

COMPARISON OF TWO PESTICIDE LEACHING INDICES<sup>1</sup>*Ricardo Diaz-Diaz and Keith Loague<sup>2</sup>*

**ABSTRACT:** Agriculture is the leading cause of regional-scale nonpoint source (NPS) pollution in the world today. Indices of pesticide leaching in the vadose zone are well suited for estimating the spatial accumulation and distribution of NPS pollutants in the near surface. In this study the Attenuation Factor (AF) and the Leaching index (Li) are used to assess the near-surface leaching potential for 32 important agrochemicals for world average agricultural soil properties and recharge rates. The AF and Li indices both require the same input data and appear to work well for nonpolar chemicals. In the effort reported here the AF and Li indices produced similar results for the 32 agrochemicals. Pesticides with high and moderate leaching potential are identified. The AF estimates were more constant than the Li estimates for changes in the compliance depth and recharge rate. The AF index is simpler to use than the Li index and, therefore, is more likely to be employed in the future for screening/ranking agrochemicals relative to regional-scale NPS ground water vulnerability.

**(KEY TERMS:** Attenuation Factor (AF); ground water vulnerability; Leaching index (Li); nonpoint source (NPS) pollution; pesticide leaching.)

1987; Laskowski *et al.*, 1982; Meeks and Dean, 1990; Pettyjohn *et al.*, 1991; Teso *et al.*, 1988). For regulatory and/or remediation purposes, pesticide leaching indices can be very useful for screening and/or ranking the vulnerability of different agrochemicals relative to their potential to contaminate ground water and/or soil resources.

The objective of the work reported in this paper was to rank, with two indices, the near-surface leaching potential of the 32 well-known chemicals listed in Table 1 that are (or have been) used in association with agriculture. In this study, the Attenuation Factor (AF) (Rao *et al.*, 1985) and the Leaching index (Li) (Bacci and Gaggi, 1993) were used to make the leaching estimates. The AF index has seen considerable use in assessing regional-scale NPS ground water vulnerability in the past ten years. Li, on the other hand, is a relatively new index for assessing pesticide-leaching potential.

## INTRODUCTION

Agriculture is the leading cause of nonpoint source (NPS) pollution in the world today (Loague *et al.*, 1998). The ability to estimate the spatial accumulation and distribution of NPS pollutants in the near surface, resulting from regional-scale agriculture activities, is a task well suited for indices of pesticide leaching in the vadose zone (Corwin and Loague, 1996; Corwin *et al.*, 1997, 1999; NRC, 1993). Several pesticide-leaching indices have been reported in the literature (e.g., Gustafson, 1991; Jury *et al.*, 1983,

## MOBILITY INDICES

The two pesticide leaching indices (AF and Li) that were compared in this study are briefly described in this section. Readers interested in the complete development of the two indices are referred for AF to Rao *et al.* (1985) and Loague *et al.* (1990), and to Bacci and Gaggi (1993) and Diaz-Diaz *et al.* (1999) for Li. The units for each of the AF and Li input parameters are given in Tables 1 and 2.

<sup>1</sup>Paper No. 99092 of the *Journal of the American Water Resources Association*. Discussions are open until April 1, 2001.

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TABLE 1. Average Physicochemical and Partitive Properties for the 32 Agrochemicals Included in This Study (abstracted from Hornsby *et. al.*, 1996).

