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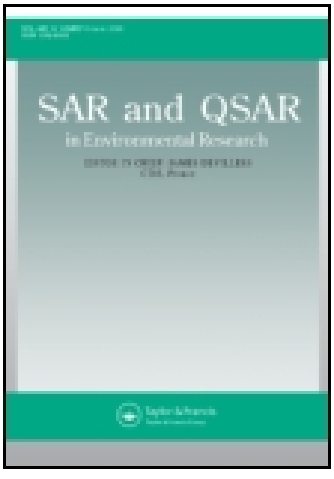

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USE OF KNOWLEDGE BASES AND QSARS TO ESTIMATE THE RELATIVE ECOLOGICAL RISK OF AGRICHEMICALS: A PROBLEM FORMULATION EXERCISE

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Ecological risk assessments can be used to establish the likelihood that an adverse effect will result from exposure to one or more chemicals. When evaluating contaminated sites with many chemicals present, risk assessors must grapple with the problem of quickly identifying the chemicals that are most likely to be of concern, based on effect and exposure assessment information. Many times data gaps exist and the risk assessor is left with decisions on which models to use to estimate the parameter of concern. In the present paper, a procedure is presented for ranking agrichemicals, utilizing the ASTER (ASsessment Tools for the Evaluation of Risk) system. The procedure was employed to rank the relative ecological risk of forty-nine pesticides historically used in agricultural sites in the Walnut Creek watershed near Ames, Iowa, USA. Empirical data from the ASTER system were used when available in the associated databases, and quantitative structure-activity relationships and expert systems were invoked when data were lacking. Separate rankings were conducted based on major species taxonomic groupings. Resulting toxic effects thresholds were compared to surface water concentrations.

KEY WORDS: risk assessment; agrichemicals; QSAR; expert system; risk ranking; pesticides.

INTRODUCTION

The U.S. Environmental Protection Agency (U.S. EPA) utilizes ecological risk assessments to evaluate the potential adverse effects that exposure to a single chemical or combination of chemicals will have on an ecosystem. The U.S. EPA has developed a framework for conducting ecological risk assessments that is divided into three components: problem formulation, analysis, and risk characterization.[1] The approach presented in this paper may be useful in the problem formulation step of the risk assessment process. Many times risk assessors are faced with a dearth of information, which impacts the final risk assessment. At other times an abundance of data is presented for a single species and/or effect and the assessor must determine the 'best' data to utilize in the risk assessment process.

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The ASTER (ASsessment Tools for the Evaluation of Risk) system was developed by the U.S. EPA, Environmental Research Laboratory-Duluth (ERL-D) to assist regulators in performing ecological risk assessments.[2] ASTER is an integration of the AQUIRE (AQUatic toxicity Information REtrieval) toxic effects database[3] and the QSAR (Quantitative Structure-Activity Relationships) system,[2] a structure-activity based expert system. When high quality empirical data are not available, ASTER uses mechanistically-based predictive models to estimate ecotoxicology endpoints, chemical properties, biodegradation, and environmental partitioning.

An example of a type of a problem formulation that can utilize an ASTER-like system is associated with the U.S. EPA, Office of Research and Development's MASTER (Midwest Agrichemical Surface/Subsurface Transport and Effects Research) program, which is designed to support ecologically sound and economically feasible agricultural management practices. A component of this research effort was to develop a computer-based risk assessment system utilizing screening-level effects and exposure assessment data for agrichemicals, and to rank the potential for adverse impacts among insecticides and herbicides registered for corn and soybeans. Forty-nine registered agrichemicals were selected for analyses, primarily herbicides (n = 36) and insecticides (n = 13) historically used in the Walnut Creek watershed, an eighteen square mile agricultural area south of Ames, Iowa in the USA (Table I).[4] Each agrichemical was scored based on acute or chronic toxicity to aquatic organisms (plants, invertebrates, and vertebrates) and birds, bioconcentration in fish, environmental partitioning, and environmental persistence. In addition to providing rankings, toxic-effect thresholds derived from ASTER were compared to reported surface water concentrations of agrichemicals as an aid in formulating more detailed risk assessment problems.

