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Water Research 38 (2004) 3485–3494

WATER RESEARCH

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Screening the leaching tendency of pesticides applied in the Amu Darya Basin (Uzbekistan)

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Received 15 September 2003; received in revised form 6 March 2004; accepted 8 April 2004

Abstract

The Amu Darya River, one of the most important water resources for Uzbekistan and Turkmenistan, was declared a World Disaster Zone in 1991. The great increase in irrigation and the use of pesticides has led to both a lack of water and drinking water contamination. The aim of the present study, part of an EU project on water management guidelines, was to evaluate the leachability of 71 organic pesticides commonly employed in the area, and to assess compounds that could potentially contaminate the river and impair drinking water quality. A multivariate approach is proposed for the pesticide screening, condensing information from different environmental partition indexes (GUS, "modified LEACH", LIN) into a single ranking, the Global Leachability Index (GLI). For a selected data set in water medium this super-index identifies three classes with a risk potential for pesticide leachability, and allows the selection of a small number of chemicals for an analytical survey.

Keywords: Pesticides; Water pollution; Leachability indexes

1. Introduction

The Amu Darya river, one of the two main affluents of the Aral sea, extends some 2550 km from its headwaters in the high mountains of Afghanistan and Tadzhikistan to the end of the delta. It is one of the most important water resources for Uzbekistan and Turkmenistan. In the Soviet period the area became well known to the world for the large scale water development that was carried out, however such development has led to many ecological problems in the region.

The most important problem is the drying up of the Aral sea, another is 'returning water'. This is water withdrawn from the river for irrigation purposes that returns to the river from the irrigated land, in lower volumes but enriched with a large content of salts and other pollutants, especially pesticides.

Irrigation covers about 1.2 million hectares in the lower Amu Darya area (in the territories of Uzbekistan and Turkmenistan) where there are more than 3 million inhabitants. Pesticide pollution and salination has led to a lack of groundwater resources for drinking water purposes, cancer is widespread and the area has the highest level of child mortality in Central Asia. In 1991 the region was declared a World Disaster Zone (UNEP, 1992)

The only fast way to ensure a sustainable supply of drinking water is to use the reservoir system of Tuyamuyn, particularly the Kaparas reservoir, to store the Amu Darya headwaters. However the large amounts

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0043-1354/$ - see front matter
doi:10.1016/j.watres.2004.04.053

of water withdrawn for irrigation, the marked salt content and the presence of other pollutants from irrigated lands have heavily compromised the use of the lower Amu Darya waters stored in the Kaparas reservoir for drinking and irrigation purposes. Thus the reservoir complex has an urgent need for management strategies that are, however, not yet available.

In an effort to remedy the situation, and provide guidelines for water management, an EU research project (EU-INTASS-IWMT—**I**ntegrated **W**ater **M**anagement **T**ools) has been set up in collaboration with the Middle Asian Scientific Research Institute of Irrigation (SANIIRI), the aim being to achieve optimal exploitation of the surface waters in the lower Amu Darya region.

The scientific literature reports no analytical data on the quality of the Amu Darya and/or Kaparas waters, so all the project data had to be taken from National Reports on water monitoring activities; unfortunately such data relate only to traditional water quality parameters.

General information on the Amu Darya river basin can be found in the literature where papers address water management problems (Saeijs and van Berkel, 1999; O'Hara and Sarah, 2000; Dukhovny and Stulina, 2001) and water quality status and effects (Rubinova, 1985; Chembarisov, 1996; Jensen et al., 1997; Kurbanaev et al., 2002).

A second project was initiated for pesticides, and a list of the chemicals commonly used in agricultural fields along the Amu Darya river was provided within the framework of EU-INTASS-OPAL (Investigation of innovative pollution clean-up and avoidance strategies for surface water and groundwater resources at the "Disaster Zone" of the Amu Darya lowers). Because of the lack of analytical facilities and the high cost of performing analyses, the project adopted the strategy to identify, from among the long list of chemicals applied in the area, those pesticides with the highest probability of being present in river water; such probability was assessed according to physico-chemical properties and environmental persistency. A second phase will consider the quantity used and the period of utilization and an analytical survey of the pesticides will then be made. Such a study could prove to be a cost-effective method for use before engaging in expensive monitoring programs, particularly in developing countries (see, for example, Calamari and Zhang, 2002).

However given the many procedures employed, and the variety in the indexes, the above described selection is not a standard task; the present paper discusses the selection pathway.

Pesticide distribution and fate in various environmental media and compartments is strongly influenced by the physico-chemical properties of the compounds themselves, and their potential for degradation (Halfon et al., 1996; Kanazawa, 1989; Altenburger et al., 1993; Tarazona et al., 2000).

Different environmental partitioning indexes like GUS, (Gustafson, 1989), LEACH (Laskowski et al., 1982) and LIN (Gramatica and Di Guardo, 2002) describe similar, but not identical, partitioning trends; such indexes do not result in homogeneous chemical rankings as they are based on different properties and algorithms. Thus, to avoid the inherent evaluation error of a particular method it is necessary to combine, by multivariate techniques, information derived from various approaches.