Chemical	P (Pa)	S (mg/L)	K <sub>oc</sub> (m <sup>3</sup> /kg)	t <sub>1/2</sub> (days)	MW (g/mol)
Alachlor (2-chloro-N-(2,6-diethylphenyl)-N-(methoxymethyl)acetamide)*	1.87x10 <sup>-3</sup>	240	0.17	15	269.8
Aldicarb (2-methyl-2-(methylthio)-propionaldehyde O-(methylcarbamoyl)oxime)*	4.00x10 <sup>-3</sup>	6000	0.03	30	190.3
Atrazine (2-chloro-4-ethylamino-6-isopropylamino-S-triazine)* <sup>1</sup>	3.85x10 <sup>-5</sup>	33	0.1	60	215.7
Bromacil (5-bromo-3-(sec-butyl)-6-methyluracil)*	4.13x10 <sup>-5</sup>	700	0.032	60	261.1
Carbaryl (1-naphthyl-N-methylcarbamate)*	1.60x10 <sup>-4</sup>	120	0.3	10	201.2
Carbofuran (2,3-dihydro-2,2-dimethyl-7-benzofuranyl-n-methylcarbamate)*	8.00x10 <sup>-5</sup>	351	0.022	50	221.3
Carboxin (5,6-dihydro-2-methyl-1,4-oxathiin-3-carboxanilide)*	2.40x10 <sup>-5</sup>	195	0.26	3	235.3
Chlorothalonil (tetrachloroisophthalonitrile)*	1.33x10 <sup>-1</sup>	0.6	1.38	30	265.9
Cyanazine (2[[[4-chloro-6(ethylamino)-S-triazin-2-yl]amino]-2-methylpropionitrile]*	2.13x10 <sup>-7</sup>	170	0.19	14	240.7
2,4-D (2,4-dichlorophenoxy acetic acid)*	1.07x10 <sup>-3</sup>	890	0.02	10	221.0
2,4-DP (butoxyethyl ester of (±) 2-(2,4-dichlorophenoxy)propanoic acid) <sup>1</sup>	4.00x10 <sup>-4</sup>	50	1	10	335.1
Dalapon (2,2 dichloropropionic acid (sodium salt))*	0.0	900000	0.001	30	165.0
DBCP (1,2-dibromo-3-chloropropane) <sup>1</sup>	1.20x10 <sup>2</sup>	1000	0.07	180	236.4
DCPA (dimethyl 2,3,5,6-tetrachloro-1,4-benzenedicarboxylate)*	3.33x10 <sup>-4</sup>	0.5	5	100	331.9
Diazinon (O, O-diethyl-O-(2-isopropyl-4-methyl-6-pyrimidinyl)phosphorothioate)* <sup>1</sup>	8.00x10 <sup>-3</sup>	60	1	40	304.3
Dicamba (2-methoxy-3,6-dichlorobenzoic acid)* <sup>1</sup>	0.0	400000	0.002	14	221.0
1,2-Dichloropropane (1,2-Dichloropropane)* <sup>1</sup>	6.67x10 <sup>3</sup>	2700	0.050	700	113.0
Dinoseb (2-sec-butyl-4,6-dinitrophenol)*	6.67x10 <sup>-3</sup>	52	0.03	30	240.2
Diphenamid (N,N-dimethyl-α-phenylbenzeneacetamide)*	4.00x10 <sup>-6</sup>	260	0.21	30	239.3
Disulfoton (O,O-diethyl S-[2-(ethylthio)ethyl]phosphorodithioate)*	2.00x10 <sup>-2</sup>	25	0.6	30	274.4
Diuron (3-(3,4-dichlorophenyl)-1,1-dimethylurea)* <sup>1</sup>	9.20x10 <sup>-6</sup>	42	0.48	90	233.1
EDB (1,2-dibromoethane) <sup>1</sup>	1.51x10 <sup>3</sup>	4300	0.034	100	187.9
Methomyl (S-methyl-N-(methylcarbamoyl)oxy-thioacetamidate)*	6.67x10 <sup>-3</sup>	58000	0.072	30	162.2
Metolachlor (2-chloro-N-(2-ethyl-6-methylphenyl)-N-(2-methoxy-1-methylethyl)acetamide)*	4.18x10 <sup>-3</sup>	530	0.2	90	283.8
Metribuzin (4-amino-6-(1,1-dimethylethyl)-3-(methylthio)-1,2,4-triazin-5(4H)-one)	1.33x10 <sup>-3</sup>	1220	0.06	40	214.3
Oxamyl (methyl 2-(dimethylamino)-N-[(methylamino)carbonyl]oxy-2-oxoethanimidodithioate)*	3.07x10 <sup>-2</sup>	282000	0.025	4	219.3
Prometon (6-methoxy-N,N'-bis(1-methylethyl)-1,3,5-triazine-2,4-diamine) <sup>1</sup>	1.03x10 <sup>-3</sup>	720	0.15	500	225.3
Prometryn (N,N'-bis(1-methylethyl)-6-(methylthio)-1,3,5-triazine-2,4-diamine) <sup>1</sup>	1.65x10 <sup>-4</sup>	33	0.4	60	241.4
Propazine (6-chloro-N,N'-bis(1-methylethyl)-1,3,5-triazine-2,4-diamine) <sup>1</sup>	1.75x10 <sup>-5</sup>	8.6	0.154	135	229.7
Simazine (2-chloro-4,6-bis(ethylamino)-s-triazine)* <sup>1</sup>	2.95x10 <sup>-6</sup>	6.2	0.13	60	201.7
Tebuthiuron (N-[5-(1,1-dimethyl)-1,3,4-thiadiazol-2-yl]-N,N'-dimethylurea)*	2.67x10 <sup>-4</sup>	2500	0.08	360	228.3
Trifluralin (2,6-dinitro-N,N-dipropyl-4-(trifluoromethyl)benzenemamine)*	1.47x10 <sup>-2</sup>	0.3	8	60	335.3

\*Identificated by U.S. EPA (1988) as high risk relative to ground water contamination; <sup>1</sup>Detected in ground water in California (Domagalski and Dubrovsky, 1992); P is the vapour pressure, S is the water solubility, K<sub>oc</sub> is the soil organic carbon/water partition coefficient, t<sub>1/2</sub> is the half-life in soil, and MW is the molar mass.