METHODS

Data Sources

ASTER[2] was the primary shell used to access empirical data (e.g., AQUIRE), QSAR models and expert systems. ASTER is a VAX-based system located at ERL-D and the U.S. EPA, National Computer Center. ASTER includes QSAR models for estimating acute toxicity, chronic toxicity, and bioconcentration factor (BCF), and expert systems for predicting biodegradation half-life and environmental partitioning. To obtain QSAR estimates for chemicals without empirical data, structural information was stored for each compound as SMILES (Simplified Molecular Input Line Entry System) strings.[5,6,7]

To augment empirical data within ASTER, several additional databases were also consulted. The U.S. EPA, Office of Pesticide Programs Ecological Effects Database (OPP-EED), which contains unpublished pesticide registration data, was used to augment the effects assessment information. In addition, the OPP-EED includes toxicity data for avian species, a taxonomic group not included in AQUIRE. The Finnish Ministry of the Environment, Environmental Protection Department compilation of environmental properties and toxic effects data for industrial chemicals[8] was also used in a few instances when empirical data from the ASTER or OPP-EED

Table I List of chemicals used in the agrichemical ranking exercise (n = 49).

CAS RN	*Common Name*	*Trade name*
Herbicides		
62476-59-9	Acifluorfen-sodium	Blazer
15972-60-8	Alachlor	Lasso
834-12-8	Ametryn	Trinatox
1912-24-9	Atrazine	Aatrex
25057-89-0	Bentazon	Basagran
42576-02-3	Bifenox	Modown
1689-84-5	Bromoxynil	Brominex
2008-41-5	Butylate	Sutan+
133-90-4	Chloramben salts	Amiben
90982-32-4	Chlorimuron-ethyl	Classic
101-21-3	Chlorpropham	Chloro IPC
81777-89-1	Clomazone	Command
21725-46-2	Cyanazine	Bladex
1918-00-9	Dicamba	Banvel
94-75-7	2,4-D acid	Weedtrol
94-82-6	2,4-DB	Butyrac
759-94-4	EPTC and inerts	Eptam
55283-68-6	Ethalfluralin	Sonalan
66441-23-4	Fenoxaprop-ethyl	Option
69806-50-4	Fluazifop-butyl	Fusilade
1071-83-6	Glyphosate	Roundup
81335-77-5	Imazethapyr	Pursuit
77501-63-4	Lactofen	Cobra
330-55-2	Linuron	Malurane
51218-45-2	Metolachlor	Dual
21087-64-9	Metribuzin	Sencor
40487-42-1	Pendimethalin	Prowl
1610-18-0	Prometon	Pramitol
7287-19-6	Prometryn	Primatol Q
1918-16-7	Propachlor	Satecid
139-40-2	Propazine	Milo-Pro
76578-14-8	Quizalofop-ethyl	Assure
74051-80-2	Sethoxydim	Poast
122-34-9	Simazine	Totazina
886-50-0	Terbutryn	Prebane
1582-09-8	Trifluralin	Treflan
Insecticides		
1563-66-2	Carbofuran	Furadan
2921-88-2	Chlorpyrifos	Lorsban
60-51-5	Dimethoate	Cygon 400
298-04-4	Disulfoton	Insyst-D
13194-48-4	Ethoprop	Jolt
51630-58-1	Fenvalerate	Ectrin
944-22-9	Fonofos	Dyfonate
121-75-5	Malathion	Calmathion
10265-92-6	Methamidophos	Monitor
52645-53-1	Permethrin	Pounce
298-02-2	Phorate	Thimet
13071-79-9	Terbufos	Counter
2686-99-9	Trimethacarb	Landrin

databases and QSAR estimates were unavailable. Finally, field half-life data from Wauchope *et al.*[9] were used when biodegradation data could not be estimated.

Data Selections

The risk ranking exercise was based on effects to three major taxonomic groups representing aquatic vascular and nonvascular plants, aquatic invertebrates, and aquatic vertebrates. Additionally, one avian species, the mallard, was selected to represent waterfowl. Separate rankings for each species group were made which allowed examination of sensitivities between taxonomic groupings. Because this project focused on agrichemicals used in the Walnut Creek watershed, only data for freshwater test organisms were examined. Species indigenous to the Walnut Creek watershed or the central United States were selected over non-native species.

Ranking scores for each species group were determined for five categories of data: acute and chronic toxicity (i.e., effect potential), and BCF, persistence and environmental partitioning (i.e., exposure potential). For the purposes of this study an acute toxicity test was less than or equal to 4 days duration and a chronic toxicity test was greater than 4 days duration.

A number of criteria were established for minimum data requirements. If either acute or chronic toxicity data were not available for at least one of the five species groups, or at least two exposure assessment parameters were not available, then these chemicals were not considered in the final risk ranking. Exact and discrete toxicity values were selected first, or if unavailable, approximate values, reported as 'greater than' (>) or 'less than' (<) values in the databases were selected. Ranges of toxicity values were not considered in this ranking exercise. Based on codes stored for each AQUIRE database entry, preference was given to those studies with the most complete documentation of test methods. These criteria were also applied to the OPP-EED database. If no empirical data were available, QSAR estimations were used.

