A Comprehensive Assessment of the Pesticide Leaching: Insights from the Hindon River Basin, India

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Table S1: Pesticide leaching indices based on pesticides physicochemical and Hindon river basin hydrogeological properties

Pesticides leaching potential index description and formula	Criteria
Groundwater Ubiquity Score (GUS): The GUS index quickly and efficiently estimates pesticide movement toward groundwater and helps to evaluate its pollution potential during agricultural management planning (Gustafson, 1989). $$GUS = [4 - log(K_{oc})] \times log\left(t_{1/2}\right)$$	> 2.8: Leachable 1.8–2.8: Transition < 1.8: Not leachable
LEACH and Modified Leach (M. LEACH): The LEACH Index estimates considering soil properties, chemical half-life, and adsorption characteristics (Papa et al., 2004; Pérez-Lucas et al., 2016). $$LEACH = \frac{S_w \times t_{1/2}}{V_p \times K_{oc}} \text{ and } M.LEACH = \frac{S_w \times t_{1/2}}{K_{oc}}$$	>1: High Leaching Potential <1: Low Leaching Potential
Hornsby index (HI): The HI is specifically designed to assess the leaching potential of pesticides considering solubility, degradation rate, and soil adsorption (Hornsby, 1992). $$HI = \frac{K_{oc}}{t_{1/2}} \times 10$$	≤ 10: High leaching potential ≥ 2000: Low leaching potential
Leachability index (LIX): The LIX Index simplifies the estimation of pesticide leaching by focusing primarily on the degradation rate and adsorption characteristics (Spadotto, 2002). $$LIX = exp(-\frac{0.693}{t_{1/2}} \times K_{oc})$$	1: Maximally leachable 0.1–1: Leachable 0 – 0.1: Transition 0: Non-leachable
Leaching Index (LIN): The LIN index accounts for multiple pesticide characteristics, including KH, Koc, Kow, Sw, and Vp, offering a broader perspective on their environmental fate (Gramatica and Guardo, 2002). $$LIN = -0.531 \log K_{ow} + 0.518 \log S_w - 0.495 \log K_{oc} - 0.023 \log V_p - 0.452 \log K_H$$	> 0: Potentially leachable < 0: Non-leachable

Global Leachability Index (GLI): The GLI index combines multiple indices such as the GUS, LIN, and M. LEACH scores to assign low, medium, and high leachability criteria (Papa et al., 2004). GLI = 0.579 LIN + 0.558 GUS + 0.595 MLEACH	> 1: High -0.5 to 1: Medium < -0.5: Low
Retardation Factor (RF): The RF estimates how a contaminant moves through the soil relative to the groundwater flow. It indicates the degree to which a contaminant is retarded due to adsorption and other soil interactions compared to the movement of the groundwater itself (Meeks and Dean, 1990). $RF = [1 + \frac{\rho_b \times f_{oc} \times K_{oc}}{\theta_{FC}}]$	1: Very mobile 1-2: Mobile 2 -3: Moderately mobile 3 - 10: Moderately immobile ≥ 10: Very immobile
Briggs RF: The Briggs RF estimates the mobility of pesticides based on soil environments, primarily focusing on how easily a pesticide can leach through the soil profile into groundwater (Briggs, 1973). $Log\left({}^{1}/_{Rf} - 1\right)$ =Log (K_{ow}) + Log (OM) – 1.33	0.90-1.0: Very high 0.65-0.89: High 0.35-0.64: Medium 0.11-0.34: Low 0–0.1: Very low
Leachate Pollution Index (LPI): LPI is helpful in understanding the behaviour of pesticides in the subsurface environment where managing groundwater quality is crucial (Meeks & Dean, 1990). $LPI = \frac{1000 \times t_{1/2} \times q}{0.693 \times RF \times Z}$	90: Very high 75 – 89: High 50 -74: Moderate 25 – 49: Low 0 – 24: Very low
Vulnerability Index (VI): The VI is a composite metric designed to assess the vulnerability of groundwater to contamination by pesticides based on a combination of soil, pesticide properties, and hydrological factors (Schlosser et al., 2002; Rossetto et al., 2020). $VI = \frac{200 \times k \times \theta_{FC}}{d \times \rho_b \times (\%OM)} \times \frac{t_{1/2}}{K_{oc}} \times F_{DGW}$	0-9: Low 9-99: Medium > 99: High