AF

The Attenuation Factor (AF), described by Rao *et al.* (1985), is defined as:

$$AF = \frac{M}{M_0} = \exp(-k \tau) = \exp\left(\frac{-0.69 d RF \theta_{FC}}{q t_{1/2}}\right) \quad (1)$$

where  $M$  is the mass leached to the depth  $d$ ,  $M_0$  is the initial mass applied,  $k$  is the first-order degradation rate coefficient,  $\tau$  is the advective transport travel time,  $d$  is the distance to a compliance depth from the surface,  $RF$  is the retardation factor,  $\theta_{FC}$  is the soil-water content at field capacity,  $q$  is the net recharge rate (taken here as the flux in the surface soil zone), and  $t_{1/2}$  is the pesticide half-life. Pesticide transformation is accommodated in  $AF$  using a first-order degradation approximation.  $RF$  is defined as:

$$RF = 1 + \frac{\rho_b f_{oc} K_{oc}}{\theta_{FC}} + \frac{n_a K_H}{\theta_{FC}} \quad (2)$$

where  $\rho_p$  is the soil bulk density,  $f_{oc}$  is the soil organic carbon,  $K_{oc}$  is the pesticide sorption coefficient,  $n_a$  is the soil air-filled porosity (i.e.,  $n_a = n - \theta_{FC}$ ),  $n$  is the soil porosity (i.e.,  $n = 1 - \rho_b/\rho_p$ ),  $\rho_p$  is the particle density,  $K_H$  is the dimensionless Henry's constant (i.e.,  $K_H = 1/RT \cdot P/S$ ),  $R$  is the universal constant for an ideal gas (i.e.,  $8.314 \text{ Pa m}^3 \text{ Mol}^{-1} \text{ K}^{-1}$ ),  $T$  is the temperature (taken here as  $293 \text{ }^\circ\text{K}$ ),  $P$  is the vapor pressure, and  $S$  is the water solubility. The second and third terms in Equation (2) are related, respectively, to sorption and volatilization. The simplifying assumptions and major limitations of the  $AF$  index are given by Kleveno *et al.* (1992), Loague *et al.* (1990), and Rao *et al.* (1985).

Li

The Leaching index (Li), described by Bacci and Gaggi (1993), is defined as:

$$Li = \frac{LM_t}{M_0} = \frac{J_{L(0)}}{M_0 k_{dis}} [1 - \exp(-k_{dis} t)] \quad (3)$$

where  $LM_t$  is the mass leached from a soil layer in the time interval  $t_2 - t_1$ ,  $J_{L(0)}$  is the initial leaching flux from the soil surface, and  $k_{dis}$  is the disappearance rate constant. The  $LM_t$  term in Equation (3) is defined as:

$$LM_t = \int_{t_1}^{t_2} J_{L(t)} dt = \frac{J_{L(0)}}{k_{dis}} [\exp(-k_{dis} t_1) - \exp(-k_{dis} t_2)] \quad (4)$$

where  $J_{L(t)}$  is the mass flux leached (assuming first-order kinetics) at time  $t$ , as:

$$J_{L(t)} = J_{L(0)} \exp(-k_{dis} t) \quad (5)$$

The two variables determining  $Li$  are  $J_{L(0)}$  and  $k_{dis}$ . The  $J_{L(0)}$  and  $k_{dis}$  terms are defined as:

$$J_{L(0)} = \frac{M_0}{V_T Z_T} q \frac{S}{P} \quad (6)$$

and

$$k_{dis} = \frac{\ln 2}{t_{1/2}} + \frac{q}{V_T Z_T} \frac{S}{P} + \frac{D_v}{V_T Z_T} \quad (7)$$

where  $V_T$  is the total volume,  $Z_T$  is the total fugacity capacity, and  $D_v$  is the volatilization reaction parameter. The three terms in Equation (7) are related, respectively, to the reaction, leaching, and volatilization processes. Sorption is accounted for in Equation (7) in both the second and third terms.