The methodological aim of this work has been to search for, and propose, a pesticide screening/ranking approach that condenses the information included in various environmental partition indexes (GUS, LEACH, LIN); this has resulted in a single ranking tool named Global Leachability Index (GLI).

The final goal is to use GLI to identify, in the selected data set, three leaching-risk classes for pesticides in water medium. These classes will then be used in last, practical, phase of the project, i.e. the analysis of a limited set of pesticides.

2. Methods

2.1. Data set

We built up a data set of molecules to be studied by identifying, from trade formulation names, the active ingredient of the parent molecule in the Pesticide Manual (Tomlin, 1997). The studied compounds can all be found in the different pesticide classes such as insecticides, acaricides, herbicides, fungicides, and plant growth factors, that had been used in the area over recent decades. The 71 molecules of the selected data set were characterized by the CAS registry number, the organic structure and the principal physico-chemical properties, and a bibliographic search was done (Tomlin, 1997; Mackay et al., 1997; Howard et al., 1991; Gramatica et al., 2000; Gramatica and Di Guardo, 2002; U.S.-EPA softwares EPIWIN, 2000; PBT profiler, 2003; PHYSPROP—Physical Properties database, 2004) to collect data on water solubility, vapour pressure, *n*-octanol/water partition coefficient, organic carbon partition coefficient, Henry's law constant and half-life in soil. A range of minimum and maximum half-life values (mainly field data) was collected, the maximum then being used to calculate indexes considered for a "worst case" scenario. When there were no available half-life experimental data (12 compounds) the analysis considered PBT profiler predicted data (medium value in soil).

All the data used for calculating indexes are reported in Appendix.

2.2. Leachability indexes

Three indexes were applied to calculate leachability. Two traditional, the Groundwater Ubiquity Score (GUS) (Gustafson, 1989). and the Leaching Index (LEACH) (Laskowski et al., 1982), and a third, recently introduced by Gramatica and Di Guardo (LIN—Leachability Index), based on principal component analysis (PCA) of pesticide physico-chemical properties (Gramatica and Di Guardo, 2002).

2.2.1. GUS index

The GUS index assesses the leachability of molecules and the possibility of finding these compounds in groundwater. It is calculated by the equation:

$$\mathrm{GUS} = \log_{10}(t_{1/2}) \times [4 - \log_{10}(\mathrm{Koc})]$$

This index is based on two parameters: mobility in soil, given by the organic carbon partition coefficient (Koc, adimensional), and soil persistence, quantified by the disappearance half-life in the soil, defined in field conditions and expressed in days ($t_{1/2}$). The index allows pesticides to be split according to trigger values, as explained in the discussion.

2.2.2. LEACH index

The leaching index (LEACH) (Laskowski et al., 1982), assesses the potential degree of groundwater and river water contamination. It is calculated by the equation:

$$\mathrm{LEACH} = (\mathrm{Sw}\times t_{1/2})/(V\mathrm{p} \times \mathrm{Koc})$$

where Sw is water solubility (mg/L), $t_{1/2}$ is the degradation half-life in soil (d), Vp is the vapour pressure (Pa) and Koc (adimensional) is the organic carbon partition coefficient. The leaching index has no trigger value: the lower the LEACH value the lower the risk of contamination. LEACH values are expressed on a logarithmic scale to allow comparison with other indexes.

Since the literature lacks experimental data for degradation half-life in soil for the compounds, disappearance half-life in soil, in field conditions, was considered for a "modified LEACH" calculation. The original equation was then modified without taking vapour pressure into account, in order to avoid a double counting of volatilization which is already considered in disappearance half-life in-the-field. Thus, the final equation for this "modified LEACH" calculation is defined:

$$\text{“modified LEACH”} = (\mathrm{Sw}\times t_{1/2\mathrm{field}})/(\mathrm{Koc}).$$

2.2.3. LIN and principal components analysis

LIN (Leaching Index) is an environmental partition index (Gramatica and Di Guardo, 2002) derived from a linear combination by PCA of those physico-chemical properties more relevant to the determination of environmental partitioning (solubility in water (Sw, mg/L)), organic carbon partition coefficient (Koc, adimensional), *n*-octanol/water partition coefficient (Kow, adimensional), vapour pressure (Vp, mmHg), Henry's law constant (H, atm m^3/mol)).

The data, measured at 25°C, were always transformed into logarithmic units. The multivariate technique of PCA was performed on autoscaled data by the SCAN (1995) program.

3. Results and discussion

3.1. GUS index

The application of the GUS index splits the studied pesticides into three groups: "leachers", "non-leachers" and "borderline compounds", based on sorption and persistence properties in soil. The GUS values were calculated for each compound, see Table 1.

