

Evaluation of Some New Tracers for Soil Water Studies¹

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ABSTRACT

Six anions which showed potential as tracers of soil water movement were evaluated in laboratory and field experiments. The anions included iodide (I^-), thiocyanate (SCN^-), and four fluorobenzoates: *m*-(trifluoromethyl)benzoic acid (*m*-TFMBA), *o*-(trifluoromethyl)benzoic acid (*o*-TFMBA), pentafluorobenzoic acid (PFBA) and 2,6-difluorobenzoic acid (2,6-DFBA). The sorption and mobility characteristics of the six potential tracers were compared to those of bromide (Br^-), which served as an index tracer in all experiments. Initial tracer concentrations ranged from 20 to 100 mg L⁻¹. The anions were quantified simultaneously in sub-mL samples of soil solution using a high performance liquid chromatography technique. Batch equilibrations (28 d), and breakthrough curves (7 to 10 d) in a 2.5-m column of loamy sand, under both ponded and trickle-irrigated conditions, indicated that all the tracers except SCN^- were conservative and were not sorbed. SCN^- was not retarded in the column studies but did show a negative mass balance, most likely due to chemical and/or biological transformation. Distribution of a tracer solution applied to a field soil was monitored for 69 d in soil water from suction samplers (1.0- and 1.8-m depth) and in extracts from core samples. SCN^- , I^- , and *m*-TFMBA showed reduced concentrations relative to Br^- at all sampling times and depths; *o*-TFMBA, PFBA, and 2,6-DFBA had distributions similar to that of Br^- . These latter three fluorobenzoates show promise as laboratory and field tracers of soil water, particularly where multiple tracing tests or totally exotic tracers are required.

Additional Index Words: anions, benzoates, bromide, fluorinated organics, iodide, solute transport, thiocyanate.

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TRACERS have long been used to follow the movement of soil water in the laboratory and in the field. Although the perfect chemical tracer probably does not exist, there are three main requirements for an effective soil water tracer: (i) the tracer should not be significantly sorbed or otherwise retarded by the soil of interest; (ii) the tracer should be exotic to the soil environment, or should be present naturally at low concentrations; (iii) the tracer should be conservative in that it is not significantly degraded chemically or biologically during the course of an experiment. Other considerations in choosing a tracer include ease of quantitation in a soil solution matrix, and the potential for adverse environmental impacts, particularly important if the tracer is to be used in unconfined field studies.

Many compounds have been used as tracers in soils, groundwater, and surface water. An excellent review of groundwater tracers has been provided by Davis et al. (1980). Among tracers used for monitoring surface and groundwater flow, many are unsuitable for use in soil water studies due to the greater surface activity and solid/water ratio of soils, which result in increased

sorption. Fluorescent dyes, such as the rhodamines, and other high molecular weight dyes are generally unsuitable soil water tracers for this reason (Smart and Laidlaw, 1977; Smettem and Trudgill, 1983). Tracers commonly used for soil water studies have included chloride (Cl^-), nitrate (NO_3^-), bromide (Br^-), and deuterated and tritiated water (HDO and HTO). Cl^- is a useful soil water tracer in soils lacking significant anion exchange capacity; however, Cl^- suffers the disadvantage of having high native concentrations (often exceeding several hundred mg L⁻¹) in many irrigation waters and soil solutions. NO_3^- is subject to an array of chemical and biological transformations which can cause it to be a nonconservative tracer under both aerobic and anaerobic conditions. Water molecules labelled with heavy isotopes of hydrogen are likely the most ideal soil water tracers. Unfortunately, deuterated water is expensive to use at required enrichment rates, and the mass spectroscopic analysis needed for greatest sensitivity is both time-consuming and costly. Tritiated water is inexpensive, and analysis by liquid scintillation counting is rapid and accurate; since it is radioactive, however, the use of HTO is precluded in most field studies. Of the common soil water tracers, Br^- is the most generally suitable. Br^- is usually present in natural waters at levels less than one percent of the Cl^- concentration (Davis et al., 1980), is not sorbed by most soils, and is not subject to chemical or biological transformations. In addition, Br^- is readily analyzed by several methods, including ion selective electrode (Abdalla and Lear, 1975; Onken et al., 1975; Orion Research, 1982), automated colorimetric detection (Moxon and Dixon, 1980; Pyen et al., 1980), and high performance liquid chromatography (Bowman, 1984; Pyen and Erdmann, 1983; Stetzenbach and Thompson, 1983). The first two techniques are subject to a variety of interferences, such as the presence of other ions or of colored materials, effects which tend to be exacerbated in soil solution extracts.