According to the fugacity approach (Mackay, 1991), the concentration of a given chemical in a given compartment (i.e., air, water, and organic matter) is equal to the product of its escaping tendency (from the compartment) and the fugacity capacity. At equilibrium, the fugacity (i.e., escaping tendency) is the same for all communicating compartments (Diaz-Diaz *et al.*, 1999). The  $V_T$  and  $Z_T$  terms in Equations (6) and (7) are defined as:

$$V_T = [(A d n_a) + (A d \theta_{FC}) + (A d f_{oc}) + (A d (1 - n - f_{oc}))] \quad (8)$$

$$Z_T = \left[ \frac{1}{RT} + \frac{S}{P} + \left( \frac{S}{P} K_{oc} \rho_b \right) + \left( \frac{S}{P} K_{mn} \rho_b \right) \right] \quad (9)$$

where  $A$  is the soil surface area, and  $K_{mn}$  is the soil mineral matter/water partition coefficient. The four terms in Equations (8) and (9) are related, respectively, to the air, water, organic matter, and mineral matter components. The fourth term in Equation (9) is taken as zero in this study as only nonpolar chemicals

are considered. The complete development of the  $D_v$  term (i.e., from Jury *et al.*, 1984) in Equation (7) is given by Diaz-Diaz *et al.* (1999).

The Li index, as used in this study, is based upon a constant time interval. Our selection of a one-year time interval is based on the assumption that this duration is sufficient to eliminate more than 90 percent of the residues of most chemicals from the surface soil layer. The simplifying assumptions and major limitations of Li are given by Bacci (1994), Diaz-Diaz *et al.* (1999), and Mackay (1991).

### Summary

The AF and Li indices both represent mass emission from surface soils, assuming first-order chemical decay during vertical transport. The AF and Li indices both represent fractions of applied mass and, therefore, they are dimensionless. The AF index is derived by assuming piston flow and zero mixing, while the Li index results from the assumption of perfect mixing in the leaching zone. AF represents the mass fraction that will eventually leach past the compliance depth, while Li represents the mass fraction moving past the compliance depth within a one-year period after application. It should be pointed out that although Li is a more process-based approach than AF, both indices require the exactly the same input data. The range of possible values for both AF and Li is between zero and one. The larger the value of an AF or Li estimate, the more likely it is that more of the chemical will leach past the compliance depth.

### DATA

#### Pesticides

Table 1 lists the chemical formulae for the 32 agrochemicals included in this study. Twenty-six of the chemicals listed in Table 1 were selected for this effort because they have been classified (U.S. EPA, 1988) as high risk relative to ground water contamination. The remaining six chemicals listed in Table 1 were selected for this study because they have been detected in ground water in California (Domagalski and Dubrovsky, 1992). The physicochemical and partitive properties (abstracted from Hornsby *et al.*, 1996), which are required as input to the AF and Li indices, are summarized in Table 1 for all 32 chemicals.

There are six ionizable chemicals listed in Table 1 (i.e., Bromacil, 2,4-D, 2,4-DP, Dalapon, Dicamba, and Dinoseb). These six chemicals all have acid properties

and, therefore, they are each dissociated to form anions at the pHs commonly found in agricultural soils. For the six anionic compounds included in this study, the sorption of the nonionized form is what is assumed to be significant.

#### Soils, Recharge, and Compliance Depth

The world average agricultural soil properties used in this study, based upon the unit world environment approach of Mackay (1991), were taken from Bacci (1994). The *base case* recharge rate used for all the AF and Li estimates in the work reported here was 2.0 mm/day (Bacci, 1994). The *base case* compliance depth ( $d$ ) was conservatively set in this study to be 0.1 m (Bacci, 1994). Table 2 lists the values used for the physical and hydrologic parameters for the AF and Li estimates reported in this study.

TABLE 2. Physical and Hydrologic Parameters and Values Used in This Study for Calculating the AF and Li Indices (Bacci, 1994).

Parameter	Value	Index
$d$ (L)	0.1 m	AF, Li
$A$ ( $L^2$ )	1 m <sup>2</sup>	Li
$q$ ( $LT^{-1}$ )	2 mm/day	AF, Li
$f_{oc}$ (dimensionless)	0.01	AF, Li
$\theta_{FC}$ (dimensionless)	0.1	AF, Li
$\rho_b$ ( $ML^{-3}$ )	1,325 kg/m <sup>3</sup>	AF, Li
$\rho_p$ ( $ML^{-3}$ )	2,650 kg/m <sup>3</sup>	AF, Li

Note:  $d$  is the soil layer depth of interest,  $A$  is the soil surface area,  $q$  is the recharge rate,  $f_{oc}$  is the soil organic carbon,  $\theta_{FC}$  is the volumetric fraction of soil-water content at field capacity,  $\rho_b$  is the soil bulk density, and  $\rho_p$  is the soil particle density.

