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Fuzzy Systems Modeling of In Situ Bioremediation of Chlorinated Solvents

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Abstract. The full-scale in situ bioremediation demonstration conducted at DOE's Savannah River Site revealed a wide range of spatial and temporal variations of concentrations of VOCs, enzymes, and biomass in groundwater and vadose zone monitoring boreholes over the field site. One of the powerful modern approaches to analyze uncertain and imprecise data is based on the use of methods of fuzzy systems modeling. Using fuzzy modeling we analyzed the spatio-temporal TCE and PCE concentrations and methanotroph densities in groundwater to assess the effectiveness of different campaigns of air stripping and bioremediation, and to determine the fuzzy relationship between these compounds. Our analysis revealed some details about the processes involved in remediation, which were not identified in the previous studies of the SRS demonstration. We also identified some future directions for using fuzzy systems modeling, such as the evaluation of the mass balance of the vadose zone - groundwater system, and the development of fuzzy-ruled methods for optimization of managing remediation activities, predictions, and risk assessment.

Savannah River Bioremediation Experiment. In 1992-93, a large-scale vadose zone-groundwater bioremediation demonstration was conducted at the Savannah River Site by injecting several types of gases (ambient air, methane, and nitrous oxide and triethyl phosphate mixtures) through a horizontal well in the groundwater at a 175 ft depth. Simultaneously, soil gas was extracted through a parallel horizontal well in the vadose zone at a 80 ft depth (Hazen et al., 1997). Table 1 presents the regimes of remediation campaigns, involving in situ air stripping (Campaigns 1 and 2) and bioremediation (Campaigns 3-6). Groundwater samples were taken from 11 monitoring wells. According to the conventional statistical analysis of concentrations measured in all wells, the nitrous oxide and triethyl phosphate injection (Campaign 6) appeared to be the most efficient type of bioremediation (Hazen et al., 1997). The demonstration revealed significant special and temporal variations of VOCs, enzymes, and biomass in boreholes over the field site. An example of time variations of TCE concentration is shown in Figure 1. Such variations in concentrations make some of the results seem ambiguous and difficult to be used in describing spatio-temporal behavior of bioremediation processes over the field site.

Table 1. Types of injections and corresponding times

Campaign	Injection	Start date	End date	Duration (days)
1	No air injection - air extraction only	2/26/92	3/18/92	21
2	Air injection	3/19/92	4/20/92	32
3	1% CH4 and air	4/21/92	8/5/92	106
4	4% CH4 and air	8/6/92	10/23/92	78
5a	Long Pulsing CH4 and air	10/24/92	12/20/92	57
5b	Short Pulsing CH4 and air	12/21/92	1/25/93	35
6	Pulsing 4% CH4, air and continuous nitrous oxide and triethyl phosphate	1/26/93	5/1/93	95

The goal of this research is to evaluate the performance of in situ remediation of chlorinated solvents carried out at the Savannah River Site in 1992-93, using fuzzy systems modeling that is well suited to the analysis of imprecise and uncertain measurements of concentrations in monitoring wells, and to illustrate the directions of further application of this method for remediation.

Essential Features of Fuzzy Systems Modeling. Fuzzy systems modeling is an effective method to simulate the performance of a system that is uncertain because of vagueness or "fuzziness," which are inherent in the

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system behavior, rather than the randomness alone (Ross, 1995). Fuzzy theory is based on the process of "fuzzification" to generalize specific, crisp (or discrete) numbers to a continuous (fuzzy) form. A fuzzy set is considered to be a family of pairs $R=\{x, \mu_R(x)\}$, where x is the variable, and $\mu_R(x)$ is the membership function of x. For a particular data set, the continuous membership function ranges in [0,1], indicating a gradual degree of a possibility p for variable x to occur in fuzzy set R:

$$\mu_R(x) = p, \text{ for } 0<p<1, \text{ if } x \text{ partially belongs to } R$$

A fuzzy membership function can be determined from the probability density function (PDF) function for a real data set by normalizing the PDF to the maximum value of the PDF. Figure 2 illustrates the concept of a comparison of two fuzzy numbers. In this figure, an α-cut level indicates a minimum degree of membership that a crisp value must obtain before it becomes a member of the fuzzy set. The value of x for $\mu(x)\leq\alpha$ is not considered a member of fuzzy set R. Figure 2 illustrates a concept of fuzzy ranking (comparison) of fuzzy numbers using their FMFs.