The classification was: 15 "leachers", GUS values higher than 2.8, compounds with a high risk for contamination, 13 "borderline" compounds, with GUS values between 1.8 and 2.8 and 43 "non-leachers", pesticides with GUS values lower than 1.8.

3.2. Modified LEACH index

The LEACH index is based on the assumption that mobility in soil is inversely proportional to the rate of decomposition in soil, and that movement by leaching through soil is directly proportional to the quantity of chemical in the water of the air/water/soil system. The leaching index did not present a trigger value to group the compounds: those with higher leachability in the environment were indicated by the higher values. Since no experimental data for each compound's degradation half-life in soil, required for the LEACH index, were available in the literature, soil disappearance half-life in field condition was considered for a "modified LEACH" calculation, as described below. This avoided a double counting of volatilization, which is already considered in disappearance half-life in-the-field.

Comparing the "modified LEACH" (Table 1) and GUS values, it can be noted that several compounds classified as "leachers" by GUS also have a high "LEACH" value, nevertheless other pesticides rank differently.

3.3. LIN

In this study LIN (Leaching Index), obtained by a PCA of physico-chemical properties relevant to the determination of environmental partitioning, was also

Table 1
Summary of leachability indexes calculated for 71 pesticides and risk classes

ID	CAS	Pesticides	LIN	GUS	Modified LEACH	GLI	Leaching risk	Class
1	030560-19-1	Acephate	4.02	3.70	6.61	3.50	High	1
2	135410-20-7	Acetamiprid	1.09	0.20	0.60	0.42	Medium	2
3	082657-04-3	Bifenthrin	−2.50	−2.89	−4.28	−2.56	Low	3
4	034681-10-2	Butocarboxim	2.15	2.20	3.88	1.94	High	1
5	000063-25-2	Carbaryl	0.76	2.32	1.13	0.98	Medium	2
6	002921-88-2	Chlorpyrifos	−1.39	0.62	−1.47	−0.70	Low	3
7	068359-37-5	Cyfluthrin-Beta	−2.13	−1.48	−6.22	−2.44	Low	3
8	091465-08-6	Cyhalothrin-Lambda	−3.20	−3.23	−6.05	−3.23	Low	3
9	052315-07-8	Cypermethrin	−2.78	−2.05	−5.35	−2.64	Low	3
10	052315-07-8	Cypermethrin-Zeta	−2.32	−0.75	−4.42	−1.96	Low	3
11	000050-29-3	p,p′-DDT	−3.22	−4.34	−4.56	−3.25	Low	3
12	052918-63-5	Deltamethrin	−2.96	−1.41	−7.37	−2.92	Low	3
13	000115-32-2	Dicofol	−0.56	4.25	0.03	0.84	Medium	2
14	000060-51-5	Dimethoate	2.44	3.25	4.30	2.40	High	1
15	000115-29-7	Endosulfan	−1.56	−0.17	−2.74	−1.22	Low	3
16	066230-04-4	Esfenvalerate	−2.23	0.68	−3.97	−1.45	Low	3
17	153233-91-1	Etoxazole	−2.20	−1.61	−5.10	−2.28	Low	3
18	064257-84-7	Fenpropathrin	−2.66	−0.33	−5.62	−2.19	Low	3
19	111812-58-9	Fenpyroximate	−2.55	−2.61	−5.68	−2.78	Low	3
20	051630-58-1	Fenvalerate	−2.18	0.00	−4.80	−1.78	Low	3
21	120068-37-3	Fipronil	−0.17	2.76	−0.08	0.55	Medium	2
22	002540-82-1	Formothion	2.13	0.00	2.41	1.06	High	1
23	078587-05-0	Hexythiazox	−1.32	0.19	−3.19	−1.13	Low	3
24	138261-41-3	Imidacloprid	2.03	−0.24	−1.71	0.16	Medium	2
25	144171-61-9	Indoxacarb DPX-JW062	−0.26	0.29	−3.19	−0.75	Low	3
26	173584-44-6	Indoxacarb DPX-KN128	−0.26	0.29	−3.19	−0.75	Low	3
27	000121-75-5	Malathion	0.43	0.77	−0.06	0.22	Medium	2
28	000298-00-0	Parathion-methyl	−0.22	0.49	−0.48	−0.15	Medium	2
29	002310-17-0	Phosalone	−0.79	0.45	−2.17	−0.69	Low	3
30	002312-35-8	Propargite	−1.14	0.79	−1.91	−0.66	Low	3
31	024017-47-8	Triazophos	−0.61	−0.54	−1.83	−0.82	Low	3
32	000052-68-6	Trichlorfon	2.93	4.96	5.73	3.30	High	1
33	034256-82-1	Acetochlor	0.21	0.81	0.25	0.22	Medium	2
34	120162-55-2	Azimsulfuron	2.90	3.93	2.99	2.48	High	1
35	083055-99-6	Bensulfuron-methyl	1.94	3.07	1.66	1.67	High	1
36	025057-89-0	Bentazone	1.29	2.62	2.20	1.44	High	1
37	001689-84-5	Bromoxynil	0.82	1.36	0.48	0.61	Medium	2
38	099129-21-2	Clethodim	−0.33	0.13	−3.11	−0.80	Low	3
39	000094-75-7	Desormone (2,4 D)	0.90	1.88	1.90	1.05	High	1
40	079241-46-6	Fluazifop-p-butyl	−1.18	0.35	−2.31	−0.87	Low	3
41	098967-40-9	Flumetsulam	2.18	3.61	1.50	1.87	High	1
42	002164-17-2	Fluometuron	0.95	4.00	2.04	1.67	High	1
43	077501-90-7	Fluoroglycofen-ethyl	−0.84	0.06	−4.76	−1.31	Low	3
44	069377-81-7	Fluroxypyr	2.75	2.73	0.78	1.68	High	1
45	069806-34-4	Haloxyfop	1.46	4.10	1.69	1.80	High	1
46	002212-67-1	Molinate	0.42	2.91	2.46	1.28	High	1
47	001836-75-5	Nitrophene	−1.21	0.21	−1.82	−0.82	Low	3
48	040487-42-1	Pendimethalin	−1.54	0.63	−2.14	−0.88	Low	3
49	000709-98-8	Propanil	0.58	2.15	1.19	0.88	Medium	2
50	094051-08-8	Quizalofop-p	0.39	2.36	−1.39	0.37	Medium	2
51	100646-51-3	Quizalofop-p-ethyl	−0.91	0.00	−4.13	−1.23	Low	3
52	101200-48-0	Tribenuron-methyl	2.69	1.98	1.63	1.63	High	1
53	017804-35-2	Benomyl	0.61	−0.07	−2.80	−0.48	Medium	2
54	116255-48-2	Bromuconazole	−0.16	−0.95	−0.68	−0.56	Low	3
55	010605-21-7	Carbendazim	1.14	4.22	1.11	1.61	High	1
56	005234-68-4	Carboxin	1.08	0.00	−0.11	0.22	Medium	2
57	083657-24-3	Diniconazole	−1.21	−0.64	−1.63	−1.01	Low	3