### RESULTS AND DISCUSSION

Table 3 is a ranked list of AF and Li estimates, with volatilization, for the 32 chemicals in Table 1 for the world average standard soil properties and recharge rates given in Table 2. Table 4 is similar to the ranked list of AF and Li estimates in Table 3, but without volatilization. Inspection of Tables 3 and 4 leads to two general observations:

- There is (as should be expected) tremendous variability in the estimates of AF and Li for the 32 different agrochemicals.

• The differences in the ranked order of AF and Li for 1,2-Dichloropropane, DBCP, and EDB are due to volatilization. With no volatilization, the ranked order of the AF and Li estimates for the 32 chemicals confirm each other.

*Vulnerability Assessments*

Estimates of AF and Li, for world average agricultural soil properties (Mackay 1991; Bacci, 1994), are

plotted against each other at different soil-water contents in Figure 1. Inspection of Figure 1 shows that, in general, there are two linear results, which can be associated with high leaching (left to right) and moderate leaching (far left) chemicals. A total of 21 chemicals (with AF > 0.02 and Li > 0.2) are associated with high leaching in Figure 1 (also see Table 4). All of these chemicals have been frequently detected in ground water (Barbash and Resek, 1996). Of course, any classification, such as the scheme used here to assess vulnerability with the AF and Li indices, is

TABLE 3. Ranked List of AF and Li Estimates for the 32 Agrochemicals Included in This Study With Volatilization.

AF	Li
1,2-Dichloropropane	0.961
Tebuthiuron	0.894
Dalapon	0.877
Prometon	0.865
EDB	0.823
DBCP	0.820
Carbofuran	0.762
Bromacil	0.739
Dicamba	0.731
Propazine	0.577
Aldicarb	0.563
Dinoseb	0.563
Metribuzin	0.461
Atrazine	0.439
Simazine	0.349
Metolachlor	0.347
Methomyl	0.296
2,4-D	0.282
Diuron	0.083
Prometryn	0.044
Diphenamid	0.036
Oxamyl	0.024
Alachlor	0.004
Cyanazine	0.002
Disulfoton	9.2x10 <sup>-05</sup>
Diazinon	9.5x10 <sup>-06</sup>
Carbaryl	7.4x10 <sup>-07</sup>
Chlorothalonil	5.9x10 <sup>-10</sup>
DCPA	1.0x10 <sup>-10</sup>
Carboxin	1.7x10 <sup>-18</sup>
2,4-DP (Dichlorprop)	8.1x10 <sup>-21</sup>
Trifluralin	2.4x10 <sup>-27</sup>

TABLE 4. Ranked List of AF and Li Estimates for the 32 Agrochemicals Included in This Study Without Volatilization.

AF	Li
1,2-Dichloropropane	0.963
Tebuthiuron	0.894
Dalapon	0.877
Prometon	0.865
EDB	0.826
DBCP	0.821
Carbofuran	0.762
Bromacil	0.739
Dicamba	0.731
Propazine	0.577
Aldicarb	0.563
Dinoseb	0.563
Metribuzin	0.461
Atrazine	0.439
Simazine	0.349
Metolachlor	0.347
Methomyl	0.296
2,4-D	0.282
Diuron	0.083
Prometryn	0.044
Diphenamid	0.036
Oxamyl	0.024
Alachlor	0.004
Cyanazine	0.002
Disulfoton	9.2x10 <sup>-05</sup>
Diazinon	9.5x10 <sup>-06</sup>
Carbaryl	7.4x10 <sup>-07</sup>
Chlorothalonil	6.0x10 <sup>-10</sup>
DCPA	1.0x10 <sup>-10</sup>
Carboxin	1.7x10 <sup>-18</sup>
2,4-DP (Dichlorprop)	8.1x10 <sup>-21</sup>
Trifluralin	2.5x10 <sup>-27</sup>