For each effect and exposure assessment parameter, a data value was selected for the ranking exercise. Based on the data value selected, a score was assigned. The strategy for assigning scores for each parameter is presented in Table II.

Toxicity Data

Within each species group, the most potent toxicity endpoints were selected for the final ranking, with the following exceptions. If more than one data point was available for a species, with the same effect and test duration, the data with measured exposure concentrations were selected over data based on unmeasured (nominal) exposure levels. The geometric mean of toxicity values was used when the selected data reported the same chemical concentration type (measured or unmeasured concentrations), species, effect and test duration.

If empirical toxicity data were not available and the octanol/water partition coefficient could be calculated, the toxic endpoint was estimated using a QSAR, with the exception of toxic effects for plant and avian species groups for which QSAR models were unavailable. The octanol/water partition coefficient was the only independent variable used in toxic effect QSARs, which was estimated using CLOGP™

Table II Criteria used in assigning scores to effects and exposure assessment parameters.

Score	*Acute toxicity*[a] (μg/l)	*Chronic toxicity*[a] (μg/l)	*Acute avian toxicity* (mg/kg)	*BCF*	*Environmental persistence (days)*	*Environmental partitioning*[b] *(%)*
5	< 1	< 0.1	< 1	$\geqslant 5000$	$\geqslant 15$	$\geqslant 80 - 100$
4	$\geqslant 1 - 50$	$\geqslant 0.1 - 5$	$\geqslant 1 - 50$	$\geqslant 1000 - 5000$	–	$\geqslant 60 - 80$
3	$\geqslant 50 - 500$	$\geqslant 5 - 50$	$\geqslant 50 - 500$	$\geqslant 500 - 1000$	$4 - 15$	$\geqslant 40 - 60$
2	$\geqslant 500 - 1000$	$\geqslant 50 - 100$	$\geqslant 500 - 1000$	$\geqslant 100 - 500$	–	$\geqslant 20 - 40$
1	$\geqslant 1000$	$\geqslant 100$	$\geqslant 1000$	< 100	< 4	< 20
0	No empirical data or estimated value available					

[a]Used for ranking aquatic vascular/non-vascular plants, aquatic invertebrates and aquatic vertebrate species groups.

[b]The sum of the partitioning percentages for water and sediments.

software.[10,11] Selection of QSARs used to estimate acute toxicity were made based on the acute mode of action. When empirical data or QSARs were unavailable for a chemical, a score of zero (0) was assigned. However, if a neurotoxic or reactivity-based mode of action was predicted, a score of five (5) was assigned to acute and chronic toxic effects for aquatic plant, invertebrate and vertebrate species. This assignment was based on the assumption that chemicals acting by these mechanisms would be very toxic to aquatic organisms.

EC50 and LC50 calculations were preferentially selected for use in evaluating aquatic plant species, but because of a lack of data, other endpoints such as changes in abundance, biomass, chlorophyll content, population growth and population diversity, were used. Acute toxicity scores for invertebrate and vertebrate species groups were assigned using only EC50 and LC50 results. For cladocerans and midges EC50 toxicity data of 2 day duration were used preferentially.

For chronic toxicity exposures for aquatic plant species, EC50 and LC50 results were preferentially selected for use in the determination of a score. If EC50 or LC50 values were not available for aquatic plants, then other effect endpoints such as changes in abundance, biomass, chlorophyll content, population growth and population diversity, were used in the assessment. For aquatic invertebrate and vertebrate species, LC50, EC50, reproduction, or growth test data were used preferentially. If data were not available for these effects, behavior, biochemical, or physiological test data were used. When data points were not available for any of these effects, the most sensitive indicator of chronic toxicity was selected.

Data selected for the effect assessment that reported a no observable effect concentration (NOEC) were assigned risk scores of 1 because the toxic effect is at an unknown concentration greater than the NOEC value reported.

