probe has been installed in one well to determine whether poplars have caused dissolved oxygen levels to increase in groundwater. To date, he said, fluctuations in this parameter seem only to correlate with rainfall occurrences. He said that some preliminary efforts have been made to determine the fate of the groundwater PAH and BTEX. These contaminants have been detected in tree leaves, but it is unclear whether these chemicals originated in the groundwater or came from some other source.

Before closing, Landmeyer presented information on another site, located in Beaufort, South Carolina, which has a BTEX and MTBE plume emanating from an underground storage tank. He said that oak trees established themselves at the site about 40 years ago. In 1997, researchers initiated evaluations to determine whether these oaks were effecting groundwater contaminants. They concluded that hydraulic capture has not been achieved because groundwater flow rates are too fast and portions of the plume are too deep. However, they did find strong evidence that contaminants are being taken up into the oak trees. Landmeyer said that the trees were cored and evaluated using gas chromatography/mass spectrometry, and that BTEX, MTBE and trimethylbenzene isomers were detected in those trees that had extended roots into the groundwater table. Landmeyer said that the oaks might be transpiring a significant amount of MTBE, which could cause some people to express concern about cross-media contamination. He said that it may be more effective to decrease MTBE concentrations by using plants that release MTBE to the air (where it has a half-life on the

order of hours or days) than to allow MTBE to be transported in anaerobic aquifer systems (where its half-life is on the order of years).

Modeling Plume Capture at Argonne National Laboratory-East (ANL-E)
John Quinn, Argonne National Laboratory

John Quinn described some of the modeling activities that were performed for the phytoremediation project at ANL-E's 317/319 area. He noted that this site was described earlier in the conference, but offered the following information as a brief summary: (1) the groundwater is contaminated with VOCs and tritium, (2) 13 extraction wells were installed as an interim measure to control groundwater, (3) the contaminated groundwater plume is about 25 to 30 feet deep, (4) the site's subsurface stratigraphy is extremely complex, (5) the aquifer is fairly thin—about 5 feet thick—but varies widely in texture and permeability, (6) groundwater flows towards the Waterfall Glen Forest Preserve and a recreational path, (7) contaminants have appeared in downgradient seeps, (8) an engineered phytoremediation system has been installed to control site contamination, and (9) fences have been installed to prevent deer from contacting the planted system.

Quinn described the phytoremediation system that has been installed at the site. He said that a herbaceous cover has been installed to minimize water infiltration and soil erosion. In addition, trees have been installed near the site's french drain in an effort to enhance the remediation of subsurface VOCs. (Quinn said that the downward migration of tree roots should not be hindered by subsurface heterogeneities, because the area around the french drain was homogenized by deep soil mixing a couple of years earlier.) Also, Quinn said, TreeWells® have been installed in an effort to achieve hydraulic control. He said that these trees were planted in 30-foot-deep, lined, large-diameter boreholes. Thus, roots are cut off from any shallow water sources and forced to grow vertically in search of deeper groundwater sources.

Quinn described modeling efforts that have been conducted on the aquifer that lies 25 to 30 feet below the site. He said that MODFLOW was used to model transient groundwater flow under pre- and post-phytoremediation conditions. For the latter, he said, TreeWell® evapotranspiration estimates were provided by Ray Hinchman and Edward Gatliff. Quinn showed computer simulations for the pre- and post-conditions, and told attendees that these could be viewed more leisurely by visiting http://web.ead.anl.gov/phyto. In both simulations, Quinn pointed out, water levels pulsate, with the highest levels predicted in spring, during snow melt events, and the lowest levels predicted during late summer and early fall. Quinn said that he also performed particle tracing studies to evaluate groundwater flow throughout the plantation. Summarizing the results of his studies and simulations, Quinn made the following conclusions about the ANL-E site: (1) mature plantations will achieve groundwater containment, even during the dormant winter months; (2) the site's 13 extraction wells can be phased out in the future; (3) groundwater that is pulled into microbially active rhizosphere areas will have a residence time of 5 to 17 months; and (4) de-watering of the perched aquifer could occur.

In closing, Quinn listed some of the activities that are ongoing or planned at the ANL-E site. These include collecting groundwater samples, making water-level measurements, collecting weather data, sampling tree tissues, evaluating transpirate, analyzing subsurface soils, and installing viewing tubes so that miniature cameras can be used to view root development.

Phytoremediation Potential of a Chlorinated Solvents Plume in Central Florida
Stacy Lewis Hutchinson, EPA, National Exposure Research Laboratory

Stacy Lewis Hutchinson said that models can be used to predict whether a plant-based system will be able to control groundwater at a site. She said that water balance can be determined by evaluating groundwater flow patterns and the amount of water that plants withdraw from aquifers. She presented the water balance equation—a calculation that is incorporated into predictive models—and listed parameters included in it: hydraulic conductivity, aquifer thickness, hydraulic head, sources and sinks of water, precipitation, irrigation, surface runoff, and evapotranspiration. The latter two, she said, are often estimated, and therefore tend to have more error associated with them.

