



Project Summary

Sorption of Ionizable Organic Compounds to Sediments and Soils

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An important process affecting the ultimate fate of pesticides and other pollutants in the environment is the sorption of these compounds to soils, sediments and aquifer materials. Besides affecting the physical transport of these compounds in the environment, sorption may significantly impact the magnitude of biological and chemical degradation processes, including anaerobic and aerobic microbial degradation, photodegradation, hydrolysis, and chemical reduction. Therefore, an understanding of sorption processes is necessary, not only to understand transport of chemicals through the environment, but also to resolve the significance of these other processes in determining the ultimate fate of chemicals in the environment.

This report examines the partition reactions of organic acid and base compounds to sediments and soils, as well as the interactions of an anionic surfactant with sediment components. In contrast to the partition reactions of non-polar organic compounds, the interactions of these classes of compounds with sedimentary materials has not previously received the same level of quantitative interpretation necessary to determine their environmental fate, *a priori*. This is despite the significance of these compounds as pesticides (such as 2,4-D, Silvex, etc.) or as other pollutants (chlorophenols, nitrophenols, anilines, etc.).

This Project Summary was developed by EPA's Environmental Research Laboratory, Athens, GA, to announce

key findings of the research project that is fully documented in a separate report of the same title (see Project Report ordering information at back).

Organic Acids

Organic acids may sorb to sedimentary materials as either neutral or ionic species. The significance of each form (neutral or ionic) depends upon the pH of the aqueous phase and the acid dissociation constant of the particular compound. The sorption of the neutral form of organic acids is similar to the sorption of other neutral organic compounds in that the predominant interactions result from hydrophobic forces. As a result, reasonable estimates concerning the extent of sorption can be made from knowledge of the organic carbon content of the sedimentary material and the hydrophobicity of the compound (as measured by the water solubility or the octanol-water partition coefficient). Sorption of the anionic form of organic acids is thought to occur primarily through modified hydrophobic interactions. Because most sediment-associated humic material is negatively charged, however, the sorption of the organic anions is less than that of the corresponding neutral species by 1 to 2 orders-of-magnitude. In addition, the sorption of organic anions is somewhat pH-dependent, as changes in pH affect not only the dissociation of the organic acid, but also the charge on sedimentary humic material.

To quantitatively describe these partition reactions, three mass action equations and several material balance constraints are required. The mass action equations



include equations describing (1) sorption of the neutral species, (2) sorption of the anionic species, and (3) acid dissociation in the aqueous phase. Model results and experimental data are given for the sorption of pentachlorophenol onto two sediments as a function of sediment concentration and pH.

Organic Bases

Organic bases of environmental concern include the nitrogen-heterocyclic compounds (NHCs) and the aromatic amines. Reaction processes of organic bases with soil and sediment components include partition reactions through hydrophobic or modified-hydrophobic mechanisms, cation or ligand exchange type reactions, and chemical reactions leading to the formation of covalent bonds through nucleophilic addition or oxidative processes (which is important only for the amines). Differentiating among these processes is

necessary if predictive fate models are to be developed. However, in soil and sediment systems, this can be problematic, as all processes occur simultaneously and influence the magnitude of one another. Currently, no models exist that can quantitatively estimate *a priori*, the reactions or organic base compounds with sedimentary materials through knowledge of compound and sorbent properties. Experimental data are given in the complete report on the loss of substituted anilines to sediment as a function of time, pH, and substituent. The data indicate that sorption processes (both hydrophobic and ionic), as well as chemical reaction, occur simultaneously for these compounds.

Surfactants

Recently, surfactants have received considerable attention because of their solubilizing effects on relatively water-in-

soluble compounds. This interest stems from both a concern over the environmental fate of surfactants *per se* and their effects on other chemicals (surfactants are contained in most pesticide formulations), and an appreciation for the potential of surfactants to enhance the desorption of pollutants from contaminated soils and sediments as a stage in decontamination treatment. For the neutral and anionic surfactants, the interactions with sediments and soils include (1) sorption reactions of both the anionic and neutral surfactant, (2) precipitation reactions of anionic surfactant with calcium, and (3) aqueous phase micelle formation at high concentrations of both anionic and neutral surfactants. Results describing the significance of each of these processes for dodecylsulfate are given in the complete report.

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The complete report, entitled "Sorption of Ionizable Organic Compounds to Sediments and Soils," (Order No. PB91- 181 941/AS; Cost: \$15.00, subject to change) will be available only from:

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