Table 1 (*continued*)

ID	CAS	Pesticides	LIN	GUS	Modified LEACH	GLI	Leaching risk	Class
58	106325-08-0	Epoxiconazole BAS 480F	0.01	1.47	−0.47	0.18	Medium	2
59	136426-54-5	Fluquinconazole	0.27	2.80	−0.39	0.64	Medium	2
60	076674-21-0	Flutriafol	0.65	−1.88	−0.07	−0.42	Medium	2
61	066246-88-6	Penconazole	0.17	3.50	1.78	1.22	High	1
62	060207-90-1	Propiconazole	0.24	2.18	1.07	0.75	Medium	2
63	107534-96-3	Tebuconazole	−0.18	−0.66	−0.68	−0.49	Medium	2
64	023564-05-8	Thiophanate-methyl	0.58	1.07	−1.27	0.11	Medium	2
65	000137-26-8	Thiram	0.84	−0.35	−1.65	−0.26	Medium	2
66	043121-43-3	Triadimefon	0.87	1.91	0.63	0.81	Medium	2
67	026644-46-2	Triforine	0.72	2.25	0.50	0.82	Medium	2
68	000052-51-7	Bronopol	3.72	5.91	6.88	4.05	High	1
69	051707-55-2	Thidiazuron	1.72	4.61	1.79	2.04	High	1
70	004602-84-0	Farnesol	−1.70	1.30	−1.54	−0.64	Low	3
71	007212-44-4	Nerolidol	−1.62	1.83	−0.96	−0.36	Medium	2

To allow comparison with other indexes "modified LEACH" values are expressed in logarithmic units