Only oral dosing studies (LD50) were used to assess the avian species score. Feeding studies (LC50) were not used in this exercise because of uncertainty of the actual toxic dose and cause of death attributed to these studies in general.[12,13]

Exposure Data

Empirical BCF data were used from tests which had the most complete methods documentation and were conducted under flow-through conditions, reporting measured, non-ranged concentration values. If more than one BCF value meeting the same criteria existed for a species, the geometric mean of the concentration values was used. A QSAR estimate from Veith and Kosian[14] was used if the above data requirements were not met. Environmental persistence was estimated using the biodegradation half-life model by Niemi *et al.*[15] When the expert system could not estimate the environmental persistence, field half-life values were used.[9] Environmental partitioning was estimated using the Mackay Level 1 fugacity model.[16,17] Mackay's model estimates partitioning into five compartments; air, water, suspended solids, sediments and biota. The emphasis in this exercise was to assess potential exposure of organisms associated with the aquatic ecosystem, therefore partitioning into the air was not included in our assessment. To assess the potential exposure to aquatic and benthic organisms from the water column and sediment respectively, the environmental partitioning score was based on the sum of the partition percentages for the water and sediment compartments. The suspended

solid compartment was not used because of difficulty in determining whether chemicals bound to suspended solids are bioavailable to aquatic organisms; however, accumulation potential in biota was addressed by the BCF parameter.

Risk Ranking Algorithm

The scores assigned to each hazard and exposure assessment parameter were used to determine the relative ecological risk for each compound. Relative risk was determined using two tiers. The first involved the calculation of a risk score (RS) from a species group score (SG_{sc}). This is based on an approach described by Sheehan *et al.*,[18] and previously unpublished algorithms developed at ERL-D (Jarvinen, personal communication). A SG_{sc} was calculated for each taxonomic group relative to exposure duration, if applicable, using the following equation:

$$SG_{sc} = [(T_{sc} \times 10) + [((BCF_{sc} + PERS_{sc} + PART_{sc}) \times 10)/N_{esc}]]/N_{te} \quad (1)$$

where: T_{sc} is the toxicity score (either acute or chronic), BCF_{sc} is the bioconcentration factor score, $PERS_{sc}$ is the persistence score obtained from biodegradation half-life, $PART_{sc}$ is the environmental partitioning score based on Mackay's Level 1 fugacity model, N_{esc} is the number of exposure assessment parameters (BCF, PERS, and PART) with a score > 0, and N_{te} is a number assigned relative to the number of toxicity and exposure assessment parameters used in calculation of the score, with $N_{te} = 2$ if $T_{sc} > 0$ and the score of at least one exposure assessment parameter is > 0, or $N_{te} = 1$ if data were available for either the T_{sc} or any of the exposure assessment parameters, but not both.

The SG_{sc}s were rounded to the nearest whole number prior to calculating the RS using Eq. (2):

$$RS = (SG_{sc-p} + ((SG_{sc-ia} + SG_{sc-ic})/2) + ((SG_{sc-va} + SG_{sc-vc})/2) + SG_{sc-m})/4 \quad (2)$$

where SG_{sc-p} is the species groups score for aquatic plants, SG_{sc-ia} and SG_{sc-ic} are the aquatic invertebrate acute and chronic species groups scores, respectively, SG_{sc-va} and SG_{sc-vc} are the aquatic vertebrate acute and chronic species groups scores, respectively, and SG_{sc-m} is the species group scores for mallards.

The RS provides a means of ranking risk based on a final calculated score, but does not take into consideration how each chemical was ranked within each taxonomic group. For instance, a chemical could be ranked as having high risk using the RS method, but when RSs are ordered within each taxonomic group, species sensitivity may alter the final ranking. Therefore, a second tier for ranking was used by ordering the SG_{sc} within each taxonomic group, using averages of the acute and chronic SG_{sc} for aquatic invertebrates and vertebrates, and assigned a number from 1 to 49 depending on the relative risk, with 1 being the highest risk to 49 equal to the lowest risk. The rankings for each species groups were then averaged to obtain a risk ranking (RR) using the following equation:

$$RR = (PR + IR + VR + MR)/4 \quad (3)$$

where PR = rank based on the aquatic plant SG_{sc}, IR = rank based on the mean of the acute and chronic aquatic invertebrate SG_{sc}, VR = rank based on the mean

of the acute and chronic aquatic vertebrate SG_{sc}, and MR = rank based on the mallard SG_{sc}.

RESULTS AND DISCUSSION

Data Availability

The number of data points available by assigned score (0–5) and parameter assessed are presented in Table III. Of the parameters for which data were collected, aquatic plant toxicity data had the most gaps, with only 8% of the pesticides examined having acute toxicity data and 53% having chronic toxicity data. All chemicals with acute toxicity data had chronic test data available. Because of the reduced acute toxicity data set for this group of species, only the chronic plant data were used in determining the SG_{sc} and RR. The lack of freshwater aquatic plant data is unfortunate, considering that 17 of the 21 chemicals without data are registered herbicides.

The majority of pesticides had acute toxicity data for aquatic invertebrates and vertebrates (90% and 96%, respectively), but less chronic effects data were available (41% and 80%, respectively). For all chemicals having chronic toxicity data, corresponding acute toxicity data were also available. Mallard toxicity data were available for only 59% of the pesticides.