The present study was undertaken to evaluate some new compounds regarding their suitability as tracers in laboratory and field studies of soil water movement. The larger purpose was to identify a series of tracers which could be used to label successive pulses of irrigation water, and which could be analyzed simultaneously in small soil water samples using a single technique.

The tracers evaluated included two inorganic and four organic anions: iodide (I^-), thiocyanate (SCN^-), *m*-(trifluoromethyl)benzoic acid (*m*-TFMBA), pentafluorobenzoic acid (PFBA), *o*-(trifluoromethyl)benzoic acid (*o*-TFMBA), and 2,6-difluorobenzoic acid (2,6-DFBA). I^- was of interest because of its chemical similarity to Cl^- and Br^- , although potential conversion of I^- to one of a variety of oxidized species was anticipated due to the low oxidation potentials for these reactions (Cotton and Wilkinson, 1980). SCN^- was of interest since this anion has been successfully used as a ground-water tracer and to follow water movement in oil-bearing formations (Geo-

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logic Testing Consultants Ltd., 1983. Evaluation of ground water tracers for nuclear fuel waste management studies. Report prepared for Atomic Energy of Canada, Ltd.). Tamm and Troedsson (1957) used SCN^- to follow water movement in a forest soil, but they did not evaluate potential sorption or degradation of this ion. The four fluorinated benzoic acid derivatives (Fig. 1) seemed likely candidates as soil water tracers, based on results of groundwater studies and due to their apparent resistance to chemical and microbial degradation in natural environments. Malcolm et al. (1980) determined that benzoate was conservative in comparison with bromide in groundwater tracing tests. *m*-TFMBA and PFBA have been used successfully as groundwater tracers (Stetzenbach et al., 1982; McCray et al., 1983). *m*-TFMBA is being used as a water tracer in the Swiss national program for radioactive waste storage (NAGRA 1982a, 1982b) and by the U.S. Dep. of Energy at the WIPP site in southeastern New Mexico (H.W. Bentley, personal communication). The remaining organic anions, *o*-TFMBA and 2,6-DFBA, are readily available commercially, and were considered promising due to their chemical similarities to the other two fluorobenzoates (Fig. 1).

In the experiments described below, emphasis was placed on evaluating similarities among tracers in describing water movement for a given soil under a given set of conditions, rather than using the tracers to investigate a specific physical system. Bromide served as the index tracer for each experiment. A difference in sorption or mobility between Br^- and any of the other six tracers was taken as an indication of the unsuitability of that chemical as a soil water tracer under the given conditions.

MATERIALS AND METHODS

Initial concentrations were chosen such that the tracers could be accurately quantified after 100-fold dilution by soil solutions. The initial concentrations for all studies described below were 100 mg L^{-1} for Br^- ; 40 mg L^{-1} for I^- , SCN^- , and PFBA; 30 mg L^{-1} for 2,6-DFBA; and 20 mg L^{-1} for *m*-TFMBA and *o*-TFMBA. Tracer solutions were prepared in tap water (pH 7.2, electrical conductivity 0.89 dS m^{-1}). Si-

multaneous analyses of the seven tracers in samples of soil solution were performed using a high performance liquid chromatographic technique described earlier (Bowman, 1984). Injection volumes ranged from 25 μL to 100 μL .

Batch Sorption Studies

For the batch equilibrations, one set of samples and blanks was prepared at the tracer concentrations noted above, and another set prepared using a tenfold dilution of that solution. Aliquots (20 mL) of the tracer mixture were added to 10 g of loamy sand subsoil which underlies a Laveen loam (coarse-loamy, mixed, hyperthermic Typic Calciorrhids) in the Salt River Valley of Arizona. The cation exchange capacity and organic carbon content were 0.031 mol (Na^+) kg^{-1} and 0.05%, respectively. Samples were contained in 50 mL screwcap polypropylene centrifuge tubes. Blanks containing tracer but no soil, and blanks containing soil but no tracer, were also prepared. The supernatant pH of samples and blanks which contained soil was 7.4. All samples and blanks were prepared in triplicate for each equilibration period and tracer concentration. Tubes, stored in the absence of light at 20 to 25°C, were shaken by hand once daily to suspend the soil. After 1, 3, 7, 14, and 28 days equilibration, a set of samples and blanks at each initial concentration was centrifuged. The supernatant solutions were analyzed for tracer concentrations.