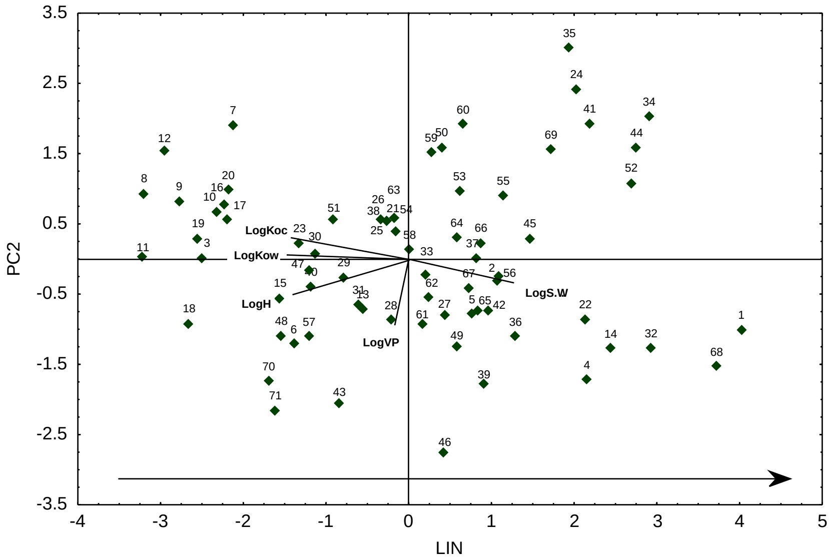

Fig. 1. LIN calculated by PCA of 71 pesticide properties. The chemicals (the points) are ranked according to the multivariate analysis of their physico-chemical properties, represented by the corresponding loadings (the arrows). The cumulative explained variance of this PCA is 88.3% of the total variance, the first principal component (PC1: LIN index) accounts for 60.04% of data variability.

used to describe a pesticide's potential leachability in soil.

PCA is the multivariate explorative technique that, by linear combination of the studied properties, allows a fast screening of the studied chemicals according to their distribution tendency in the different media. The plot of scores (coordinates of objects on the new variables, PC1 and PC2) gives information about the similarity of chemical behaviour, while the plot of loadings (weights of original variable in the PCs) shows correlations among the original variables. A biplot (a combined plot of scores and loadings) gives condensed information.

Fig. 1 shows the biplot of the PCA for 71 pesticides, the chemicals (the points) being ranked according to the partitioning tendency in the different media. The PC1 score, according to the orientation of loadings in the PCA graph (solubility and sorption coefficients playing opposite roles on this axis), represents the LIN index (values reported in Table 1) and tends to discriminate between the relatively more soluble/less sorbed pesticides (on the right of the graph) and more sorbed/less soluble (on the left).

3.4. *Comparison of leachability indexes: definition of a global leachability index (GLI)*

The leachability indexes (values reported in Table 1) calculated for the selected pesticides rank them according to their water partitioning tendency, obtained by different approaches. The comparison of these values shows, as expected, some discrepancies due to the mathematical algorithms and/or various properties included in the index calculations, giving rise to different rankings for the studied pesticides. Nevertheless, one of the aims of this work was to propose a method, based on the multivariate approach, able to evaluate the partition tendency in the selected data set, and also useful to screen general pesticide behaviour in a holistic view. Thus to obtain a single GLI, we combine, by PCA, all the information included in the different GUS, ''modified LEACH'' and LIN leachability indexes. The derived new ranking, that gives an integrated view of the leaching potentiality, is more realistic and holistic than the information derived from each single index.

The first two principal components give 96.7% of the information included in the studied indexes, and PC1 alone explains 87.5% of the total variance. In the biplot of Fig. 2 it is evident that all the original variables (the indexes) are oriented in the same direction and have similar weights (loadings) on the first component, therefore the different indexes have a similar influence on the total ranking.

Along PC2 (explained variance 9.2%) it is evident that ''modified LEACH'' and LIN are closely related, and that GUS gives different information, being based only on $t/2$ and Koc and not on solubility. The correlation of LIN and ''modified LEACH'' on PC2 is clearly understandable from the similarity of the information included in their calculation (both deal with solubility and disappearance by volatilization).

Therefore, since the first principal component alone synthesizes most of the information included in all the indexes, and all the loadings are oriented along the same direction, this PC1 score is proposed as a GLI to rank pesticides according to their leaching tendency.

Some chemicals show extreme behaviour, lying towards the extreme sides of the graph: on the right Bronopol (68), Acephate (1), Trichlorfon (32), Azimsulfuron (34), Dimethoate (14) appear as the most leachable chemicals, contemporarily showing the highest values of GUS, LIN and ''modified LEACH'' and obviously with the highest derived GLI scores, while on the left side of Fig. 2, p, p′-DDT (11), Cyhalothrin-Lambda (8), Deltamethrin (12), Fenpyroximate (19), Cypermethrin (9) and Bifenthrin (3) show the lowest GLI values, in accordance with the low values of the used indexes.

Some structural features can justify this partition behaviour: for instance, the chemicals identified as the most leachable are generally of limited dimension and have molecular structures characterized by the presence of electronegative atoms (O or N), relevant to hydrogen bonding with water and therefore giving rise to an increase in solubility.

On the contrary these structural features are not present in the chemicals that lie on the opposite side of the graph, which have, in general, a more complex structure.