Ninety-five percent of the effects data used in the ranking exercise were obtained from toxic effects databases, while 5% were estimated using QSARs, Eighty-five percent of the data extracted from the AQUIRE and OPP-EED databases had extensive methods documentation. Mallard toxicity data for propachlor and algae toxicity data for prometon were obtained from Nikunen *et al.*[8] The default assignment of an effect score of 5 for neurotoxicants or reactive toxicants occurred 3 times for the QSAR derived data. Four effect concentrations for invertebrates and vertebrates were based on NOECs, and 12 of the 29 mallard risk scores were based on NOECs.

Table III Number of pesticides (n = 49) assigned scores of 0 to 5 for effect and exposure parameters used in determining the species group scores (SG_{sc}).

Parameter	*Score*					
	0	1	2	3	4	5
Aquatic non-vascular and vascular plants-toxic effects						
Acute	45	2	0	0	2	0
Chronic	23	14	0	8	3	1
Aquatic invertebrates-toxic effects						
Acute	5	26	2	5	4	7
Chronic	29	6	1	3	8	2
Aquatic vertebrates-toxic effects						
Acute	2	29	0	9	6	3
Chronic	10	25	1	7	6	0
Mallard-toxic effects	20	21	1	1	4	2
BCF	2	19	13	3	5	7
Persistence	0	0	N/A	12	N/A	37
Partitioning	2	0	0	14	8	25

Estimated environmental persistence data were available for all but six chemicals, which were evaluated using field half-life values. BCF and environmental partitioning data were available for all but two compounds, imazethapyr and glyphosate. Environmental persistence was scored high for most compounds, with only 12 pesticides having an estimated or measured environmental persistence of less than 15 days.

Ranking Studies

Based on the previously established criteria, three compounds were removed from the final risk ranking. Lactofen was removed because toxicity data were not available for any of the taxonomic groups. Imazethapyr and glyphosate were removed because persistence was the only exposure assessment parameter available.

A distribution of overall scores observed for this data set of 46 chemicals is presented in Table IV. Chemicals are listed in order of the RR. The mean RS was 31 and the median RS was 30. The minimum RS was 20 ($n = 1$) and the maximum RS was 42 ($n = 1$), with 9% of the chemicals having a RS less than 25 and 4% of the chemicals having a RS greater than 40. Seventy-seven percent of the insecticides and 33% of the herbicides had a RS greater than the mean score of 31.

Many of the chemicals lacked effect data for certain taxonomic groups. Figure 1 is a subset of the 46 chemicals for which data were available for all exposure assessment parameters (BCF, environmental persistence and environmental partitioning), and for which either acute or chronic toxicity data were available for each taxonomic group. This subset of the database represents 10 herbicides and 8 insecticides. Chemicals in Figure 1 are listed in the order of RR, decreasing from left to right. Differences can be observed between the SG_{sc}. For instance, aquatic plants, aquatic invertebrates and aquatic vertebrates have SG_{sc} for fenvalerate and permethrin above 40, while the SG_{sc} for mallards are in the moderate range (~ 25). In addition, the specific herbicidal activity of ethoprop and atrazine can be evidenced by the high SG_{sc} for aquatic plant species and the lower SG_{sc} for the other taxonomic groups. Simazine had a relatively low SG_{sc} for all four taxonomic groups.

In addition to providing initial insights regarding relative risks of agrichemicals, the effects data gathered from this exercise can also be used to initiate more extensive chemical-specific risk assessments. For example, Figure 2 compares effects data to measured surface water concentrations for alachlor, atrazine, cyanazine, metolachlor and metribuzin observed at various field locations. These surface water concentration data are ranges of maximum values from a number of Lake Erie tributaries draining agricultural watersheds.[19] These surface water data represent numerous samples from April 1983 to December 1991. Ninety-six hour EC50 values for *Selenastrum capricornutum* were obtained for consistency in evaluating effects to aquatic plants associated with these specific surface water concentrations. Data for alachlor and metribuzin are from Fairchild *et al.*,[20] the atrazine EC50 value is from Turbak *et al.*,[21] and cyanazine and metolachlor data are from St Laurent *et al.*[22]

The RSs for these five compounds ranged from 26 for alachlor to 32 for metribuzin (Table IV). All five compounds have high scores for environmental persistence with estimated biodegradation rates greater than 15 days. Alachlor and metolachlor have relatively high octanol/water partition coefficients (3.99 and 4.05,

Table IV Risk ranking (RR), species group scores (SG_{sc}), and risk score (RS) for 46 agrichemicals. SG_{sc} for invertebrate and vertebrate species are averages of the acute and chronic SG_{sc}.