Column Mobility Studies

Relative mobilities of Br^- and the six tracers were observed in a laboratory soil column under both ponded and trickle irrigated conditions. Water fluxes were adjusted to simulate reasonable infiltration and redistribution rates. The column, which had been used previously for sewage effluent leaching experiments (Lance and Whisler, 1972), was 0.1 m in diam and packed with 2.5 m of loamy sand above a 0.06-m bed of pea gravel. Porous ceramic sampling ports had been installed at intervals, allowing determination of positive or negative pressure heads along the length of the column. The soil (Carrizo series, sandy-skeletal, mixed, hyperthermic Typic Torrifluvents) had a cation exchange capacity of 0.011 mol (Na^+) kg^{-1} , a clay content of 2.5%, and an organic carbon content of 1.5%. The soil had been packed to an average bulk density of 1.6 Mg m^{-3} . A drain equipped with a switching valve was located at the soil-gravel interface. The switching valve, connected to a timer, periodically diverted column effluent to an automatic fraction collector; the rest of the time, effluent was directed to waste. Effluent fractions were analyzed for their tracer concentrations. The pH of the effluent was 7.2 under both irrigation regimes.

For the ponded study, the column was initially wetted with tap water from the bottom. A constant head of 0.105 m was then maintained via a Mariotte syphon, and the column allowed to drain freely until a steady state outflow rate of 0.0363 m h^{-1} was obtained. Under these conditions, positive water pressures were present along the entire length of the column. The tap water leaching solution was replaced with tracer solution, and a 0.73-m pulse added to the column under the same hydraulic head. Following the tracer pulse, leaching with tap water was resumed.

For the trickle irrigated study, water was dripped on the soil surface using six 0.89-mm i.d. plastic tubes. Water input was provided by a peristaltic pump connected to a tap water reservoir. The column was loosely covered to minimize evaporation. At steady state, positive water pressures were present in a capillary fringe extending between 0.2 and 0.6 m above the column outlet. At greater elevations the column water was under negative pressure, as indicated by the lack of free water in the sampling ports. The steady state outflow

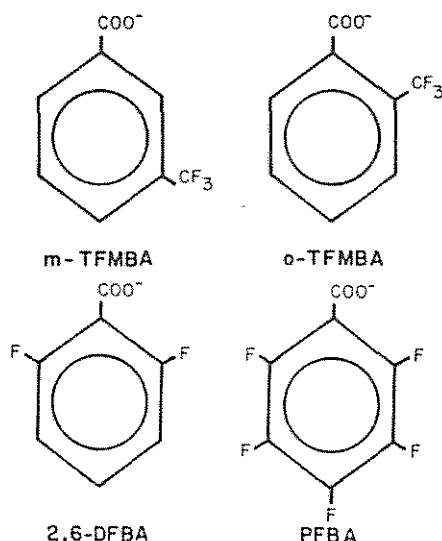


Fig. 1—Structures of the fluorinated benzoic acid derivatives.

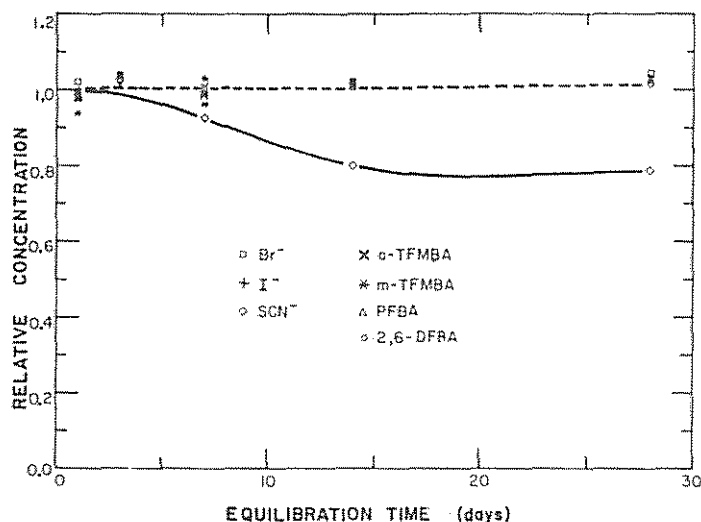


Fig. 2—Batch sorption study, no dilution. Initial concentrations: Br^- , 100 mg L^{-1} ; I^- , SCN^- , and PFBA, 40 mg L^{-1} ; 2,6-DFBA, 30 mg L^{-1} ; *m*-TFMBA and *o*-TFMBA, 20 mg L^{-1} . Plotted points are averages of three replicates.

rate was 0.0192 m h^{-1} . A 0.47-m pulse of tracer solution was added to the column at the same flux rate, after which leaching with tap water resumed. For this study only, the tracer mixture was enriched in deuterium at the rate of $0.67 \text{ mL D}_2\text{O}$ (99.8%) per liter of solution. This resulted in a δD value of $+4090$ for the Br^- solution, using Vienna Standard Mean Ocean Water (V-SMOW) as a reference. The tap water, used for leaching and tracer solution preparation, had a δD value of -64 (V-SMOW). Deuterium analyses were performed by mass spectroscopy.

