EXPERIMENTAL AND THEORETICAL MODELING
EXPERTISE OF THE
ORGANIC AND INORGANIC ENVIRONMENTAL
GEOCHEMISTRY GROUPS

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Final Report:

Environmental Geochemistry (93-DE-064)

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Text:

We are combining the experimental and theoretical modeling expertise of the Organic and Inorganic Geochemistry Groups in the Earth Sciences Division to conduct research in environmental chemistry. Our objective is to provide the fundamental basis for the development of innovative soil and ground water remedial technologies applicable to cleaning-up the DOE complex.

We have focused our attention on a particular problem site as an analog for many other similar sites. We are using laboratory experiments and geochemical modeling to determine the fundamental behavior of non-aqueous phase liquid (NAPL) contaminants and their interaction with the inorganic/aqueous system and to evaluate site response to a variety of recovery techniques, focusing initially on dynamic stripping using steam. The key component of this proposal is the integral link between experiment and theory.

We are investigating the potential for in situ degradation *via* hydrous pyrolysis of petroleum distillates (alkanes and fatty acids) and the chlorinated hydrocarbons (TCA, TCE, etc.) that comprise the dominant constituents of solvents, machining fluids, etc. We are also investigating the impact of heat and the degradation products of the petroleum distillates and chlorinated hydrocarbons on reservoir mineral stability, complexation and transport of associated metal contaminants, and finally, methods to catalyze the chemical processes to maximize degradation. Our recent results in this area have been very encouraging.

We have found that TCA decomposes readily in O₂-free water to produce primarily acetic acid, HCl and 1,1-DCE at temperatures above about 80°C. At lower temperatures the uncatalyzed reaction proceeds, but more slowly. The anaerobic conditions that we used provide a lower limit for the degradation rate. We are now investigating the influence of catalysts, including the O₂ and minerals naturally present in soils, on the reaction path. Our goal for next year is to maximize the production of "benign"

products and eliminate the production of DCE.

The petroleum distillate-based solvents (alkanes + fatty acids) produce only "benign" products (short chain alkanes and carboxylic acids). This suggests that hydrous pyrolysis will provide a convenient mechanism for cleanup. TCE is found to be more refractory than TCA (requiring higher temperatures to pyrolyze), but producing similar products (HCl, acetic acid and 1,2-DCE). Our goal with TCE, like TCA, is to maximize the production of "benign" products and eliminate the production of DCE.

Our work to date has allowed us to develop experimental capabilities and an expertise in research areas that are the new mission areas of DOE. We have already attracted funding from existing programs for related research on the effects of petroleum products. We are also now in a position to submit a TTP to EM50 for a new project in *in situ* thermal remediation techniques.

Figure 1 Caption:

Destruction of TCA *via* hydrous pyrolysis

References:

Siskin, M. and Katritzky, A.R. (1991) Reactivity of organic compounds in hot water: Geochemical and technological implications. Science v. 254, p. 231-237.

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