Chapter

Development of a Method for Prediction of Risk of Surface and Groundwater Contamination with Pesticides and Their Dangerous Aspects for Human Health

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Abstract

The probability of groundwater contamination is high enough because groundwater has different origins: a majority of them are formed by atmospheric precipitation filtration through soil layer or due to condensation of water vapors directly into the ground. Pesticides could be one of such hazardous groundwater pollutants. We developed two methods for the hazardous effect on human organism while consuming contaminated water prediction: risk acceptance assessment and integral groundwater contamination hazard index (IGCHI) evaluation in points according to special scale.

Keywords: groundwater, surface water, hazard, pesticide, leaching, health

1. Introduction

Growing of world population, agriculture, and industrial development led to the increase of ecotoxicants in environmental pollution. Among these ecotoxic substances, pesticides have a special place [1, 2]. Migrating through the soil profile, pesticides create the danger of groundwater contamination that requires their constant control and monitoring [1, 2]. Some older and cheap pesticides, whose application is forbidden in developed countries but are still used in a lot of developing countries, can persist in soil, ground, and surface water for years [3].

At the present time, around 65% of European and 70% of Ukrainian rural and urban population have been using ground (shaft wells) and middle water (artesian wells) for drinking.

As groundwater forms in two ways, (1) water from atmosphere precipitations filtrates through soil or (2) condensation of vapors into the ground, the possibility of groundwater chemical contamination is rather high [4].

That is why prediction of the risk of groundwater contamination with different classes of pesticides, as well as hygienic assessment of their impact on public health is very actual nowadays.

2. Prediction of the risk of ground and surface water contamination with pesticides and its danger to human health in areas with irrigation farming

The prediction of migration opportunities in groundwater of pesticides in different soil and climatic conditions could be carried out by a number of indices.

For example, leaching potential index [groundwater ubiquity score (GUS)] [4] is calculated using the below formula:

$$GUS = \log \tau_{50} \times [4 - \log K_{oc}],$$

where τ_{50}—half-life in soil, days; and
K_{oc}—sorption coefficient of organic carbon.

For the assessment of GUS values, we have used net approach: probability of pesticide leaching into groundwater is present (GUS > 2,8); probability of pesticide leaching into groundwater is possible (GUS < 1,8); pesticides possibly not leached into groundwater (GUS = 1,8–2,8) [5].

US Environmental Protection Agency (EPA) has developed SCI-GROW screening method for the determination of maximum pesticide concentration in groundwater [6], and this model is widely used. SCI-GROW index counts the substance's half-life period in soil, organic carbon sorption coefficient, and pesticide application rate and frequency. The calculation gives the highest possible groundwater concentration of substance in mg/l.

Unfortunately, GUS index has disadvantages. For example, not all significant parameters that can influence the behavior of pesticide in the system "groundwater" are taking into account; run-off to surface water cannot be assessed using this value.

LEACH index is better. It determines also the possibility of river contamination and takes into account the maximum number of parameters that can influence the transition of pesticides from soil into other mediums.

The index of potential contamination of groundwater and river water LEACH was calculated according to the below formula [7]:

$$LEACH_{\text{mod.}} = \frac{S_w \times DT_{50field}}{K_{oc}},$$

where S_w—water solubility, mg/l;
$DT_{50\ field}$—half-life period substances in the soil in natural conditions, day; and
K_{oc}—organic carbon (o.c.) sorption coefficient, ml/g o.c.

Evaluation of the index: 0,0–1,0-low risk of pollution (3 class), 1,1–2,0-average (moderate) risk (2 class), and >2,0-high risk (1 class).

But all the above listed indices characterize only the potential of pesticide penetration into groundwater and surface water without the possibility of evaluation of risk for human organism while consumption of contaminated water.

So, method of comprehensive assessment of pesticides leaching into the water possible adverse effects on humans developed by us has been used for the SCI-GROW evaluation [8]. The principle of complex hygienic regulation takes into account the possibility of pesticide intake through inhalation, with drinking water and food and its safe levels, is in the base of this method. Pesticide acceptable daily intake with water (PADIW) compares with pesticide maximum possible daily intake with water (PMDIW), which ways of calculations in 3 steps is given below (**Figure 1**).