RR	*Chemical*	SG_{sc} Plant	SG_{sc} *Invertebrate*	SG_{sc} *Vertebrate*	SG_{sc} *Mallard*	*RS*
1	Bifenox	43	43	40	43	42
2	Fluazifop	43	35	40	43	40
3	Trimethacarb	40	38	40	40	40
4	Quizalofop-ethyl	40	40	38	40	40
5	Fenvalerate	47	47	44	27	41
6	Ethalfluralin	35	42	42	40	40
7	Permethrin	42	44	42	27	39
8	Chlorpyrifos	40	42	40	35	39
9	Acifluorfen	43	35	27	43	37
10	Terbufos	37	41	38	37	38
11	Chlorimuron-ethyl	40	40	32	25	34
12	Pendimethalin	37	37	37	27	34
13	Carbofuran	30	35	30	40	34
14	Disulfoton	33	37	32	37	35
15	Phorate	20	38	32	40	32
16	Ametryn	40	25	25	40	32
17	Linuron	35	30	25	40	32
18	Trifluralin	25	38	40	25	32
19	Metolachlor	40	32	25	25	30
20	Terbutryn	25	32	25	40	30
21	Prometryn	25	32	25	40	30
22	Prometon	25	32	25	40	30
23	Fonofos	23	36	36	38	33
24	2,4-DB	37	30	23	37	32
25	Metribuzin	37	30	23	37	32
26	Malathion	30	38	38	20	32
27	Fenoxaprop-ethyl	25	32	38	25	30
28	Ethoprop	20	32	30	35	29
29	Dicamba	37	30	23	23	28
30	Bromoxynil	37	30	23	23	28
31	Bentazon	37	30	23	23	28
32	Propazine	23	30	23	37	28
33	Chlorpropham	23	30	23	37	28
34	Propachlor	30	28	30	25	28
35	2,4-D	33	23	23	37	29
36	Cyanazine	33	30	23	23	27
37	Methamidophos	30	30	20	30	28
38	Clomazone	37	23	23	23	26
39	Dimethoate	20	35	20	35	28
40	Alachlor	25	25	28	25	26
41	Chloramben	23	30	23	23	25
42	Atrazine	37	27	22	22	27
43	Sethoxydim	30	25	20	20	24
44	Butylate	30	25	20	20	24
45	EPTC	20	25	20	20	21
46	Simazine	20	20	20	20	20

respectively), which resulted in higher BCF scores. Cyanazine and metribuzin received the highest environmental partitioning scores, which reflect that over 90% of the chemical resides in the water. Alachlor and metolachlor have slightly lower environmental partitioning scores, but they represent significant distribution into

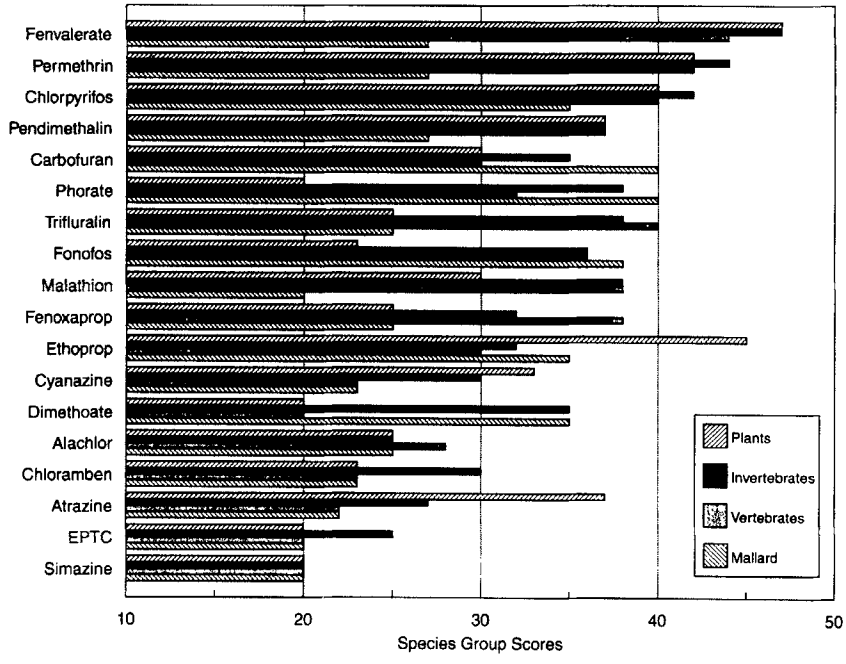

Figure 1 Species group scores (SG_{sc}) for chemicals with complete data sets. Chemicals listed in order of risk ranking (RR) from highest risk (left) to lowest risk (right). SG_{sc} for invertebrate and vertebrate species are the mean of the acute and chronic SG_{sc}.