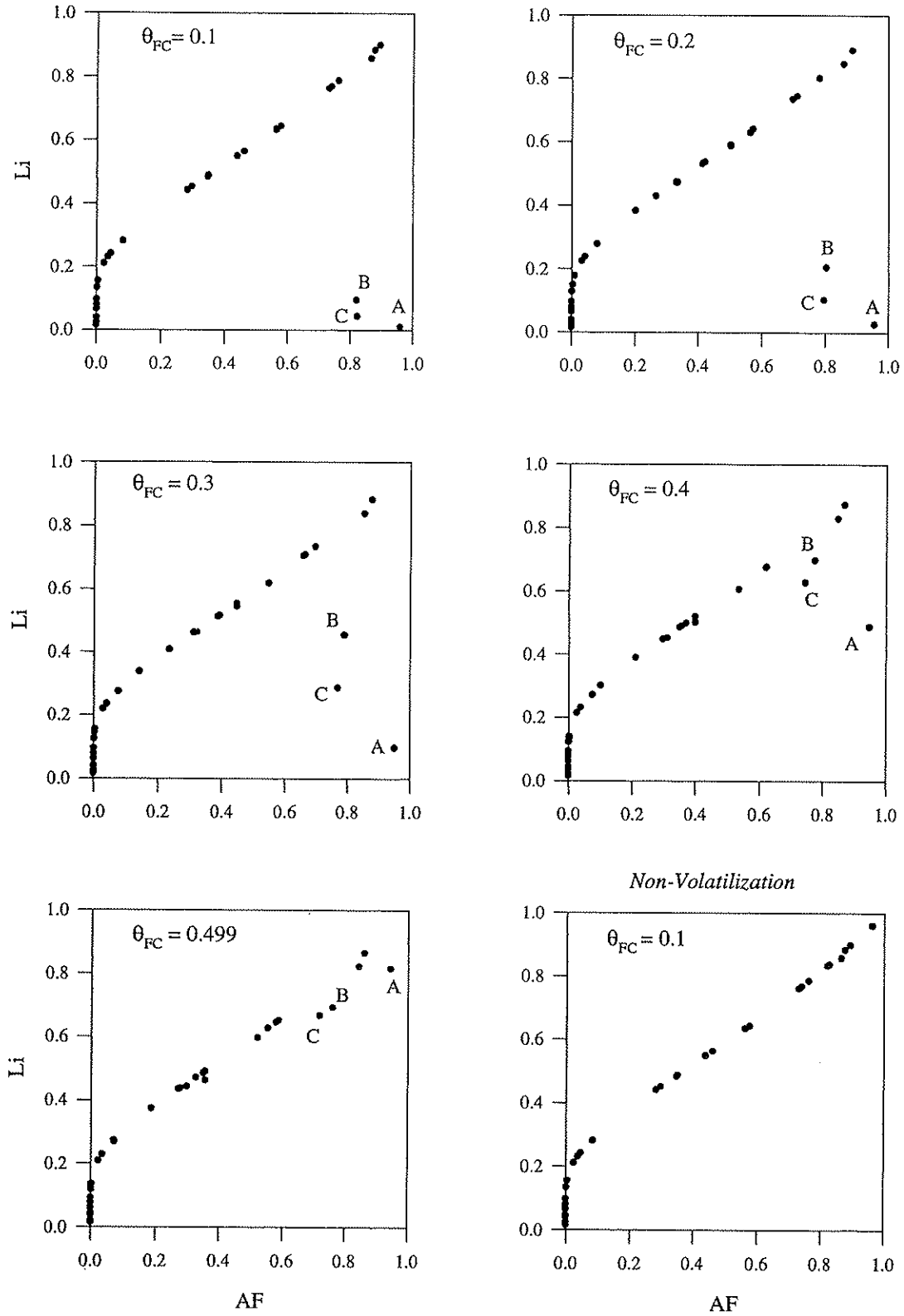


Figure 1. AF and Li Estimates for the World Average Standard Soil Properties and Recharge Rate Given in Table 2 [with volatilization, plotted against each other for five different soil-water contents (i.e., between 0.1 and 0.499) and at a soil-water content of 0.1 without volatilization.] The points A, B, and C are: (A) 1,2-Dichloropropane, (B) DBCP, and (C) EDB.

arbitrary and indicates only the relative likelihood of contamination.

The pesticides with high leaching potential in Figure 1, in general, have long half-lives, high water solubility, and are nonvolatile. The three outliers in Figure 1 (i.e., 1,2-Dichloropropane, DBCP, and EDB) each have a high vapor pressure and water solubility (see Table 1) and, as should be expected, correspond well with the other leachable compounds as soil-water content increases. The value of the dimensionless air/water partition coefficient ( $K_H$ ), for the three outliers in Figure 1 (i.e., 1,2-Dichloropropane = 0.114, DBCP = 0.012, and EDB = 0.027), indicates how far each of these chemicals is from the overall linear relationship. It should be pointed out that for assessment purposes, volatilization can be ignored for 1,2-Dichloropropane, DBCP, and EDB, each of which is a soil fumigant, applied to the soil via injection to reduce volatility.