Field Evaluation

A 2-m by 2-m field plot, separated from the surrounding soil by galvanized steel borders set 0.2 m into the ground, was established in a bermudagrass lawn on Avondale silty clay loam (fine loamy, mixed, hyperthermic Torrifluventic Haplustolls). The surface 0.15 m of the soil had a saturated paste pH of 7.9, a cation exchange capacity of $0.215 \text{ mol (Na}^+) \text{ kg}^{-1}$, and an organic carbon content of 0.97%. The clay percentage of the soil profile varied from 21 at the surface to a maximum of 42 at the 1.5-m depth.

The plot was instrumented with a neutron probe access tube set to a 2-m depth in the center of the plot, and with two porous ceramic suction samplers (0.025 m o.d. by 0.055 m in length), set to depths of 1.0 and 1.8 m using copper extension tubing. The samplers were placed opposite one another, each 0.3 m from the plot center. The ceramic samplers and the copper tubing had been previously shown not to sorb any of the tracers.

The plot was flood irrigated several times prior to tracer addition, resulting in a mean volumetric water content of 0.32 (range 0.30 to 0.34) between the surface and the 2-m depth. A 0.058-m pulse of tracer solution was then applied by flood irrigation. The plot was covered with plastic to minimize evaporation. An additional 0.2 m of unlabelled irrigation water was added to the plot by flooding 26 days after the tracer addition.

Soil water samples were collected daily for 69 days using the two suction samplers. Fourteen days after the tracer addition, core samples were taken at a single location 0.3 m from the plot center and equidistant from the suction sampler positions. Cores were collected at 0.05-m depth increments to a depth of 2 m using a 0.05-m diam bucket auger.

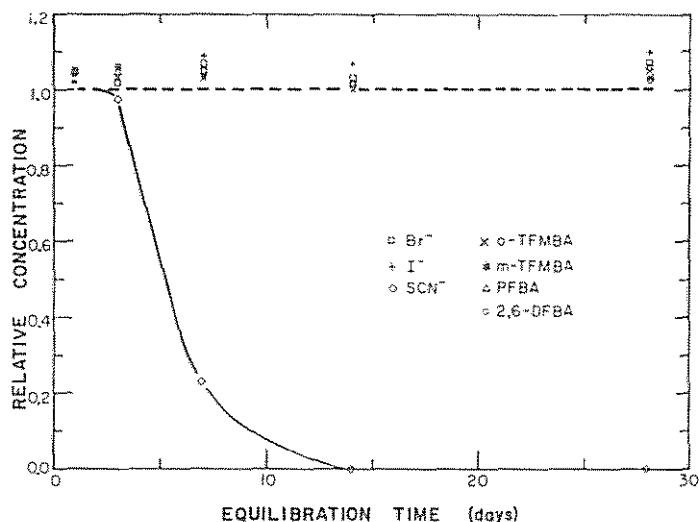


Fig. 3—Batch sorption study, tenfold dilution. Initial concentrations: Br^- , 10 mg L^{-1} ; I^- , SCN^- , and PFBA, 4 mg L^{-1} ; 2,6-DFBA, 3 mg L^{-1} ; *m*-TFMBA and *o*-TFMBA, 2 mg L^{-1} . Plotted points are averages of three replicates.

The water content of each core was determined on a subsample, and the remaining subsample used to prepare a saturation extract. Suction samples and core sample extracts were analyzed for tracer concentrations.

RESULTS AND DISCUSSION

Figures 2 and 3 show results of the batch sorption studies for the undiluted and tenfold diluted tracer concentrations, respectively. The data are plotted in terms of the relative concentration, C/C_0 (measured concentration at time of sampling divided by the initial concentration), vs. equilibration time. For each tracer except SCN^- , the relative concentration remained approximately 1.0 at both initial concentrations for 28 days. SCN^- began to show a loss in concentration in both systems within one week; in the more dilute solution, which had an initial SCN^- concentration of 4 mg L^{-1} (Fig. 3), the SCN^- level had fallen to zero within two weeks. The batch data therefore indicated that under saturated, anaerobic conditions, each of the tracers except SCN^- was stable with respect to chemical or biological degradation in the soil used for at least 28 days. SCN^- , on the other hand, was being sorbed and/or degraded.