Using concepts of fuzzy logic, the fuzzy system parameters can be characterized using linguistic terms such as small, medium, or high, etc. To determine fuzzy relationships between two fuzzy variables, we applied a method of Fuzzy C-Means clustering followed by the rule-based, Fuzzy Inference System (FIS) and Adaptive-Neuro-Fuzzy Inference System (ANFIS) analysis in the Fuzzy Logic Toolbox of Matlab®. This method partitions the data set of two fuzzy variables into clusters with particular membership functions for each of the clusters. The FMFs can then be used for predictions. One of the main advantages of the fuzzy logic approach is the use of the human, intuitive processes of conceptualization of imprecise properties of the object (Ross, 1995), which we also used in this study.

Assessing the effectiveness of bioremediation campaigns. The analysis revealed that there are two groups of wells with distinctly different concentrations of TCE: (1) Wells MHT 1C – 3C and 5C – 10, with the highest concentrations, and (2) Wells MHT 4 and 11 with much lower concentrations (see Figure 1). To determine FMFs, we used normalized PDFs, which were piece-wise approximated for α-cuts of 0, 0.1, 0.33, 0.66, and 1. Table 2 summarizes the results of pair-wise, fuzzy comparison between campaigns for PCE min, TCE min, and TCE concentrations. Figure 3 illustrates the results of comparison of fuzzy concentrations of TCE and PCE min (mineralization potential) between background conditions (BG), air stripping (Campaign 2) and bioremediation (Campaign 6). Concentrations corresponding to α < 0.1 can be considered noise and were not used in comparison. The results indicated that the air stripping (used during Campaigns 1 and 2) led to an initial decrease in the concentration of solvents, causing a decrease in the TCE min, but an increase in PCE min concentrations. Bioremediation activities (Campaigns 3-6) led to different patterns of changes in the TCE and PCE concentrations. Figure 3 shows that there are two different fuzzy membership functions for TCE and PCE mineralization for Campaign 6. The TCE mineralization decreased at some wells (solid red line), while it increased in other wells (dashed red line). The PCE mineralization only slightly increased in some wells (solid red line) and significantly increased in other wells (dashed red line).

Table 2. Comparison of fuzzy concentrations for TCE, PCE, TCE min, and PCE min (for Wells 1C-3C and 5C-10C)

Comparison of campaigns	**TCE min**	**PCE min E**	**TCE**
Background (BG) - C1	C1 < BG for α>0.5	C1 < BG for α>0.8	C1 > BG
C1 - C2	C2 ~ C1	C2 < C1 for α>0.4	C2 < C1 for α>0.5
C2 - C3	C3 > C2 for α>0.9	C3 ~ C2	C3 > C2 for α>0.5
C3 - C4	C4 < C3 for α>0.9	C4 < C3 for α>0.1	C4 > C3 for α>0.75
C4 - C5a	C5a < C4 for α<1	C5a > C4	C5a < C4 for α>0.8
C5a - C5b	C5b > C5a for α<1	C5b > C5a	C5b ~ C5a
C5a - C6	1 group - C6 > C5b 2 group - C6 > C5b	C6 > C5b C6 > C5b	C6 < C5b

Despite the overall trend of the increase in the methanotroph densities as the TCE concentration decreased during bioremediation (which indicates efficient results of bioremediation), these values varied significantly in different wells. As an example, Figure 4 shows a clustering approximation of a fuzzy graph (Zadeh, 1995) between the TCE concentration and methanotroph densities for a group of Wells 1C-3C and 5C-10C. These data were then used to crease a set of simple fuzzy *if-then* rules:

if TCE is high then methanotrophs is small
if TCE is medium then methanotrophs is medium
if TCE is small then methanotrophs is high.

with corresponding FMFs for the TCE and methanotroph concentrations, which are shown along the axes on Figure 4. These rules were then used in the Fuzzy Inference System created in the Fuzzy Logic Toolbox of Matlab® for predictions.