#### *Compliance Depth and Recharge*

The *base case* compliance depth ( $d$ ) of 0.1 m used in this study for both AF and Li was somewhat of an arbitrary value (taken from Bacci, 1994). Other depths could have been selected. For example, 0.25 m could have been used to represent an average arable depth, or 0.5 m could have been used to represent an average root zone depth. Figure 2 shows a comparison of the AF versus Li results with and without volatilization using 0.25 and 0.5 m for the compliance depth. The plots in Figure 2 show the same two linear results as already seen in Figure 1 for the *base case* (i.e.,  $d = 0.1$  m). In Figure 2, the numerical values for both indices are obviously smaller with compliance depths of 0.25 and 0.5 m. The overall ranking of the chemicals does not change with the different compliance depths with the AF index. The chemical ranking does change for Li with different compliance depths. However, these changes are minimal, affecting only those chemicals with similar *base case* Li estimates. One can easily see, when comparing Figure 2 with Figure 1, that there are two new outliers when the 0.25 and 0.5 m compliance depths are considered (i.e., Prometon and Tebuthiuron). These pesticides, *albeit* very different than 1,2-Dichloropropane, DBCP, and EDB (see Table 1), can also be considered as extremes due to their properties [e.g., long half-life ( $t_{1/2}$ ) and high water solubility ( $S$ )]. For the *base case* recharge rate of 2.0 mm/day, 1,2-Dichloropropane, DBCP, and EDB move up in the overall ranking for the larger compliance depths (i.e., less volatilization with depth).

The impact of using 2.0 mm/day as the *base case* recharge rate in this study was investigated by also considering 0.5 and 4.0 mm/day recharge rates for the AF and Li indices for the 32 agrochemicals. For AF, the ranking of the chemicals did not change with changes in the recharge rate. The AF values were, as should be expected, larger for the greater recharge rates. For Li, the ranking of the chemicals did change with changes in the recharge rate (i.e., with larger recharge, there was less sorption with the same  $K_{oc}$ ). The changes in ranking were, however, only minimal, affecting only those chemicals with similar *base case* Li estimates.

In general, the effect of the compliance depth and the recharge rate were found to be the same for the AF and Li estimates in this study. For example, a greater compliance depth with more recharge has (generally) the same impact, in terms of either an AF or Li estimate, as a shallower compliance depth with less recharge. Therefore, it appears that estimates from either the AF and Li indices can be scaled to the compliance depth and/or recharge rate.

#### *AF Versus Li*

The AF and Li indices are best utilized for non-polar chemicals. Li is a more process-based representation of pesticide leaching behavior than AF, using the fugacity approach (i.e., equilibrium partitioning). Based solely upon the mathematical gymnastics of the two indices, AF is a simpler method to use than Li for assessing pesticide leaching potential. In general, for the chemical properties, soil characteristics, and recharge rates considered in this study, the AF and Li estimates of leaching potential are the same. The similar results for AF and Li suggest that it may be sufficient to use the AF index (in lieu of Li) for the extension to regional-scale ground water vulnerability assessments of the type reported by Diaz-Diaz *et al.* (1999) and Diaz-Diaz and Loague (2000).

#### *Uncertainty*

The AF and Li indices should only be used to screen and/or rank the approximate leaching potential of agrochemicals of concern. The assessment of regional-scale NPS pollution vulnerability rests upon chemical, recharge, and soils data that are all extremely sparse and contain considerable uncertainty (e.g., Foussereau *et al.*, 1994; Loague *et al.*, 1996; Nofziger *et al.*, 1996). For a given location, it is possible to estimate the uncertainty in assessments