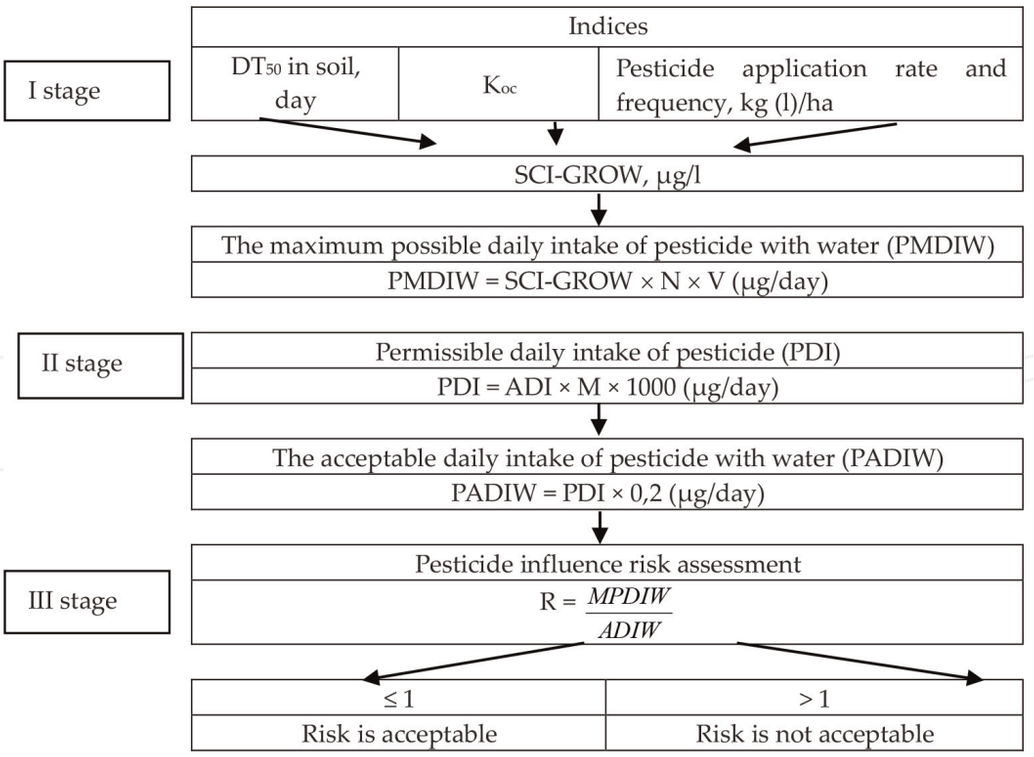

Figure 1.
A method for assessing the risk of adverse effects of pesticides on human health when consuming contaminated water. Notes: SCI-GROW—screening concentrations of pesticides in groundwater, μg/l; V—daily intake of water by human, l (3 l—in temperate climate, 5–10 l—in hot climate); ADI—acceptable daily intake of pesticide, mg/kg; M—average weight of person (60 kg); 1000—factor for conversion in micrograms.

Initially, one needs to calculate the SCI-GROW using computer program from EPA official Website. This indicator is based on the actual results of field studies; therefore, it gives the most realistic values. In order to obtain the maximum possible value of pesticide intake with water (PMDIW) by humans, SCI-GROW index is multiplied by the average daily consumption of water (for persons living in temperate climate-3 L, for those living in hot climate-5 to 10 L).

To evaluate the obtained indicator, it is necessary to calculate the permissible level of pesticide intake with water (PADIW). For this, firstly, the allowable daily dose (ADI) must be multiplied by the average weight of a person (M) (60 kg for nonprofessional contingents and 70 kg for professionals). Based on the principles of complex hygienic regulation, the amount of pesticide that entered the human body with water should not exceed 20% of the permissible daily intake. Therefore, the indicator obtained earlier is multiplied by 0.2.

Finally, the values of PMDIW and PADIW should be compared (R). If the R value is ≤1, risk is considered to be acceptable; and if R > 1, risk is not acceptable.

Also, we recommend integrated assessment of the potential hazard of pesticide exposure on the human organism when consuming contaminated drinking water to use the scale with four gradations (**Figure 2**). The scale includes three indices: LEACH, τ_{50} in water, and acceptable daily intake (ADI) [9, 10].

These three indicators mostly reflect the danger of a pesticide, when ingested with water. LEACH displays the maximum possible risk of contamination of water supply sources, both underground and surface, taking into account, the physical properties of the main pesticide and stability in soil. τ_{50} displays the possibility and duration of the presence of the pesticide in the potentially drinking water. ADI, the main and integral pesticide toxicity index, shows the possibility of the realization of the toxic effects of a substance, when it is present in water for a long period.

Indices	$LEACH_{\text{mod.}} = \frac{S_w \times \tau_{50\,field}}{K_{oc}}$, where Sw – water solubility, mg/l; τ_{50} field – half-life period substances in the soil in natural conditions, day; Koc – organic carbon (o.c.) sorption coefficient, ml/g o.c.	τ_{50} in water, day	Acceptable daily intake (ADI), mg/kg

Points, depends on index value			
Points	LEACH	τ_{50} in water	ADI
1	<0,01	<5	>0,02
2	0,01-0,1	5-10	0,0051–0,02
3	0,11-1,0	11-30	0,0021–0,005
4	>1,0	>30	≤0,002

Integral groundwater contamination hazard index (IGCHI)
IGCHI = LEACH + τ_{50} + ADI (points)

IGCHI evaluation and determination of hazard class	
3 and 4 points	substances are low hazardous for human (4 class)
5 and 6 points	moderately hazardous (3 class)
7 and 8 points	hazardous (2 class)
9 and 10 points	highly hazardous (1B class)
11 and 12 points	extremely hazardous (1A class)

Figure 2.
Method of hazard prediction of contaminated water by pesticide water effect on human body. Note. Evaluation of the LEACH index: 0,0–1,0—low risk of pollution (3 class), 1,1–2,0—average (moderate) risk (2 class), and >2,0—high risk (1 class).