Breakthrough curves (BTCs) for the ponded column experiment are shown in Fig. 4 and 5. These and the following BTCs are presented in terms of cumulative outflow rather than column pore volumes, due to the lack of precise column water content data. Figure 4 shows the six BTCs for Br^- and the other tracers except SCN^- . Each of the BTCs in Fig. 4 shows the same peak position and magnitude, indicating that the anions were not retained by the soil or were sorbed or excluded to an identical degree. The individual concentration measurements for Br^- , I^- , and the four fluoroorganics fluctuate about a single, mean BTC. BTCs for Br^- and SCN^- for the ponded column study are compared in Fig. 5. Although the same peak position was observed for both anions, the peak magnitude was lower for SCN^- . Mass recoveries for Br^- , SCN^- , and the other tracers are presented in Table 1.

$\delta \text{D} = \left[\frac{(\text{D}/\text{H})_{\text{tracer}}}{(\text{D}/\text{H})_{\text{reference}}} - 1 \right] \times 1000$.

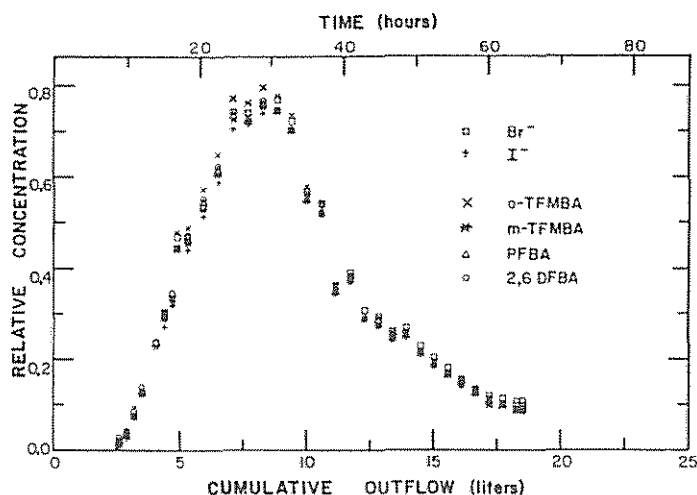


Fig. 4—Breakthrough curves for all the anions except SCN^- , ponded column study.

The mass balance calculations assumed a relative concentration of zero for each anion at a cumulative outflow of 25 L. The relative recoveries indicated a loss of SCN^- during flow through the ponded column. The recovery of SCN^- was only 94%, compared to recoveries of 99 to 105% for the other anions.

Loss of SCN^- , also seen in the batch equilibration study, was likely due to degradation rather than irreversible sorption, as indicated by the position of the SCN^- peak in relation to the other tracers (Fig. 5). Degradation of SCN^- appeared to be biologically me-

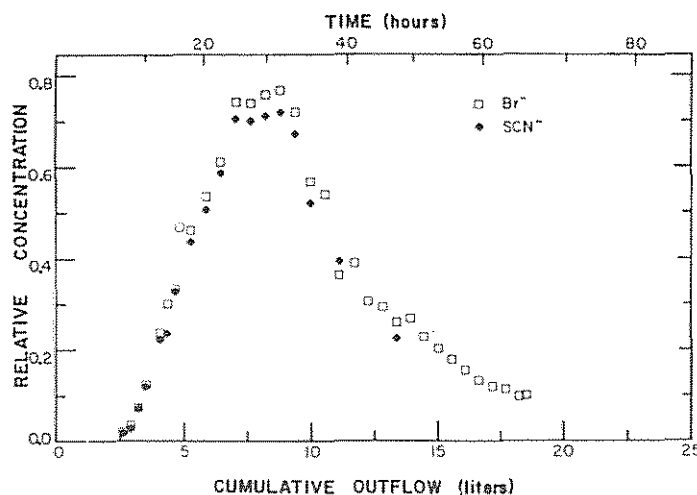


Fig. 5—Breakthrough curves for Br^- and SCN^- , ponded column study.

diated. Individual column effluent samples showed decreasing SCN^- levels over time. The low number of SCN^- points on the tail of the BTC (Fig. 5) resulted from loss of SCN^- when samples were stored at room temperature for more than a few hours prior to analysis. In contrast, tracer solutions which had no contact with soil (e.g., tracers made up in tap water) showed constant SCN^- levels over a period of months. Microorganisms present in the column effluent likely continued SCN^- degradation following elution from the soil.

Similar relationships among BTCs for the anions were seen under trickle irrigated conditions. The BTCs for all the anions except SCN^- are presented in Fig. 6. As in the ponded column experiment, Br^- , I^- , and the fluoroorganics yielded a single BTC. A comparison of BTCs for Br^- and SCN^- (Fig. 7) shows an even greater loss in mass of SCN^- than occurred under ponded conditions. Br^- and SCN^- peak positions were the same, however, indicating that the two anions moved through the column at the same average velocity. The recovery of SCN^- from this study was 85%, compared to recoveries of $106 \pm 1\%$ for the other 6 anions (Table 1). Recoveries of greater than 100% were

Table 1—Recoveries of tracers in laboratory column studies.