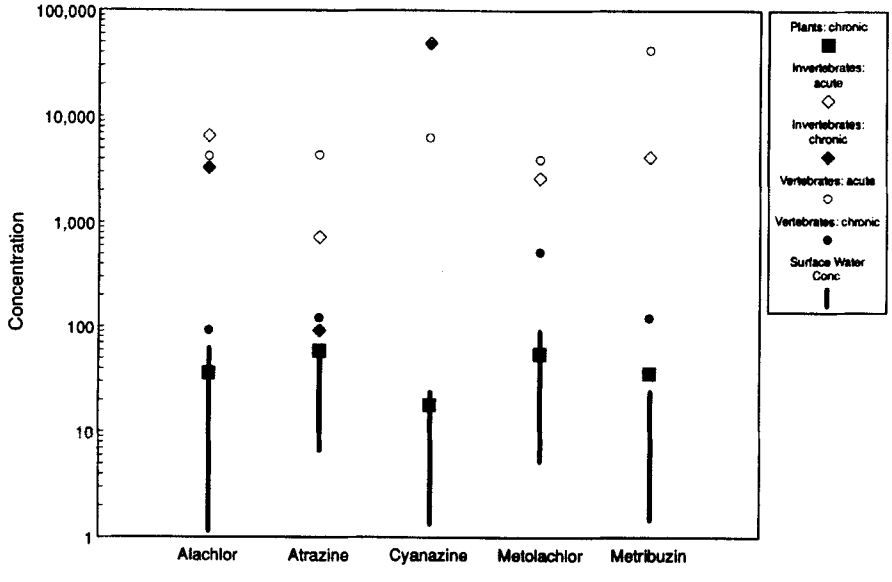

Figure 2 Comparison of toxicity data to surface water concentrations for alachlor, atrazine, cyanazine, metolachlor and metribuzin. Surface water concentrations are ranges of maximum values sampled from Lake Erie tributaries.[19] Concentration units are μg/l for plant, invertebrate and vertebrate species and mg/kg for mallards.

both the water column and sediment (approximately 30% in the sediment and 40% in the water column).

Atrazine, alachlor, cyanazine, and metolachlor surface water concentrations are within the range where toxicity was observed for aquatic plants in laboratory bioassays (Figure 2). Acute toxicity values for aquatic invertebrates and aquatic vertebrates are outside the range of the surface water concentrations. The maximum surface water concentrations for atrazine, alachlor, and metribuzin approach the chronic invertebrate and vertebrate toxicity values, however, these comparisons should be viewed with caution since these are surface water maximum concentrations observed over a 7 year period. In addition, although these concentrations approach a chronic toxicity value, the duration of the concentration in the exposure water may not be long enough to cause detrimental effects to these species.

CONCLUSION

The ranking techniques used in this exercise illustrate the means whereby screening-level risk assessments can be facilitated. In addition, these techniques and associated knowledge bases can also be used to efficiently establish a conceptual model within the problem formulation stage of an ecological risk assessment. This exercise also illustrated that many assessments are hampered by limited exposure and effects data. Clearly, this approach is not appropriate for more detailed risk assessments, where dose-response relationships are required and where impacts on population, community or ecosystem structure and function are identified as assessment endpoints. In addition, this analysis deals only with single chemicals, therefore additive, synergistic, or antagonistic effects of pesticides and their formulations are not addressed. To assess the risk of agrichemicals to communities and ecosystems will require physical and mathematical models, with parameters specified appropriately for intended applications, to evaluate and forecast responses as a function of current or future agrichemical concentrations in water, sediment and biota.

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References

1. U.S. EPA (1992). *Framework for Ecological Risk Assessment.* U.S. Environmental Protection Agency, EPA/630/R-92/001, Risk Assessment Forum, Washington, DC, p. 41.
2. Russom, C.L., Anderson, E.B., Greenwood, B.E., and Pilli, A. (1991). ASTER: an integration of the AQUIRE data base and the QSAR system for use in ecological risk assessments. *Sci. Total Env.* **109/110,** 667–670.
3. Russo, R.C. and Pilli, A. (1984). AQUIRE: *aquatic information retrieval toxicity data base. Project description, guidelines and procedures.* Report No. EPA-600/8-84-021. U.S. Environmental Protection Agency, Office of Research and Development, Duluth, MN 55804.