For testing proposed by us, methods of risk assessment of pesticide-contaminated drinking water, we have studied widely used in agriculture representatives of the most perspective chemical classes of herbicides, fungicides, and insecticides (**Tables 1–3**). The main physical and chemical properties of studied compounds are given in **Table 1–3**.

The conditions of studied pesticides application and stability are given in **Table 4**.

International IUPAC classification [15] was used to assess the literature data about the stability and mobility of substances in the soil. The first includes three classes: 1-highly persistent (with DT_{50} more than 100 days), 2-moderately persistent (30–100 days), and 3-low persistent (less than 30 days).

According to IUPAC classification [15], most of fungicides and insecticides by persistence in soil may be attributed to moderately persistent (2 class); all herbicides, to low persistent (3 class). Exceptions are highly persistent insecticides, imidacloprid and chlorantraniliprole; fungicides, sedaxane, boscalid, fluxapyroxad, and azoxystrobin; and moderately persistent herbicides, triasulfurone and imazethapyr (**Table 3**). It should be noted that these literature data are very average. For example, in the soil and climatic conditions of the southern and southeastern European countries, including Ukraine, the transformation of the studied substances occurs much faster due to microbiological degradation (typical for these regions, black soils are rich in microflora) [8].

Trade name	Chemical name (IUPAC)	lg K_{ow}	Solubility in water, mg/l	K_{oc}
Triazoles				
Difenocona-zole	3-chloro-4-[(2RS.4RS;2RS.4SR)-4-methyl-2-(1H-1.2.4-triazol-1-ylmethyl)-1.3-dioxolan-2-yl]phenyl 4-chlorophenyl ether	4.2	15.0	3760
Tebuconazole	(RS)-1-p-chlorophenyl-4.4-dimethyl-3-(1H-1.2.4-triazol-1-ylmethyl)pentan-3-ol	3.7	32.0	769
Penconazole	(RS)-1-[2-(2.4-dichlorophenyl)pentyl]-1H-1.2.4-triazole	3.72	73.0	2205
Strobilurines				
Pyraclostrobin	methyl {2-[1-(4-chlorophenyl)pyrazol-3-yloxymethyl]phenyl}(methoxy)carbamate	3.99	1.9	9304
Azoxystrobin	methyl (E)-2-{2-[6-(2-cyanophenoxy)pyrimidin-4-yloxy]phenyl}-3-methoxyacrylate	2.5	6.7	589
Trifloxystrobin	methyl (E)-methoxyimino-{(E)-α-[1-(α.α.α-trifluoro-m-tolyl)ethylideneaminooxy]-o-tolyl}acetate	4.5	0.61	2377
Ethylene-bis-dithiocarbamate				
Metiram	zinc ammoniate ethylenebis(dithiocarbamate) - poly (ethylenethiuram disulfide)	1.76	2.0	998
Mancozeb	manganese ethylenebis(dithiocarbamate) (polymeric) complex with zinc salt	1.33	6.2	500,000
Cyanopyrrole				
Fludioxonil	4-(2.2-difluoro-1.3-benzodioxol-4-yl)-1H-pyrrole-3-carbonitrile	4.12	1.8	145,600
Anilidepyrimidines				
Cyprodinil	4-cyclopropyl-6-methyl-N-phenylpyrimidin-2-amine	4.5	13.0	2277
Pyrimethanil	N-(4.6-dimethylpyrimidin-2-yl)aniline	2.84	0.121	301
Valifenale	methyl N-(isopropoxycarbonyl)-L-valyl-(3RS)-3-(4-chlorophenyl)-β-alaninate	3.11	24.1	1686
Pyrazolecarboxamides				
Fluxapyroxad	3-(difluoromethyl)-1-methyl-N-(3′.4′.5′-trifluorobiphenyl-2-yl)pyrazole-4-carboxamide	3.13	3.44	728
Isopyrazam	mixture of 2 isomers 3-(difluoromethyl)-1-methyl-N-[(1RS.4SR.9RS)-1.2.3.4-tetrahydro-9-isopropyl-1.4-methanonaphthalen-5-yl]pyrazole-4-carboxamide and 2 isomers 3-(difluoromethyl)-1-methyl-N-[(1RS.4SR.9SR)-1.2.3.4-tetrahydro-9-isopropyl-1.4-methanonaphthalen-5-yl]pyrazole-4-carboxamide	4.25	0.55	2416
Penthiopyrad	(RS)-N-[2-(1.3-dimethylbutyl)-3-thienyl]-1-methyl-3-(trifluoromethyl)pyrazole-4-carboxamide	4.62	1.375	804
Sedaxane	mix of: trans-isomers 2′-[(1RS.2SR)-1.1′-bicycloprop-2-yl]-3-(difluoromethyl)-1-methyl-1H-pyrazole-4-carboxanilide and 2 cis-isomers 2′-[(1RS.2RS)-1.1′-bicycloprop-2-yl]-3-(difluoromethyl)-1-methyl-1H-pyrazole-4-carboxanilide	3.3	14.0	534

Trade name	Chemical name (IUPAC)	lg K_{ow}	Solubility in water, mg/l	K_{oc}
Anilides				
Benalaxyl-M	methyl N-(phenylacetyl)-N-(2.6-xylyl)-D-alaninate	3.67	33.0	7175
Boscalid	2-chloro-N-(4′-chlorobiphenyl-2-yl)nicotinamide	2.96	4.6	772

Table 1.
Physical and chemical properties of the studied fungicides [11, 12].