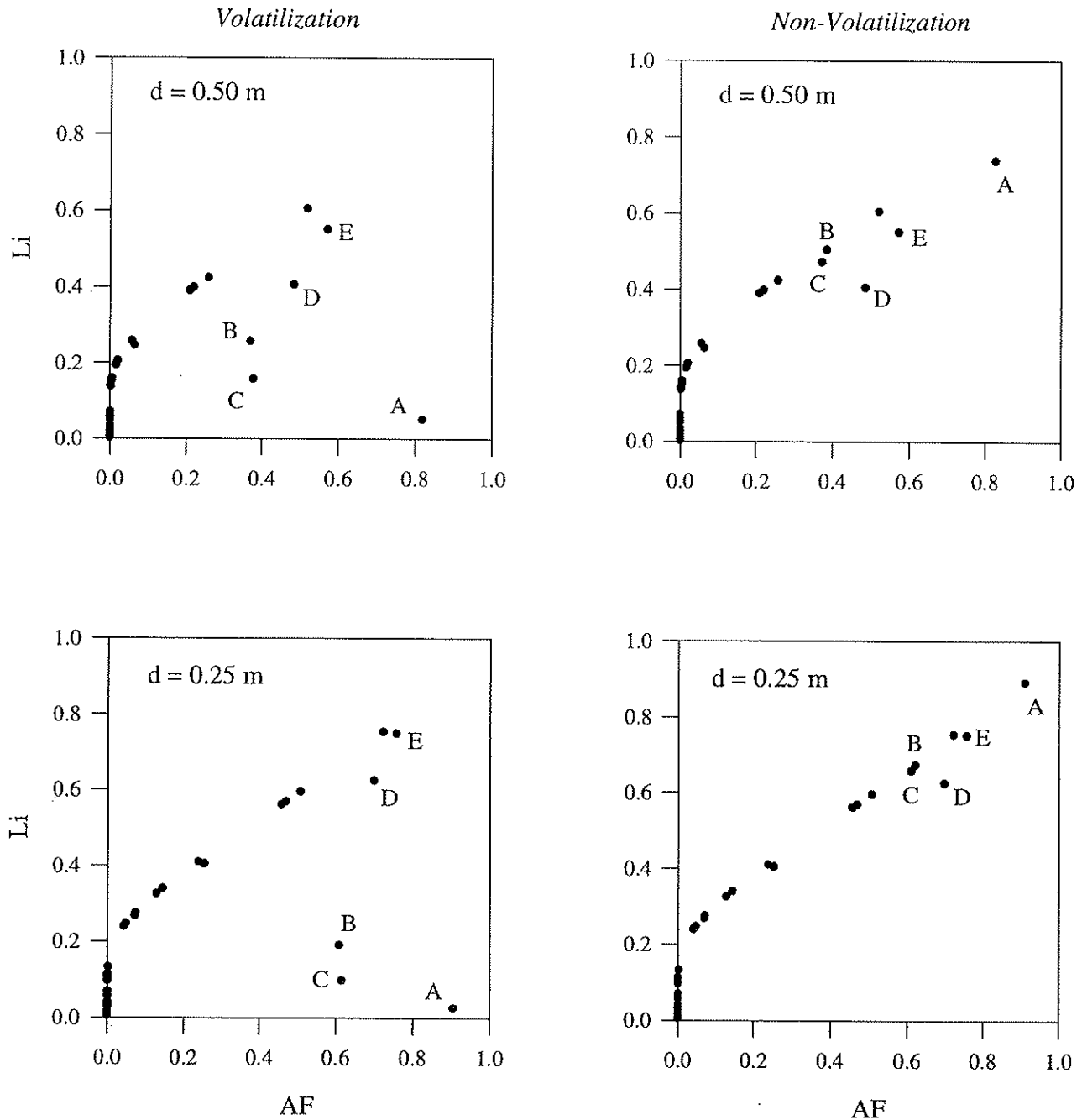


Figure 2. AF and Li Estimates for the World Average Standard Soil Properties and Recharge Rate Given in Table 2 [plotted against each other, with and without volatilization, and for two different compliance depths (0.25 and 0.5 m)]. The points A, B, C, D, and E are: (A) 1,2-Dichloropropane, (B) DBCP, (C) EDB, (D) Prometon, and (E) Tebuthiuron.

of chemical leaching with either the AF and Li indices given information on the uncertainties in the chemical, recharge, and soils data. For example, such assessments have recently been made using first-order uncertainty analysis, for the Canary Island of Tenerife with the AF index (Diaz-Diaz *et al.*, 1999) and with the Li index (Diaz-Diaz and Loague, 2000).

## CONCLUSIONS

In the effort reported here for 32 important agrochemicals, the AF and Li indices of pesticide leaching potential produced comparable results. Based upon the AF and Li results, the relative leaching vulnerability for the 32 chemicals was quantitatively

assessed. These results facilitated the division of the 32 different chemicals into two general classes – high leaching potential and moderate leaching potential.

The AF estimates were more constant, than the Li estimates for changes in the compliance depth and recharge rate. The AF and Li indices have the same results for normal chemical properties [i.e., the half-life in soil ( $t_{1/2}$ )], the soil organic carbon/water partition coefficient ( $K_{oc}$ ), the vapor pressure (P), and the water solubility (S). The AF and Li results are different for chemicals with extreme properties [e.g., those with very high vapor pressure (1,2-Dichloropropane, DBCP, and EDB)] or those with high water solubility and soil organic carbon/water partition coefficients (Prometon and Tebuthiuron).

The AF and Li indices work well for nonpolar chemicals. Both indices require exactly the same chemical, recharge, and soils data. The range of use is greater for Li than for AF, as Li is a more process-based approach. AF is the simpler index for estimating pesticide leaching potential and, therefore, is more likely to be used in the future for screening/ranking agrochemicals relative to regional-scale NPS ground water vulnerability.

#### ACKNOWLEDGMENTS

The effort reported in this paper is a CESIR contribution. The first author is grateful to the Ministerio de Educacion y Cultura (Spain) for a "Beca del Programa Nacional de Formacion del Personal Investigador en el Extranjero (Subprograma de Perfeccionamiento de Doctores y Tecnologos)" fellowship.

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