Hutchinson talked briefly about the evapotranspiration parameter, noting that plants that exhibit high values may be able to reduce average net recharge to subsurface aquifers, prevent plume diving, and create an upward flux of groundwater. A plantation's capability of achieving these results, she said, is influenced by geography and climate. For example, she said, evidence suggests that plants are more likely to achieve hydraulic control in the Southwest than in the Southeast. (Both areas are hot and exhibit fairly equivalent evaporation energies, but precipitation rates differ between the two. In the wet Southeast, plant roots are more likely to use precipitation as a water source. In the dry Southwest, roots are forced to search for deeper groundwater aquifers.) Hutchinson described the methods that are used to determine evapotranspiration values. She said that many researchers use the Penman-Montieth equation to generate estimates, but cautioned that this equation may provide overinflated evapotranspiration values. Recently, Hutchinson said, researchers have started using sap flow collars and probes to obtain a more direct measurement of evapotranspiration.

Hutchinson described modeling efforts that were conducted at a site in Orlando, Florida. This site's groundwater, which is contaminated with PCE and TCE, flows under a paved area, to a ditch, a grassy area, and then a more densely vegetated area before discharging to a lake. Groundwater analyses, she said, reveal that there is plume diving at the site. Thus, groundwater is too deep for existing trees to tap into. In an effort to fix the plume diving problem, Hutchinson said, investigators used models to determine (1) why the plume diving is occurring and (2) how the problem could be fixed. She said that a one-dimensional analytical recharge model was used to evaluate the local patterns of aquifer recharge. Using this, researchers were able to mimic the pattern of plume diving that was observed at the site. (The model was not perfect, she said, noting that it did not precisely predict how deep the plume would dive.) Once researchers had a better understanding of recharge, a numerical model was developed for the site, using the MODFLOW code and a U.S. Geological Survey (USGS) regional calibration of the same model. Two layers of differing conductivity were incorporated into the model, and fine scale layering was incorporated to define lake bathymetry. Hutchinson said that addressing vertical discretization is important for evaluating three-dimensional flow features. She said that the model was run using three different evapotranspiration estimates: 50 cm/year (a value cited in a USGS report), 80 cm/year (a value cited in a report about the actual site), and 130 cm/year (a value cited by the Florida Agricultural Extension Service). All of these values, she noted, are less than 140 cm/year—the average annual precipitation estimate.

After the model was used to simulate existing conditions, Hutchinson said, it was used to predict the impact that different engineering solutions might have. For example, she said, simulations were performed to determine whether plume diving could be reversed by (1) diverting runoff from the ditch, and (2) planting some trees in the paved area. She noted that the latter area has no recharge, because water cannot infiltrate pavement. Thus, by dispersing some trees in this area, site managers could be assured of causing a net loss of groundwater over this area. The modeling results indicated that combining the two approaches would

reverse much of the diving that is currently observed at the site. Assuming that recharge in the paved area is zero and evapotranspiration rates are 80 cm/year, she said, vegetation would be able to capture about 77% of the plume. The percentage is even higher (88%), she said, when evapotranspiration rates are assumed to be 130 cm/year. In closing, Hutchinson stressed two important points: (1) vertical characterization is required to delineate plumes, and (2) the localized recharge distribution should be carefully assessed.

Speaker Panel and Audience Discussion

Audience members asked questions or provided comments about the following topics:

- *The role models play in obtaining regulatory approval.* Hirsh said that regulators will want to review modeling and forecasting data when trying to determine whether to approve a phytoremediation project. Having these data available, he said, will help build convincing arguments in support of phytoremediation.

- *Using evergreens.* A participant asked whether evapotranspiration rates at the ANL-E site could have been enhanced by including evergreens in the phytoremediation design. Quinn said that this was a good question, but that he did not have an answer. Quinn said that evergreens do transpire water for a longer portion of the year, but pointed out that their evapotranspiration rates are lower than those exhibited by poplars and willows. McMillan acknowledged that the rates are lower, but thought it might be beneficial to include evergreens in a tree mix, since they actively transpire during early spring and late fall—two critical recharge periods that occur when poplars and willows are not transpiring optimally.

- *Public perception on genetic enhancements.* One meeting attendee said that the public might express concern about genetically enhanced plants and GEM. She asked Burken if he had any recommendations on how to handle this. He suggested hiring someone with public relations experience to address the public's concerns. He said that the public would need to be educated on these topics. For example, he said, it is important for the public to understand that the GEM that are being created have suicide implantations.
- *GEM.* Phil Sayre advised researchers who are creating GEM to be careful if they are working with the *Burkholderia cepacia* complex, which has been reported to cause death in people with cystic fibrosis. Sayre also advised investigators to evaluate GEM for resistance to antibiotics.