Trade name	Chemical name (IUPAC)	lg K_{ow}	Solubility in water, mg/l	K_{oc}
Organophosphates				
Chlorpyrifos	O.O-diethyl O-3.5.6-trichloro-2-pyridyl phosphorothioate	4.7	1.05	8151
Dimethoate	2-dimethoxyphosphinothioylthio-N-methylacetamide	0.704	39,800	28.3
Pyrethroid				
Bifenthrin	2-methyl-3-phenylbenzyl (1RS)-cis-3-(2-chloro-3.3.3-trifluoroprop-1-enyl)-2.2-dimethylcyclopropanecarboxylate	6.6	0.001	236,610
Cypermethrin	(RS)-α-cyano-3-phenoxybenzyl (1RS.3RS;1RS.3SR)-3-(2.2-dichlorovinyl)-2.2-dimethylcyclopropanecarboxylate	5.3	0.009	156,250
Alpha-cypermethrin	Racemate comprising (R)-α-cyano-3-phenoxybenzyl (1S)-cis-3-(2.2-dichlorovinyl)-2.2-dimethylcyclopropanecarboxylate and (S)-α-cyano-3-phenoxybenzyl (1R)-cis-3-(2.2-dichlorovinyl)-2.2-dimethylcyclopropanecarboxylate	6.94	0.004	57,889
Lambda-cyhalothrin	(R)-a-cyano-3-phenoxybenzyl (1S)-cis-3-[(Z)-2-chloro-3.3.3-trifluoropropenyl]-2.2-dimethylcyclopropanecarboxylate and (S)-a-cyano-3-phenoxybenzyl (1R)-cis-3-[(Z)-2-chloro-3.3.3-trifluoropropenyl]-2.2-dimethylcyclopropanecarboxylate	5.5	0.005	283,707
Neonicotinoid				
Thiamethoxam	(EZ)-3-(2-chloro-1.3-thiazol-5-ylmethyl)-5-methyl-1.3.5-oxadiazinan-4-ylidene(nitro)amine	−0.13	4100	56.2
Imidacloprid	(E)-1-(6-chloro-3-pyridylmethyl)-N-nitroimidazolidin-2-ylideneamine	0.57	610	225
Pyrazolium				
Tebufenpyrad	N-(4-tert-butylbenzyl)-4-chloro-3-ethyl-1-methylpyrazole-5-carboxamide	4.93	2.39	5992
Chlorantraniliprole	3-bromo-4′-chloro-1-(3-chloro-2-pyridyl)-2′-methyl-6′-(methylcarbamoyl)pyrazole-5-carboxanilide	4.22	0.88	362
Benzoylurea				
Novaluron	(RS)-1-[3-chloro-4-(1.1.2-trifluoro-2-trifluoromethoxyethoxy)phenyl]-3-(2.6-difluorobenzoyl)urea	4.3	0.003	9598

Table 2.
Physical and chemical properties of the studied insecticides [11].