GLI scores were used to group the studied pesticides into three classes of potential leaching risk that can then be applied to accept or reject the controlled use of these chemicals. The first class (Fig. 2) includes chemicals with high leaching potential from soil to water (high GLI

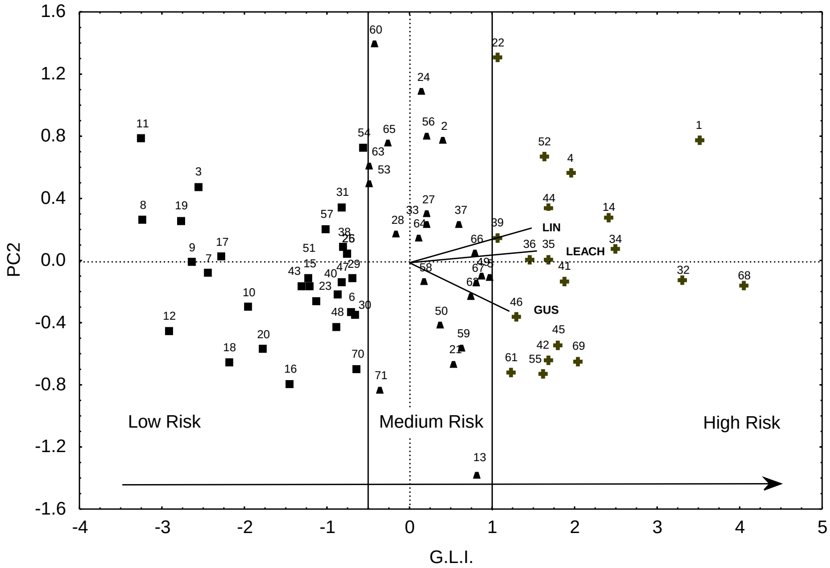

Fig. 2. GLI calculated by PCA of the leachability indexes of 71 pesticides. All the original variables (the indexes) are represented by the loadings (the lines). The cumulative explained variance of this PCA is 96.7% of the total variance , the first principal component (PC1: GLI Index) accounts for 87.5% of data variability. Three classes of risk are indicated with arbitrary cut-off values.

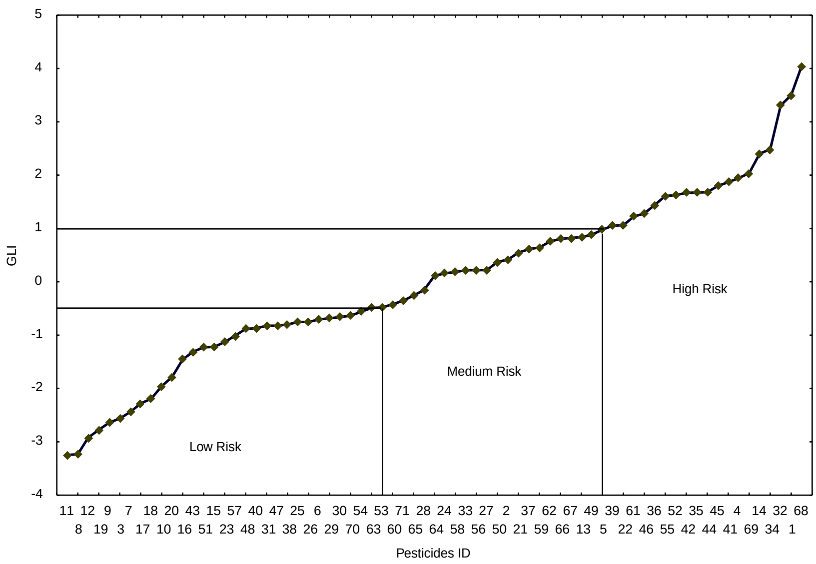

Fig. 3. Pesticides ranking according to their Global Leachability tendency. The chemicals are ranked according to their GLI value and the three risk classes for water pollution are highlighted.

score), while the third class includes chemicals with low mobility potential (low GLI score) that are therefore of less concern with regard to water. The second class collects pesticides of medium leaching tendency.

The presence of groups of chemicals allowed the setting of threshold values (-0.5 and 1). The cut-off values for the definition of the three classes are clearly arbitrary, and were chosen by observing the PC1 pesticide distribution in Fig. 2: adjustments in the cut-off values, based on expert judgment, could obviously redefine the location of some border-line chemicals. In Fig. 3 the chemicals are ranked according to their GLI value and the three classes of risk are indicated. In spite of the arbitrary trigger value definition, the method allows pesticides to be ranked for leachability and identifies, fast and clearly, the potentially most leachable pesticides. Like all ranking methods this procedure allows a qualitative and relative analysis of pesticide behaviour, and has no quantitative or absolute value.

4. Conclusions

The application of a multivariate technique like principal component analysis to different indexes of pesticide leachability allows:

- The introduction of a single "super index", the so-called Global Leachability Index (GLI), for a preliminary ranking of the data set, mainly according to soil/water partition behaviour.
- The identification of three classes of risk in the data set and a preliminary method for screening chemicals according to their leaching tendency, highlighting those pesticides of high concern for water contamination and, consequently, for impairment of drinking water.
- The possibility of making a list of the most leachable chemicals, in accordance with the need to identify potentially contaminating chemicals commonly used in agriculture along the river Amu Darya, correlated with their load, time-period of application and river flow. The eventual development of a simple model for a final screening before the analytical survey, could be a good result for the project (EU-INTASS-OPAL — Investigation of innovative pollution clean-up and avoidance strategies for surface water and groundwater resources at the "Disaster Zone" of the Amu Darya lower).
- The proposal of this multivariate approach, obviously applicable to any selected chemical data set, as an invaluable tool for an early assessment of environmental chemical distribution, especially for developing countries where there is a lack of economic resources and analytical facilities.