Tracer	Percent recovery	
	Ponded column	Trickle-irrigated column
Br^-	104	107
I^-	99.3	105
SCN^-	93.6	85.5
m-TFMBA	102	106
o-TFMBA	105	105
PFBA	104	106
2,6-DFBA	103	105
HDO	—	103

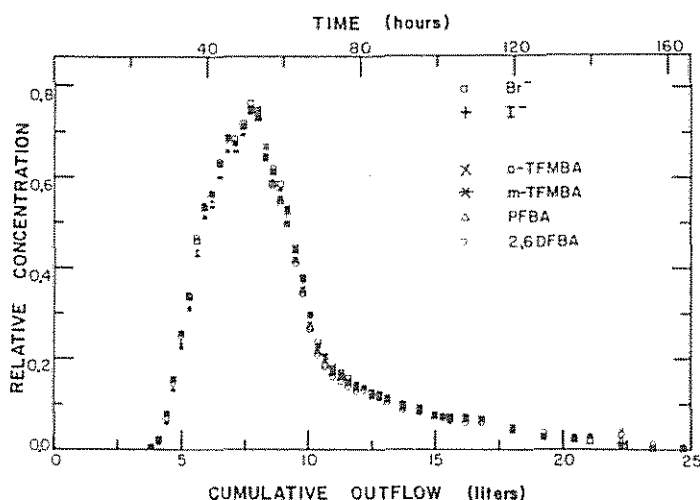


Fig. 6—Breakthrough curves for all the anions except SCN^- , trickle irrigated column study.

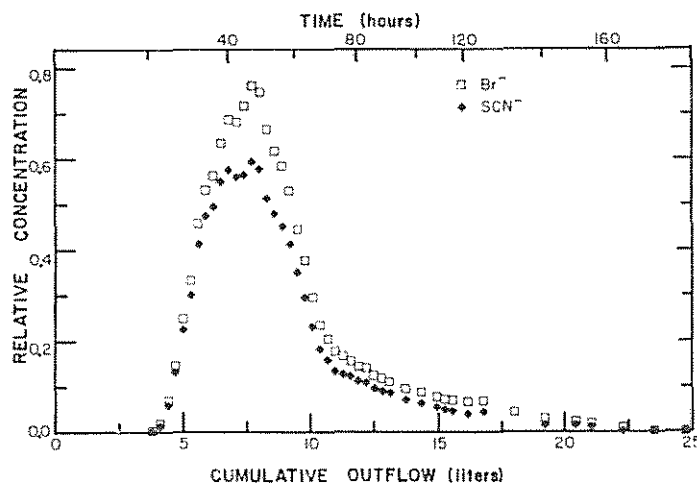


Fig. 7—Breakthrough curves for Br^- and SCN^- , trickle irrigated column study.

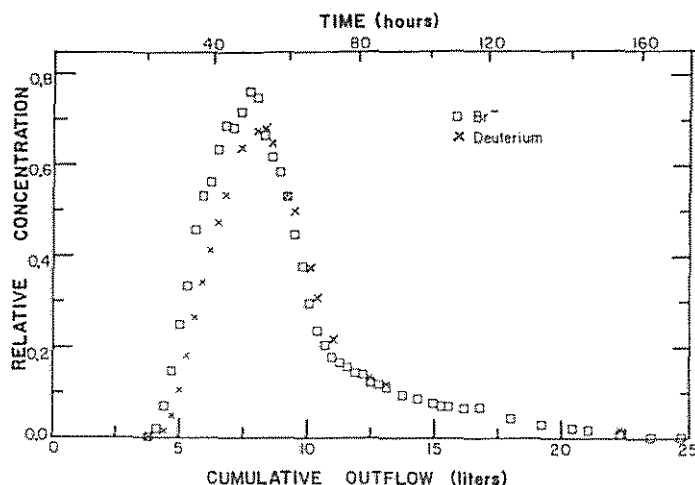


Fig. 8—Breakthrough curves for Br^- and HDO, trickle irrigated column study.

likely due to inaccuracies in quantifying the tracers at low relative concentrations. At these low levels, the chromatographic technique employed tends to yield elevated concentration measurements (Bowman, 1984).