Trade name	Chemical name (IUPAC)	lg K_{ow}	Solubility in water, mg/l	K_{oc}
Chloroacetamides				
Acetochlore	2-chloro-N-ethoxymethyl-6′-ethylacet-o-toluidide	4.14	282	156
Dimetachlor	2-chloro-N-(2-methoxyethyl)acet-2′.6′-xylidide	2.17	2300	69
Propizochlor	2-chloro-6′-ethyl-N-isopropoxymethylacet-ortho-toluidide	3.3	90.8	291
S-metolachlor	Mix of: (aRS.1S)-2-chloro-6′-ethyl-N-(2-methoxy-1-methylethyl)acet-o-toluidide and (aRS.1R)-2-chloro-6′-ethyl-N-(2-methoxy-1-methylethyl)acet-o-toluidide	3.05	480	226.1
Metasachlor	2-chloro-N-(pyrazol-1-ylmethyl)acet-2′.6′-xylidide	2.49	450	54
Sulfonil-carbonyl-triazolinone				
Thiencarbazon-methyl	Methyl 4-[(4.5-dihydro-3-methoxy-4-methyl-5-oxo-1H-1.2.4-triazol-1-yl)carbonylsulfamoyl]-5-methylthiophene-3-carboxylate	−1.98	436	100
Oxazoles				
Topramezone	[3-(4.5-dihydro-1.2-oxazol-3-yl)-4-mesyl-o-tolyl](5-hydroxy-1-methylpyrazol-4-yl)methanone	−1.52	100,000	15.0–296.7
Isoxaflutole	(5-cyclopropyl-1.2-oxazol-4-yl)(α.α.α-trifluoro-2-mesyl-p-tolyl)methanone	2.32	6.2	112
Triketones				
Mesotrione	2-(4-mesyl-2-nitrobenzoyl)cyclohexane-1.3-dione	0.11	160	80
Sulfonylurea				
Foramsulfu-rone	1-(4.6-dimethoxypyrimidin-2-yl)-3-[2-(dimethylcarbamoyl)-5-formamidophenylsulfonyl]urea	−0.78	3293	78
Iodsulfurone methyl-sodium	Sodium ({[5-iodo-2-(methoxycarbonyl)phenyl]sulfonyl} carbamoyl) (4-methoxy-6-methyl-1.3.5-triazin-2-yl)azanide	1.59	25,000	45
Phosphonoglycine				
Glyphosate	N-(phosphonomethyl)glycine	−3.2	10,500	21,699
Sulfonylurea with triazine heterrocycle				
Tritosulfuron	N-{[4-methoxy-6-(trifluoromethyl)-1.3.5-triazin-2-yl]carbamoyl}-2-(trifluoromethyl)benzene-1-sulfonamide	2.93	78.3	7.5
Prosulfuron	1-(4-methoxy-6-methyl-1.3.5-triazin-2-yl)-3-[2-(3.3.3-trifluoropropyl)phenylsulfonyl]urea	1.5	4000	14.2
Metsulfuron-methyl	Methyl 2-(4-methoxy-6-methyl-1.3.5-triazin-2-ylcarbamoylsulfamoyl)benzoate	−1.87	2790	12.0
Triasulfuron	1-[2-(2-chloroethoxy)phenylsulfonyl]-3-(4-methoxy-6-methyl-1.3.5-triazin-2-yl)urea	−0.59	815	60
Tribenuron-methyl	Methyl 2-[4-methoxy-6-methyl-1.3.5-triazin-2-yl (methyl)carbamoylsulfamoyl]benzoate	0.38	2483	35
Sulfonylurea with pyrimidine heterocycle				
Rimsulfuron	1-(4.6-dimethoxypyrimidin-2-yl)-3-(3-ethylsulfonyl-2-pyridylsulfonyl)urea	−1.46	7300	50.3

Trade name	Chemical name (IUPAC)	lg K_{ow}	Solubility in water, mg/l	K_{oc}
Nicosulfuron	2-[(4.6-dimethoxypyrimidin-2-ylcarbamoyl)sulfamoyl]-N.N-dimethylnicotinamide	0.61	7500	30
Chlorimuron-ethyl	Ethyl 2-(4-chloro-6-methoxypyrimidin-2-ylcarbamoylsulfamoyl)benzoate	0.11	1200	106
Imidazolinone				
Imazapyr	2-[(RS)-4-isopropyl-4-methyl-5-oxo-2-imidazolin-2-yl]nicotinic acid	0.11	9740	125
Imazamox	2-[(RS)-4-isopropyl-4-methyl-5-oxo-2-imidazolin-2-yl]-5-methoxymethylnicotinic acid	5.36	626,000	11.6
Imazethapyr	5-ethyl-2-[(RS)-4-isopropyl-4-methyl-5-oxo-2-imidazolin-2-yl]nicotinic acid	1.49	1400	52
Pyrimidinyl carboxy compound				
Bispyribac-sodium	Sodium 2.6-bis(4.6-dimethoxypyrimidin-2-yloxy) benzoate	−1.03	64,000	302
Semicarbazone				
Diflufenzopyr	2-{(EZ)-1-[4-(3.5-difluorophenyl)semicarbazono] ethyl}nicotinic acid	1.09	5850	87

Table 3.
Physical and chemical properties of the studied herbicides [11].

Half of the studied herbicides and insecticides are resistant or highly resistant in water, as they are poorly decomposed by photolysis and hydrolysis. Fungicides are much less resistant (**Table 3**).

It was found that according to GUS index, there is no risk of leaching into groundwater for most of the studied herbicides; for the rest, it is low. Only for one fungicide (topramezone) and most of insecticides, the risk of groundwater leaching is high (**Table 5**). It could be explained by their high toxicity (very low ADI values) and relatively high persistency in soil and water (**Table 4**).

The calculated maximum possible concentrations of the studied fungicides, herbicides, and insecticides SCI-GROW in groundwater indicate that the risk to humans when consuming such water is acceptable (**Table 5**). SCI-GROW values exceed 1 μg/l only for triasulfurone, imazamox, imazethapyr, and chlorantraniliprole. But the high risk will not be realized as shown in **Table 5**; IGHI values for these pesticides are 7, 6, 6, and 7, respectively.