4. Hartzler, R. and Wintersteen, W. (1990). *A survey of pesticides used in Iowa crop production in 1990.* Iowa Extension Office, Iowa State University, Ames, IA.
5. Anderson, E., Veith, G.D., and Weininger, D. (1987). SMILES: *a line notation and computerized interpreter for chemical structures.* Report No. EPA/600/M-87/021. U.S. Environmental Protection Agency, Environmental Research Laboratory-Duluth, Duluth, MN 55804.
6. Weininger, D. (1988). SMILES, a chemical language and information system. 1. Introduction to methodology and encoding rules. *J. Chem. Info. Computer Sci.* **28,** 31–36.
7. Weininger, D., Weininger, A., and Weininger, J.L. (1989). SMILES. 2. Algorithm for generation of unique SMILES notation. *J. Chem. Info. Computer Sci.* **29,** 97–101.
8. Nikunen, E., Leinonen, R., and Arto, K. (1990). *Environmental Properties of Chemicals.* Research Report 91/1990. Ministry of Environment, Environmental Protection Department, ISSN 0784-8129, VAPK Publishing, Helsinki, Finland, p. 1084.
9. Wauchope, R.D., Buttler, T.M., Hornsby, A.G., Augustijn Beckers, P.W.M., and Burt, J.P. (1992). The SCS/ARS/CES pesticide properties database for environmental decision-making. In, *Reviews of Environmental Contamination and Toxicology* (G.W. Ware, Ed.). Springer-Verlag Publishers, New York, NY, pp. 1–164.
10. Leo, A. and Weininger, D. (1984). MEDCHEM User Reference Manual, Release 3.52, CLOGP™ version 3.53. Pomona Medicinal Chemistry Project, Pomona College, Claremont, CA 91711.
11. Leo, A. (1985). Parameter and structure-activity data bases: management for maximum utility. *Environ. Health Perspect.* **61,** 275–285.
12. Bennett, R.S. (1989). Factors influencing discrimination between insecticide-treated and untreated foods by northern bobwhite. *Arch. Environ. Contam. Toxicol.* **18,** 697–705.
13. Bennett, R.S. (1989). Role of dietary choices in the ability of bobwhite to discriminate between insecticide-treated and untreated food. *Environ. Toxicol. Chem.* **8,** 731–738.
14. Veith, G.D. and Kosian, P. (1983). Estimating bioconcentration potential from octanol/water partition coefficients. In, *Physical Behavior of PCBs in the Great Lakes* (D. Mackay *et al., Eds.*). Ann Arbor Science Publishers, Ann Arbor, MI, pp. 269–282.
15. Niemi, G.J., Veith, G.D., Regal, R.R., and Vaishnav, D.D. (1987). Structural features associated with degradable and persistent chemicals. *Environ. Toxicol. Chem.* **6,** 515–527.
16. Mackay, D. (1988). *Level 1 Environmental Partitioning/Fugacity Model.* University of Toronto, Chemical Engineering Dept., Toronto, Ontario, M5S, 1A4, Canada.
17. Mackay, D., Joy, M., and Paterson, S. (1983). A quantitative water, air, sediment interaction (QWASI) fugacity model for describing the fate of chemicals in lakes. *Chemosphere* **12,** 981– 997.
18. Sheehan, P.J., Baril, A., Mineau, P., Harfenist, A., and Marshall, W. K. (1987). *The impact of pesticides on the ecology of prairie nesting ducks.* Technical Report Series No. 19. Canadian Wildlife Service, Headquarters, Ottawa, Canada.
19. Richards, R.P. and Baker, D.B. (1993). Pesticide concentration patterns in agricultural drainage networks in the Lake Erie basin. *Environ. Toxicol. Chem.* **12,** 13–26.
20. Fairchild, J.F, Ruessler, S., and Nelson, M.K. (1993). *Bioavailability and toxicity of agricultural chemicals in runoff from MSEA sites: potential impacts on non-target aquatic organisms.* Interim Report under EPA/IAG DW14935600-01-0. U.S. Fish and Wildlife Service, National Fisheries Contaminant Research Center, Columbia, MO 65201.
21. Turbak, S.C., Olson, S.B., and McFeters, G.A. (1986). Comparison of algal assay systems for detecting waterborne herbicides and metals. *Water Res.* **20,** 91–96.
22. St Laurent, D., Blaise, C., MacQuarrie, P., Scroggins, R., and Trottier, B. (1992). Comparative assessment of herbicide phytotoxicity to *Selanastrum capricornutum* using microplate and flask bioassay procedures. *Env. Tox. Wat. Qual.* **7,** 35–48.