Acknowledgements

This research was partially funded by the European Community through the INTAS programmes IMWT (Integrated Water Management Tools) and OPAL (Investigation of innovative pollution clean-up and avoidance strategies for surface water and groundwater resources at the "Disaster Zone" of the Amu Darya lower)

The authors are grateful to Dr. Jochen Froebrich for his collaboration.

Appendix A

Data used (properties and units) for Leachability Indexes calculations.

ID	CAS	Pesticides	Log $t_{1/2}$	V_p (mmHg)	Sw (mg/L)	H (atm*m^3/mol)	Log Kow	Log Koc
1	030560-19-1	Acephate	1	1.70E−06	8.18E+05	5.01E−13	−0.85	0.3
2	135410-20-7	Acetamiprid	0.3	7.50E−09	4.20E+03	6.92E−08	0.8	3.32
3	082657-04-3	Bifenthrin	2.1	1.80E−07	1.00E−01	1.00E−06	6	5.38
4	034681-10-2	Butocarboxim	0.9	7.95E−05	3.50E+04	5.70E−10	1.1	1.56
5	000063-25-2	Carbaryl	1.45	1.36E−06	1.20E+02	4.36E−09	2.36	2.4
6	002921-88-2	Chlorpyrifos	2.08	2.03E−05	1.40E+00	2.93E−06	4.96	3.7
7	068359-37-5	Cyfluthrin-Beta	1.48	1.50E−10	2.00E−03	1.50E−10	5.95	5
8	091465-08-6	Cyhalothrin-Lambda	1.92	1.50E−09	5.00E−03	1.48E−06	7	5.68
9	052315-07-8	Cypermethrin	2.05	3.07E−09	4.00E−03	4.20E−07	6.6	5
10	052315-07-8	Cypermethrin-Zeta	1.45	1.88E−09	4.50E−02	4.20E−07	6.6	4.52
11	000050-29-3	p,p′-DDT	3.1	1.88E−07	5.50E−03	8.32E−06	6.91	5.4
12	052918-63-5	Deltamethrin	1.36	9.30E−11	2.00E−04	3.09E−07	6.2	5.03
13	000115-32-2	Dicofol	2	3.98E−07	8.00E−01	2.42E−07	5.02	1.88
14	000060-51-5	Dimethoate	1.2	8.25E−06	2.50E+04	1.05E−10	0.78	1.3
15	000115-29-7	Endosulfan	1.85	1.73E−07	3.25E−01	6.50E−05	3.83	4.09
16	066230-04-4	Esfenvalerate	2.46	1.50E−09	2.00E−03	3.14E−07	6.22	3.72
17	153233-91-1	Etoxazole	1.28	1.64E−08	7.54E−02	1.03E−07	5.59	5.26
18	064257-84-7	Fenpropathrin	0.7	5.48E−06	1.41E−02	1.79E−04	5.7	4.47
19	111812-58-9	Fenpyroximate	1.7	5.63E−08	1.46E−02	2.14E−06	5.01	5.54
20	051630-58-1	Fenvalerate	1.9	1.50E−09	2.00E−03	3.45E−08	6.2	4
21	120068-37-3	Fipronil	2.56	2.78E−09	1.90E+00	8.42E−10	4	2.92
22	002540-82-1	Formothion	0	8.48E−07	2.60E+03	1.10E−10	1.48	1
23	078587-05-0	Hexythiazox	0.9	2.55E−08	5.00E−01	2.37E−08	5.57	3.79
24	138261-41-3	Imidacloprid	−0.8	3.00E−12	6.10E+02	1.65E−15	0.57	3.7
25	144171-61-9	Indoxacarb DPX-JW062	0.7	7.50E−07	5.00E−01	2.72E−13	4.6	3.59
26	173584-44-6	Indoxacarb DPX-KN128	0.7	7.50E−07	5.00E−01	2.72E−13	4.6	3.59
27	000121-75-5	Malathion	1.04	3.38E−06	1.45E+02	4.89E−09	2.36	3.26
28	000298-00-0	Parathion-methyl	1.64	3.50E−06	3.77E+01	1.00E−07	2.86	3.7
29	002310-17-0	Phosalone	0.6	4.54E−08	3.05E+00	3.94E−07	4.38	3.26
30	002312-35-8	Propargite	1.99	4.50E−08	5.00E−01	4.15E−08	5	3.6
31	024017-47-8	Triazophos	1.08	2.90E−06	3.90E+01	4.84E−08	3.34	4.5
32	000052-68-6	Trichlorfon	1.65	7.80E−06	1.20E+05	1.70E−11	0.51	1
33	034256-82-1	Acetochlor	1.26	3.38E−08	2.23E+02	2.23E−08	3.03	3.35
34	120162-55-2	Azimsulfuron	2.08	3.00E−11	1.05E+03	3.75E−17	0.65	2.11
35	083055-99-6	Bensulfuron-methyl	2.15	2.10E−14	1.20E+02	3.78E−15	1.8	2.57
36	025057-89-0	Bentazone	1.08	3.45E−06	5.00E+02	2.18E-09	2.34	1.57
37	001689-84-5	Bromoxynil	1	4.72E−08	1.30E+02	1.32E−10	2.8	2.64
38	099129-21-2	Clethodim	0.48	7.50E−08	1.36E+00	1.16E−11	4.21	3.72
39	000094-75-7	Desormone (2,4 D)	0.85	8.25E−05	6.77E+02	3.54E−08	2.81	1.78
40	079241-46-6	Fluazifop-p-butyl	1.45	2.48E−07	1.00E+00	6.22E−07	4.5	3.76
41	098967-40-9	Flumetsulam	1.78	2.78E−12	4.90E+01	2.47E−13	0.21	1.97
42	002164-17-2	Fluometuron	2	9.38E−07	1.10E+02	1.80E−09	2.42	2
43	077501-90-7	Fluoroglycofen-ethyl	−0.35	9.98E−01	6.00E−01	4.32E−10	3.65	4.19
44	069377-81-7	Fluroxypyr	0.95	2.84E−11	9.10E+00	1.05E−13	−1.24	1.14
45	069806-34-4	Haloxyfop	2	9.98E−09	4.34E+01	3.74E−11	1.34	1.95
46	002212-67-1	Molinate	1.4	5.60E−03	9.70E+02	4.10E−06	3.21	1.92
47	001836-75-5	Nitrophene	2.08	1.00E−07	1.00E+00	2.55E−07	4.64	3.9
48	040487-42-1	Pendimethalin	2.08	3.00E−05	3.00E−01	8.56E−07	5.18	3.7