According to IGCHI index, fungicides, penconazole and azoxystrobin; herbicides, dimetachlor, propizochlor, s-metolachlor, foramsulfurone, glyphosate, and rimsulfuron are less hazardous for human organism in case of consuming contaminated water. Fungicides, difenoconazole, pyraclostrobin, trifloxystrobin, metiram, mancozeb, fludioxonil, valifenale, fluxapyroxad, isopyrazam, penthiopyrad, and boscalid; herbicides, metazachlor, thiencarbazone-methyl, isoxaflutole, iodsulfuron methyl-sodium, metsulfuron-methyl, nicosulfuron, chlorimuron-ethyl, imazapyr, imazamox, imazethapyr, and diflufenzopyr; insecticides, thiamethoxam and imidacloprid are moderately hazardous (**Table 5**). Only insecticides, chlorpyrifos, bifenthrin, lambda-cyhalothrin, and tebufenpyrad are highly and extremely hazardous because of their high toxicity and water pollution possibility. Rest of the studied compounds is hazardous (2 class) to human organism.

Active ingredient (a.i.)	Maximum application rate of a.i., kg/ha	DT_{50} soil, day	DT_{50} water, day	Acute oral LD_{50} (mg/kg) (rat)	ADI, mg/kg	PDI, mg/day
Fungicides						
Difenoconazole	0.250	85 (20–265)	3.0	1453	0.01	0.6
Tebconazole	0.175	47.1 (25.8–91.6)	42.6	1700	0.03	1.8
Penconazole	0.160	90 (22–115)	2.0	>2000	0.03	1.8
Pyraclostrobin	0.100	32 (8–55)	2.0	>5000	0.03	1.8
Azoxystrobin	0.200	180.7 (120.9–261.9)	6.1	>5000	0.20	12.0
Trifloxystrobin	0.175	7 (2–12)	1.1	>5000	0.10	6.0
Metiram	1.750	7 (~7)	0.7	>5000	0.03	1.8
Mancozeb	1.625	18 (1)	0.2	>5000	0.05	3.0
Fludioxonil	0.250	20.5 (8–43)	2.0	>5000	0.37	22.2
Cyprodinil	0.375	45 (11–98)	12.5	>2000	0.03	1.8
Pyrimethanil	0.480	29.5 (23–54)	16.5	4150	0.17	10.2
Valifenale	0.306	1.9–12.0 hours	5.0	>5000	0.07	4.2
Fluxapyroxad	0.126	151 (53–424)	4.4	>2000	0.02	1.2
Isopyrazam	0.450	72 (9.11–173)	2.3	2000	0.03	0.6
Penthiopyrad	0.390	47 (0.8–33.3)	9.9	>2000	0.10	6.0
Sedaxane	0.025	170 (54.6–188.0)	17.3	>2000	0.10	6.0
Benalaxyl-M	0.400	44 (36–124)	38.0	>2000	0.04	2.4
Boscalid	0.668	118 (28–208)	9.0	>5000	0.04	2.4
Herbicides						
Acetochlore	2.700	12.1 (7.0–17.0)	40.5	1929	0.0036	0.220
Dimetachlor	1.200	3.2 (2.3–15.6)	10.0	1600	0.1	6.000
Propizochlor	2.160	7.63 (10.0–15.0)	8.5	2290	0.025	1.500
S-metolachlor	1.920	21.0 (11.0–31.0)	9.0	2577	0.1	6.000
Metasachlor	1.250	6.8 (26.0–114.0)	216.0	3480	0.08	4.800
Thiencarbazone-methyl	0.045	17.0 (14.0–45.0)	118	>2000	0.23	13.80
Topramezone	0.075	26.1 (10.8–69.3)	30	>2000	0.001	0.060
Isoxaflutole	0.1125	1.3 (0.5–2.4)	11	>5000	0.02	1.200
Mesotrione	0.110	5.0 (3.0–7.0)	>30	>5000	0.01	0.600
Foramsulfurone	0.045	5.5 (12.0–15.0)	10	>5000	0.25	30.00
Iodsulfurone methyl-sodium	0.0015	3.2 (0.8–10.3)	31	2448	0.03	1.800
Glyphosate	1.6654	23.79 (5.7–40.9)	2.5	>2000	0.3	18.00
Tritosulfuron	0.0500	12 (3–21)	20.0	>5000	0.15	9.0
Prosulfuron	0.0150	11.9 (3.8–38.9)	173.0	546	0.02	1.2
Metsulfuron-methyl	0.0060	13.3 (7.3–37.1)	224.3	>5000	0.22	13.2
Triasulfuron	0.0062	38.5 (16.1–92.4)	217.0	>5000	0.01	0.6