The BTCs for Br^- and HDO in the trickle irrigated flow experiment are shown in Fig. 8. The BTC for Br^- was slightly accelerated relative to that for HDO, and yielded a higher, sharper peak. The broader HDO peak indicates greater dispersion of the uncharged tracer. The difference between the BTCs for HDO and Br^- (and for the other anionic tracers as well) is consistent with the occurrence of some anion exclusion in this soil. Such acceleration of an anion pulse compared to deuterated or tritiated water has been noted by others (Thomas and Swoboda, 1970; Krupp et al., 1972; McMahon and Thomas, 1974; van de Pol et al., 1977; Cameron and Wild, 1982). Figure 8 indicates that there was no sorption of the anionic tracers by this soil.

Precise water content data were not obtained for the ponded and trickle irrigated column experiments. Comparison of Fig. 4 and 6 indicates that water contents in the two studies did not differ greatly. The relative tracer concentrations in the column effluent reached values of 0.5 after 5.5 to 6.0 L of leaching, suggesting that the column pore volume was in this range in each case. The calculated column porosity (assuming a particle density of 2.75 Mg m^{-3}) was 0.42, translating to a column pore volume of 8.2 L at saturation. Thus, even under the ponded condition, the column was less than fully saturated. The greater loss of mass of SCN^- under trickle irrigated conditions was probably due to the longer column residence time, rather than to a difference in column aeration.

Field data for the relative concentrations of the seven anions from suction samples at the 1-m depth are presented in Fig. 9. The data show some similarities and some differences to the results of the laboratory studies. SCN^- disappeared rapidly in the field soil environment, being detectable only on the first sampling date, one day after tracer application. *o*-TFMBA, PFBA, and 2,6-DFBA yielded essentially identical BTCs during the 20-day period shown. These fluoro-

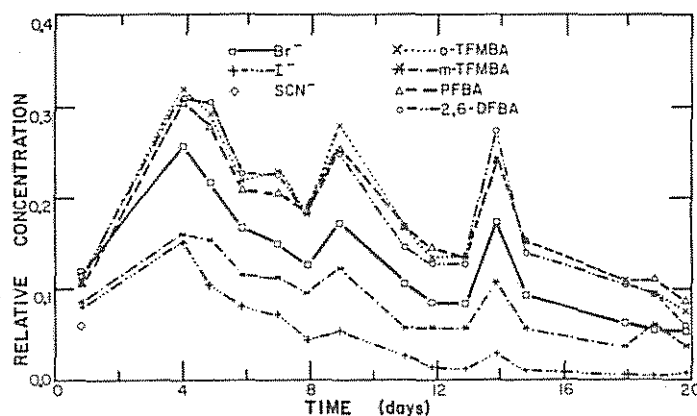


Fig. 9—Relative concentrations of the anions from suction samples at the 1-m depth in the field.

trations than Br^- . The reasons for the depressed Br^- level are not known; the Br^- curve, however, has the same shape as the *o*-TFMBA, PFBA, and 2,6-DFBA curves. The four tracers thus showed the same trends in water movement despite differences in peak magnitudes. *m*-TFMBA likewise showed the same variations in relative concentration over time, but with depressed magnitudes compared to Br^- and the other three fluoroorganics. This suggests possible degradation of *m*-TFMBA under field conditions.

I^- showed greatly reduced relative concentrations compared to Br^- and the fluoroorganics. After 12 days, the I^- level had fallen almost to zero at the 1-m depth, while the other tracers continued to show relative concentrations in the range 0.05 to 0.3.

Data for anion concentrations at the 1-m depth after 20 days, and at the 1.8-m depth for the entire 69-day sampling period (not presented), showed the same relationships among the tracers, although relative concentrations in each case were lower.

Extracts of the core samples from the field plot (Fig. 10) showed similar relationships among the fluoroorganics. In the plot position where the core samples were taken, most of the tracers remained near the soil surface two weeks after the tracer irrigation. This contrasts with the distribution obtained from the suction sampler data, where tracer concentrations began to

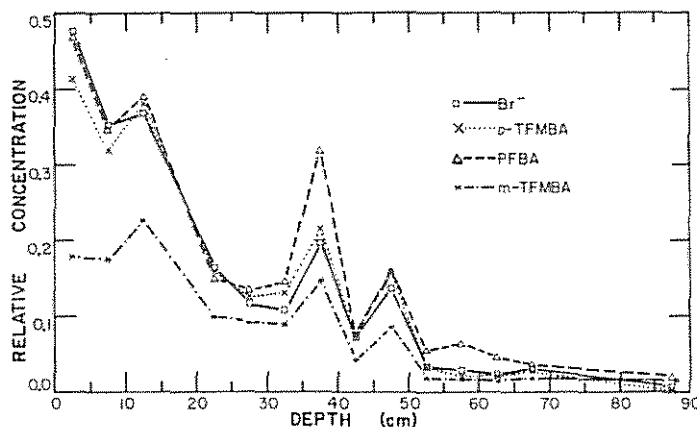


Fig. 10—Relative concentration vs. depth profile for Br^- , *o*-TFMBA, *m*-TFMBA, and PFBA in the field 14 days after tracer application, based on saturation extracts of core samples.