Conclusions and Future Research. Fuzzy modeling for the TCE, PCE and methanotroph concentrations measured in 11 monitoring groundwater monitoring wells confirmed main conclusions regarding the effectiveness of the in situ air stripping and bioremediation campaigns carried out during the SRS injection-extraction experiment. At the same time, our analysis revealed that fuzzy modeling is an effective approach to obtain a better understanding of the volume-averaged, temporal and spatial distribution of solvent concentrations. Fuzzy systems analysis can be used to supplement a conventional statistical (Pfiffner et al., 2000) and numerical (Travis and Rosenberg, 1994) analyses of bioremediation. Future analysis should reveal a set of *n*-dimensional fuzzy *if-then* rules using a combination of fuzzy logic and neural network methods (Nikravesh et al., 2000). Future research using these methods can also involve the evaluation of the mass balance of solvents and biota in the vadose zone - groundwater system, and the development of fuzzy-ruled methods for optimization of managing remediation activities, predictions, and risk assessment.

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References:

Hazen, T.C., K.H. Lombard, B.B Looney, M.V. Enzien, J.M. Dougherty, C.B. Fliermans, J. Wear, and C.A. Eddy-Dilek, Full scale demonstration of in situ bioremediation of chlorinated solvents in the deep subsurface using gaseous nutrient biostimulation, In: *Progress in Microbial Ecology*, M.T. Martins et al. (eds), pp. 597-604.

Nikravesh, M., R.D. Adams, R.A. Levey, Soft computing: Tools for intelligent reservoir characterization and (IRESC) and optimum well placement (OWP), *Journal of Petroleum Science and Engineering*, 882, 2000.

Pfiffner, S.M., A.V. Palumbo, T.J. Phelps, J.J. Beauchamp, D.B. Ringelberg, H.C. Pinkart, D.C. White, and T.C. Hazen, Microbial Monitoring as a measure of success for in situ TCE bioremediation, Submitted to *Environmental Science and Technology*, 2000.

Ross, T.J., *Fuzzy Logic with Engineering Applications*, New York: McGraw-Hill, 1995.

Travis, B.J, and N.D. Rosenberg, Numerical simulations in support of the in situ bioremediation demonstration at Savannah River, LANL Report, LA-12789-MS, 1994.

Zadeh, L. Fuzzy control, Fuzzy graphs, and Fuzzy inference, In: *Future Directions of Fuzzy Theory and Systems*, Y. Yam and K.S. Leung (eds.), pp. 1-9, Singapore, World Scientific, 1995.

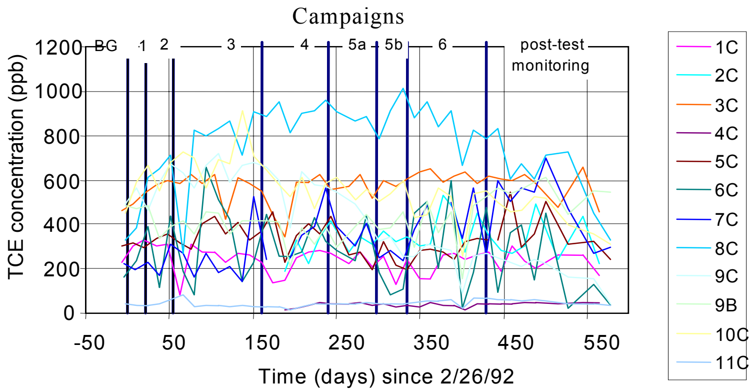

Figure 1. Time variations of TCE concentration in groundwater in 11 observation wells