Active ingredient (a.i.)	Maximum application rate of a.i., kg/ha	DT_{50} soil, day	DT_{50} water, day	Acute oral LD_{50} (mg/kg) (rat)	ADI, mg/kg	PDI, mg/day
Tribenuron-methyl	0.0188	10 (5–20)	139.0	>5000	0.01	0.6
Rimsulfuron	0.0125	10.8 (5.6–17.7)	6.0	>5000	0.1	6.0
Nicosulfuron	0.0600	19.3 (8.9–63.3)	65.0	>5000	2.0	120.0
Chlorimuron-ethyl	0.0094	28 (14–42)	21.0	>4102	0.02	1.2
Imazapyr	0.0550	11 (5.9–16.5)	30.0	>2000	2.5**	156.0
Imazamox	0.0400	16.7 (8.1–14.0)	233	>5000	9.0	540.0
Imazethapyr	0.1200	51.0 (14.0–290.0)	520	>5000	0.44	26.4
Bispyribac-sodium	0.0450	6.3 (2.1–7.6)	35.3	2635	0.01	0.6
Diflufenzopyr	0.0680	4.5 (8.0–18.0)	24.0	>5000	0.26	15.6
Insecticides						
Chlorpyrifos	0.720	27.6 (0.32–88.9)	36.5	66	0.001	0.060
Dimethoate	0.600	7.2 (4.6–9.8)	15.5	245	0.001	0.060
Bifenthrin	0.060	86.8 (5.4–267.0)	161.0	54.5	0.015	0.900
Cypermethrin	0.075	21.9 (14.0–199.0)	17.0	287	0.05	3.000
Alpha-cypermethrin	0.030	42.6 (14.0–112.0)	21.0	40	0.015	0.090
Lambda-cyhalothrin	0.0424	26.9 (10.1–47.5)	15.1	56	0.0025	0.150
Thiamethoxam	0.150	39.0 (7.0–72.0)	40.0	>1563	0.026	1.560
Imidacloprid	0.060	174 (104.0–228.0)	129.0	131	0.06	3.600
Tebufenpyrad	0.160	4.5 (0.05–22.4)	90.0	>202	0.01	0.600
Chlorantraniliprole	0.050	204.0 (123.0–561.0)	170.0	>5000	1.56	93.60
Novaluron	0.060	96.5 (33.0–160.0)	17.5	>5000	0.01	0.600

Note. PDI: permissible daily intake of pesticide.
***The table gives the initial data for the evaluation and shows the results of calculations of the index proposed by us (testing the method).*

Table 4.
The conditions of studied pesticides' application and stability [9–11, 13, 14].

Active ingredient	GUS	SCI-GROW (μg/l)	Leach		IGCHI	
			Value	Class	Value	Class
Fungicides						
Difenoconazole	0.9	1.79×10^{-2}	3.391×10^{-1}	3	6	3
Tebconazole	2.0	2.77×10^{-1}	$1.9599 \times 10^{+0}$	2	7	2
Penconazole	1.36	3.38×10^{-2}	$2.9796 \times 10^{+0}$	1	3	4
Pyraclostrobin	0.05	5.52×10^{-3}	6.500×10^{-3}	3	5	3
Azoxystrobin	2.60	1.98×10^{-1}	$2.0555 \times 10^{+0}$	1	4	4
Trifloxystrobin	0.53	1.43×10^{-5}	1.800×10^{-3}	3	5	3
Metiram	0.00	5.35×10^{-3}	1.40×10^{-2}	3	5	3

