

# 73793 Biofiltration of Volatile Pollutants: Solubility Effects

**Publication Date:** June 15, 2001

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**Graduate Students:** One master's degree candidate from the University of Tennessee will conduct his graduate research as part of this project. One BS candidate will complete a summer internship for this project during the first year.

## RESEARCH OBJECTIVE

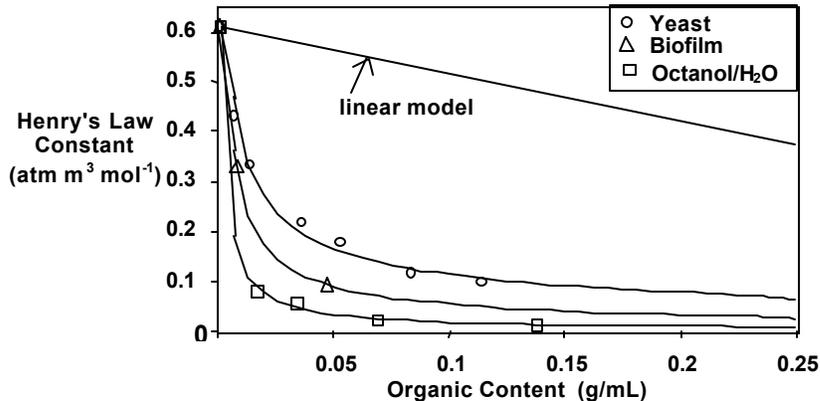
This project investigates and collects fundamental partitioning data for a variety of sparingly soluble subsurface contaminants (e.g., TCE, etc.) between vapor, aqueous phase, and matrices containing substantial quantities of biomass and biomass components. Due to the difficulty of obtaining these measurements, environmental models have generally used solubility constants of chemicals in pure water or, in a few rare cases, simple linear models. Our prior EMSP work has shown that the presence of biological material can increase effective solubilities by an order of magnitude for sparingly soluble organics; therefore, the previous simple approaches are not valid and are extremely poor predictors of actual bio-influenced partitioning. It is likely that environmental contaminants will partition in a similar manner into high-biomass phases (e.g. biobarriers and plants) or humic soils. Biological material in the subsurface can include lipids, fatty acids, humic materials, as well as the lumped and difficult to estimate 'biomass'. Our measurements include partition into these biological materials to allow better estimation. Fundamental data collected will be used in mathematical models predicting transport and sorption in subsurface environments, with the impacts on bioremediation being evaluated based on this new information. Our 2-D Win95/98 software program, Biofilter 1.0, developed as a part of our prior EMSP efforts for describing biofiltration processes with consideration given to both kinetic and mass transfer factors, will be extended to incorporate and use this information.

## RESEARCH PROGRESS AND IMPLICATIONS

This report summarizes work after 6 months of a 3-year project. Experiments have been initiated which first focus on trichloroethylene (TCE) and methyl chloride (MC) as critical contaminants of interest. We have developed a number of new protocols for precise measurements for complex multi-phase systems containing yeast, octanol, water, and a headspace. One result has been the measurement of greater-than-expected biomass partitioning into organic phases such as octanol. 'Equilibrium' mixtures have indicated that as much as 1% of aqueous-phase biomass can permeate an adjacent octanol phase, which is much higher than intuitively obvious. Yeast biomass has been harvested for all experiments and is being used in ternary phase systems (biomass/aqueous/octanol or biomass/aqueous/air) containing contaminants which distribute unevenly into the various phases.

This research will provide much-needed fundamental information regarding partitioning of priority contaminants in subsurface aquifers, vadose zones, and surface water impoundments where biological material is present. Due to the difficulty of obtaining these measurements, environmental models have generally used solubility constants of chemicals in pure water or, in

a few rare cases, simple linear models. Our work (see **Figure 1**) has shown that the presence of biological material can increase effective solubilities by more than an order of magnitude; therefore, the previous simple approaches are not valid and are extremely poor predictors of actual bio-influenced partitioning. Accurate data measurements of phase distributions of sparingly soluble organics between biomaterial/water/air are needed to replace the current assumptions using pure water data. Beyond the detailed equilibrium measurements of a variety of contaminants and biological material types, we also seek to characterize the biomass in order to understand the fundamental properties that cause different biomaterial types to have different partition constants. We will develop correlations based on these insights to allow these data to be easily utilized by developers of predictive models for subsurface transport and fate as well as bioremediation.



**Figure 1.** Published data for propane which show deviation from ideal models of partitioning between biomass and gas phases (as would be likely in vadose zones and surface impoundments). Data were collected for yeast (circles) and bacteria (triangles) over a variety of organic densities and compared to two 'ideal models' for octanol/water partitioning (squares and straight line). In both cases, actual partitioning measurements deviated significantly from idealized models for pure water/octanol mixtures.



Biomass is harvested (see picture at left) from reactor vessels ranging in size from 4 to 500 L for use in partitioning experiments. Biomass types being investigated include yeast, bacteria, and algae as well as traditional groupings of protein, lipid, and complex carbohydrates. Tightly sealed equilibrium test reactors (see picture at right) are constructed with precisely measured amounts of water, biomass, organic carrier, and target contaminant (such as TCE). Fundamental partitioning data are then incorporated into a standardized model for comparison and impact.



## PLANNED ACTIVITIES

Experiments are being conducted at bench-scale to determine the physical partitioning parameters (equilibrium aqueous/biomaterial partition constants and Henry's law constants) of priority contaminants in contact with high biological material levels. Intermediate scale columns will be used to simulate subsurface conditions as well as to validate models and parameters. The following time/table lists/describes activities:

## Tasks/Time Table

FY 01	FY 02	FY03
1.1 Measure partition coefficients for priority contaminants in saturated aqueous matrices w/varying levels of biomaterial		
1.2 Measure partition constants for priority contaminants in unsaturated (vadose) matrices with varying levels of biomaterial		
	2.1 Examine various biomasses (yeast, etc.) to correlate how compositional properties impact enhanced solubilities	
	3. Determine how mixed biota/degrader consortia display solubility effects characterized by hydrophobicity, protein content, etc.	
	4. Quantify how geochemical factors affect measured parameters	
		5 Heterogeneous matrix simulation of subsurface
	6. Validation of "intrinsic" correlations	
	7. Apply measured parameters to existing models to determine improvement of predictive estimates	
	8. Incorporate new constitutive relationships into ORNL-developed Biofilter software with subsequent validation	
		9. Enhance bioavailability by adding environmentally-friendly solvents

## INFORMATION ACCESS

Davison, B.H., J.W. Barton, K.T. Klasson, A. F. Francisco. "Influence of Biomass on Alkane Solubilities". *Biotechnology and Bioengineering*, 68:279-284, 2000.

Davison, BH, Barton, JW, Klasson, KT, Francisco AB. Effect of biomass on the measured solubility of sparingly soluble organics in aqueous bioremediation systems. Presented at the 217<sup>th</sup> ACS National Meeting, March 21-25, 1999, Anaheim, CA.