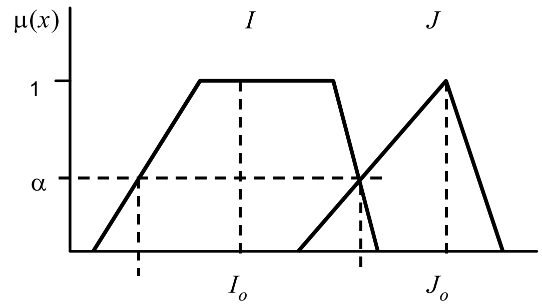

Figure 2. Comparison of two fuzzy numbers: $J > I$ for $\mu(x) > \alpha$ (I_o and J_o are crisp numbers)

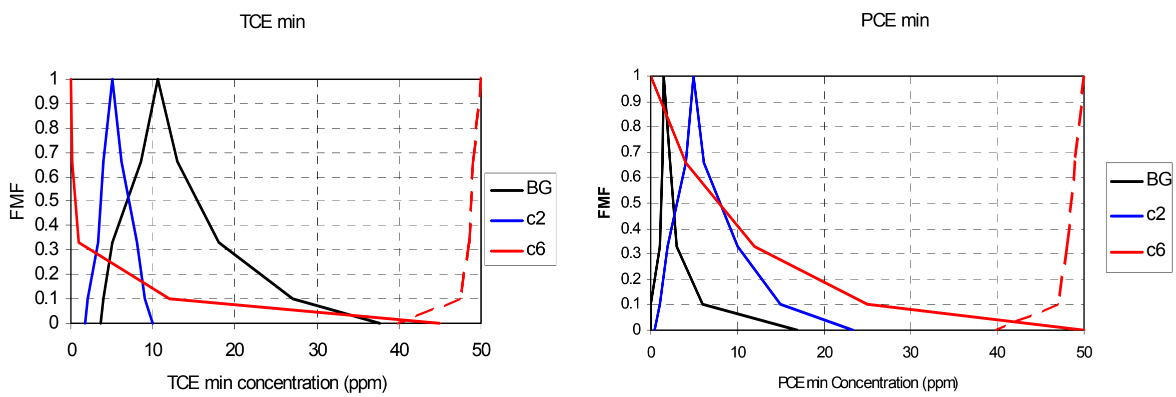

Figure 3. Fuzzy membership functions for TCE and PCE mineralization, which compare the performance of air stripping (Campaign 2 - c2) and bioremediation (Campaign 6 - c6) with background conditions (BG)

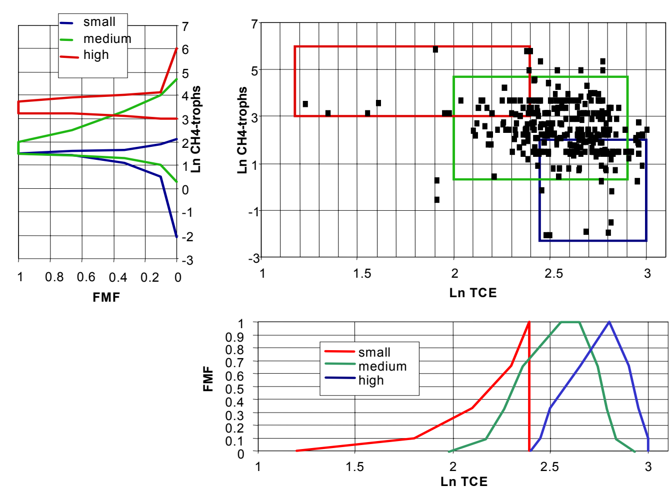

Figure 4. Fuzzy graph of the relationship between logarithms of TCE and methanotrophs concentrations for wells 1C-3C and 5C-10C and corresponding FMFs plotted parallel to the axes.