Active ingredient	GUS	SCI-GROW (μg/l)	Leach		IGCHI	
			Value	Class	Value	Class
Mancozeb	−1.00	2.84×10^{-6}	2.000×10^{-4}	3	5	3
Fludioxonil	−2.48	5.35×10^{-3}	3.000×10^{-4}	3	5	3
Cyprodinil	1.01	2.33×10^{-2}	2.569×10^{-1}	3	7	2
Pyrimethanil	2.65	1.90×10^{-1}	1.19×10^{-2}	3	7	2
Valifenale	−0.68	1.97×10^{-5}	0.0071×10^{-3}	3	6	3
Fluxapyroxad	2.57	1.85×10^{-1}	7.135×10^{-1}	3	6	3
Isopyrazam	1.47	4.01×10^{-2}	1.64×10^{-2}	3	5	3
Penthiopyrad	2.33	1.31×10^{-1}	1.57×10^{-2}	3	6	3
Sedaxane	2.59	1.85×10^{-4}	$4.46 \times 10^{+0}$	1	8	2
Benalaxyl-M	0.41	9.34×10^{-3}	2.024×10^{-1}	3	8	2
Boscalid	2.56	2.10×10^{-1}	7.031×10^{-1}	3	6	3
Herbicides						
Acetochlore	1.58	2.58×10^{-2}	$3.073 \times 10^{+1}$	1	8	2
Dimetachlor	1.76	8.68×10^{-3}	$5.20 \times 10^{+2}$	1	4	4
Propizochlor	1.36	1.26×10^{-2}	$4.68 \times 10^{+0}$	1	4	4
S-metolachlor	1.91	4.85×10^{-2}	$6.581 \times 10^{+1}$	1	4	4
Metasachlor	2.17	4.73×10^{-2}	$9.50 \times 10^{+2}$	1	6	3
Thiencarbazone-methyl	2.46	1.03×10^{-1}	$1.962 \times 10^{+2}$	1	6	3
Topramezone	5.06	0.567×10^{-1}	$2.336 \times 10^{+4}$	1	8	2
Isoxaflutole	0.59	1.28×10^{-3}	$9.244 \times 10^{+2}$	1	6	3
Mesotrione	1.47	4.13×10^{-3}	$1.400 \times 10^{+1}$	1	7	2
Foramsulfurone	1.56	4.63×10^{-3}	$6.333 \times 10^{+2}$	1	4	4
Iodsulfurone methyl-sodium	0.71	1.64×10^{-3}	$5722 \times 10^{+3}$	1	6	3
Glyphosate	−0.36	5.35×10^{-3}	$1.979 \times 10^{+1}$	1	3	4
Tritosulfuron	2.81	2.43×10^{-1}	4.00×10^{-2}	3	7	2
Prosulfuron	5.11	$4.17 \times 10^{+0}$	$3.61 \times 10^{+0}$	1	7	2
Metsulfuron-methyl	3.99	6.89×10^{-1}	$8.626 \times 10^{+3}$	1	6	3
Triasulfuron	5.12	$4.13 \times 10^{+0}$	$1.255 \times 10^{+3}$	1	7	2
Tribenuron-methyl	2.40	4.17×10^{-2}	$1.419 \times 10^{+3}$	1	7	2
Rimsulfuron	3.23	3.17×10^{-1}	$2.569 \times 10^{+3}$	1	4	4
Nicosulfuron	3.25	2.38×10^{-1}	$1.583 \times 10^{+4}$	1	6	3
Chlorimuron-ethyl	3.16	3.55×10^{-1}	$4.755 \times 10^{+2}$	1	6	3
Imazapyr	1.98	4.02×10^{-2}	$1.286 \times 10^{+3}$	1	5	3
Imazamox	6.76	$3.92 \times 10^{+1}$	$2.026 \times 10^{+2}$	1	6	3
Imazethapyr	6.19	$2.59 \times 10^{+1}$	$7.808 \times 10^{+3}$	1	6	3
Bispyribac-sodium	1.68	3.41×10^{-2}	$1.611 \times 10^{+3}$	1	7	2
Diflufenzopyr	2.36	7.85×10^{-2}	$1.210 \times 10^{+3}$	1	5	3
Insecticides						
Chlorpyrifos	0.17	6.45×10^{-3}	1.15×10^{-2}	3	11	1A

Active ingredient	GUS	SCI-GROW (μg/l)	Leach		IGCHI	
			Value	Class	Value	Class
Dimethoate	1.06	2.36×10^{-3}	$1.38 \times 10^{+4}$	1	8	2
Bifenthrin	−2.76	$5.35 \times 10 - ^{3}$	1.13×10^{-6}	3	9	1B
Cypermethrin	−2.19	5.35×10^{-3}	1.15×10^{-5}	3	7	2
Alpha-cypermethrin	−1.53	$5.35 \times 10 - ^{3}$	7.74×10^{-6}	3	8	2
Lambda-cyhalothrin	−3.28	$5.35 \times 10 - ^{3}$	8.37×10^{-7}	3	9	1B
Thiamethoxam	4.69	$3.14 \times 10^{+0}$	$5.25 \times 10^{+3}$	1	6	3
Imidacloprid	3.74	$9.29 \times 10 - ^{1}$	$6.18 \times 10^{+2}$	1	6	3
Tebufenpyrad	0.58	1.11×10^{-2}	8.93×10^{-3}	3	9	1B
Chlorantraniliprole	4.22	$1.86 \times 10^{+0}$	$1.36 \times 10^{+0}$	2	7	2
Novaluron	0.02	5.20×10^{-3}	5.00×10^{-5}	3	8	2

Table 5.
Ground and surface water migration parameters of studied pesticides [8–10, 13, 14].

The estimate presented is approximate. In each particular case, it is necessary to assess the risk of a pesticide when it enters the human body with water separately, taking into account the soil and climatic conditions of the application area, the norms of application, the groundwater depth, and other background factors.

3. Conclusions

1. It was determined that according to IUPAC classification, most of the pesticides pertain to low or moderate in soil, but for some of them, there is a risk of groundwater contamination.

2. Two methods for hazardous effect on human organism while consuming contaminated water prediction were developed by us. For integrated assessment of the potential hazard of pesticide exposure on the human organism when it enters ground and surface waters, we developed integral groundwater contamination hazard index (IGCHI), which includes assessment of three indices: LEACH, τ_{50} in water, and allowable daily intake (ADI) on a scale, which provides four gradations. For the evaluation of the parameters of SCI-GRW, a method of comprehensive assessment including establishment of the maximum possible daily intake of pesticide with water (PMDIW) and subsequently compared with acceptable daily intake of pesticide with water (PADIW) developed by us was used.

3. It was shown that when the human body reaches the majority of investigated compounds, when evaluated using first method, the risk is acceptable. According to the second method, only insecticides were highly or extremely dangerous for the human body while drinking contaminated water. The rest of the compounds are low or moderately hazardous.

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