peak at the 1-m depth after four days (Fig. 9). The differences in tracer distribution were likely due to soil spatial variability and/or some short-circuiting of the tracer solution along the suction sampler during ponding. Br^- , *o*-TFMBA, and PFBA showed identical concentration distributions with depth in the core sample extracts. *m*-TFMBA, as in the suction sampler data, had a consistently lower relative concentration at all depths than did Br^- or the other fluoroorganics. 2,6-DFBA could not be accurately quantified in these samples due to interference from high NO_2^- levels, caused by conversion of NO_3^- to NO_2^- during saturation extract preparation (Bowman, 1984). Thus, no data for 2,6-DFBA are presented in Fig. 10. Neither SCN^- nor I^- were detectable in any of the core sample extracts.

The usefulness of the tracers evaluated here will vary depending upon the specific application. Since all of these species are anions, anion exclusion and tracer pulse acceleration can be anticipated in soils with high negative surface charge densities. Anion exclusion effects would be most pronounced at low soil water contents and low electrolyte concentrations. The fluoroorganic tracers, which are acids, could display increased sorption in soils with pH values closer to their acid dissociation constants. pK_a values for the fluorinated benzoic acid derivatives are presented in Table 2. The soils used in the studies described above all had pH values several units greater than the pK_a 's listed in Table 2, and thus the acids were present mainly in the anionic form. In soils with pH values below 6, a significant proportion of the *m*-TFMBA, *o*-TFMBA, and 2,6-DFBA (pK_a 's 3.5–3.8) would be present as the uncharged organic acid. PFBA (pK_a 1.74) would be predominantly anionic in all but the most acid soils. Sorption of the organic acids might also be greater in soils with high organic matter contents.

A consideration in the use of any chemical tracer is the magnitude of the solute diffusion coefficient in relation to the dispersion coefficient for water flow through the system. Table 2 presents aqueous diffusion coefficients for the tracers evaluated in this study. The diffusion coefficients of the fluoroorganic anions are about 40% of those for Br^- and I^- , and about 33% of that for HDO. In systems where molecular diffusion

represents a significant fraction of the hydrodynamic dispersion, the fluoroorganic compounds would be expected to predict lower dispersion coefficients relative to those determined using the smaller inorganic anions or labelled water.

At present there are little data available regarding the potential health risks associated with the four fluorobenzoates described here. Although no toxicity problems with these compounds are anticipated, they should not be used where their introduction into domestic water supplies is possible.

CONCLUSIONS

The results of the laboratory and field experiments lead to the following conclusions:

- 1) SCN^- is not a suitable soil water tracer even for short-term studies, due to rapid chemical and/or biological transformation.
- 2) I^- may be a useful tracer under laboratory conditions; however, I^- is lost rapidly under aerobic field conditions.
- 3) *m*-TFMBA, despite its usefulness as a ground-water tracer, should be used as a soil water tracer with caution. The data presented above indicate that *m*-TFMBA may not be conservative under aerobic field conditions.
- 4) *o*-TFMBA, PFBA, and 2,6-DFBA move with the soil water in a manner similar to Br^- , at least under the conditions of this series of experiments. These compounds should prove to very useful soil water tracers, particularly in field studies when multiple tracing tests or totally exotic tracers are desired.

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Table 2—Acid dissociation constants and aqueous diffusion coefficients of the tracers at 25°C.

Tracer	pK_a	Diffusion coefficient ($\text{m}^2 \text{s}^{-1} \times 10^{10}$)
Br^-	—	18.7§
I^-	—	18.7§
SCN^-	—	—¶
<i>m</i> -TFMBA	3.79†	7.4†
<i>o</i> -TFMBA	3.8†	7.3#
PFBA	1.49†	7.2†
2,6-DFBA	3.5†	7.6#
HDO	—	23.4††

† Walter (1982).

‡ Estimated by the Hammett correlation (Harris and Hayes, 1982). True value likely lower due to the "ortho effect" (Morrison and Boyd, 1966).

§ Value is for a 0.1M solution of the potassium salt (Chemical Rubber Co., 1983).

¶ No value available, but likely similar to the values of Cl^- , Br^- , and I^- ($18\text{--}19 \times 10^{-10} \text{ m}^2 \text{ s}^{-1}$).

Estimated by the Hayduk and Laudie method (Tucker and Nelken, 1982).

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