49	000709-98-8	Propanil	1.18	9.08E−06	1.52E+02	1.71E−08	3.07	2.17
50	094051-08-8	Quizalofop-p	1.88	4.29E−10	3.00E−01	1.74E−13	3.57	2.74
51	100646-51-3	Quizalofop-p-ethyl	0	4.69E−09	4.00E−01	1.06E−08	4.28	3.73
52	101200-48-0	Tribenuron-methyl	0.85	3.90E−10	2.80E+02	1.02E−13	−0.44	1.66
53	017804-35-2	Benomyl	−0.1	3.70E−09	3.80E+00	4.93E−12	2.12	3.28
54	116255-48-2	Bromuconazole	2.08	3.00E−08	5.00E+01	2.99E−10	3.24	4.46
55	010605-21-7	Carbendazim	2.56	7.50E−10	8.00E+00	2.12E−11	1.52	2.35
56	005234-68-4	Carboxin	0	1.80E−07	1.99E+02	2.80E−10	2.14	2.41
57	083657-24-3	Diniconazole	2.08	3.68E−05	4.00E+00	3.97E−07	4.3	4.31
58	106325-08-0	Epoxiconazole BAS 480F	1.95	7.50E−08	6.63E+00	3.98E−10	3.44	3.25
59	136426-54-5	Fluquinconazole	2.48	4.80E−11	1.00E+00	2.06E−11	3.24	2.87
60	076674-21-0	Flutriafol	2.56	5.33E−11	1.30E+02	1.63E−13	2.29	4.74
61	066246-88-6	Penconazole	2.54	2.78E−06	7.30E+01	1.42E−08	3.72	2.62
62	060207-90-1	Propiconazole	1.85	4.20E−07	1.10E+02	4.12E−09	3.72	2.82
63	107534-96-3	Tebuconazole	2.08	1.28E−08	3.60E+01	9.87E−11	3.7	4.32
64	023564-05-8	Thiophanate-methyl	1.45	7.13E−08	3.50E+00	0.00E+00	1.4	3.26
65	000137-26-8	Thiram	−0.3	1.73E−05	3.00E+01	0.00E+00	1.73	2.83
66	043121-43-3	Triadimefon	1.26	1.50E−08	7.15E+01	8.11E−11	2.77	2.48
67	026644-46-2	Triforine	1.32	2.00E−07	3.00E+01	3.82E−09	2.2	2.3
68	000052-51-7	Bronopol	1.48	1.26E−05	2.50E+05	1.33E−11	−0.64	0
69	051707-55-2	Thidiazuron	2.16	2.30E−11	3.10E+01	3.33E−13	1.77	1.86
70	004602-84-0	Farnesol	1.48	3.94E−05	1.29E+00	2.52E−04	5.77	3.12
71	007212-44-4	Nerolidol	1.88	5.92E−04	1.53E+00	1.81E−04	5.68	3.02

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