Where: K_{oc}: carbon-water partition coefficient (mL/g organic carbon); K_{ow}: octanol-water partition coefficient (mL/g organic carbon); $t_{1/2}$: pesticide half-life in soil (days); S_w: water solubility (mg/L); V_p: pesticide vapor pressure (Pa or mm/Hg); k: degradation constant (1/day); K_H: Henry's constant (Pa m^3/mol); ρ_b: bulk density of soil (gm/cm^3); f_{oc}: soil fraction of organic carbon (%); θ_{FC}: volumetric water content at field capacity (non-dimensional); OM: soil organic matter (%); Z: water table depth (m); q: net aquifer recharge rate (m/día); d: depth to which organic matter is concentrated (m) and F_{DGW}: factor that adjusts for local groundwater dynamics

Table S2: Pesticides physicochemical used for pesticides leaching potential estimation

Pesticide	S_W (mg/l)	K_{ow}	V_p (mPa)	HLC (Pa m³ mol⁻¹)	DT_{50} (typical) (d)	DT_{50} (field) (d)	K_{oc} (mL g⁻¹)	Freundlich K_{oc} (mL g⁻¹)
Atrazine	35	501	0.039	0.00015	75	29	100	174
Carbendazim	8	30.2	0.09	0.0036	40	22	-	225
Carbofuran	322	63.1	0.08	0.00005	29	14	-	86.5
Chlorpyrifos	1.05	50100	1.43	0.478	386	27.6	5509	3954
Dichlorvos	18000	79.4	2100	0.0258	2	-	50	-
Dimethoate	25900	5.62	2.5	1.42e-06	2.5	7.2	-	28.3
Fipronil	3.78	5620	0.002	0.000231	142	65	-	727
Glyphosate	100000	0.0000005	0.0131	2.21e-08	17.3	6.45	1424	4348
Imidacloprid	610	3.72	4.00e-07	1.70e-10	191	174	-	225
Lambda-cyhalothrin	0.005	316000	0.0002	0.02	175	26.9	283707	290311
Malathion	148	562	3.1	0.001	0.17	1	1800	217
Mancozeb	6.2	200	0.056	0.0617	0.05		998	771
Metribuzin	10700	50.1	0.121	1.71e+05	7.03	19	-	48.3
Metsulfuron methyl	2790	0.0135	0.000001	2.87e-06	10	13.3	-	12
Monocrotophos	818000	0.603	0.29	-	7	30	19	-
Pendimethalin	0.33	251000	3.34	1.27	182.3	100.6	17491	13792
Propiconazole	150	5250	0.056	0.000092	71.8	35.2	1086	955
Quinalphos	17.8	27500	0.346	0.0047	21		1465	
Sulfosulfuron	1627	0.17	3.05e-05	8.83e-09	63.8	44.5	-	33
Thiophanate-methyl	18.5	25.1	0.009	0.000167	0.5	2	-	220
Thiram	18	69.2	0.02	0.000139	4.89	15	-	9629
Zineb	10	20	0.008	0.000276	30	19.5	1000	-

Table S3: Hindon river basin hydrogeological properties used for pesticides leaching potential estimation

Hydrogeological properties								
Scenario	Region	ρ_b (gm/cm³)	Recharge (mm/day)	Soil Organic Matter, %	θ_{FC} (%)	F_DGW	GWL, m	Soil Organic Carbon Fraction, %
S1	Upstream	1.45	0.82	1.53	0.40	2.50	9.13	0.90
S2	Upstream	1.50	0.82	1.02	0.40	2.50	9.13	0.60
S3	Midstream	1.50	0.51	1.02	0.40	2.00	12.54	0.60
S4	Downstream	1.50	0.37	1.02	0.40	1.00	15.60	0.60
S5	Upstream	1.45	0.82	1.53	0.40	2.50	5.09	0.90

S6	Upstream	1.50	0.82	1.02	0.40	2.50	5.09	0.60
S7	Midstream	1.50	0.51	1.02	0.40	2.05	6.33	0.60
S8	Downstream	1.50	0.37	1.02	0.40	2.05	7.50	0.60
S9	Upstream	1.45	0.82	1.53	0.40	2.00	13.18	0.90
S10	Upstream	1.50	0.82	1.02	0.40	2.00	13.18	0.60
S11	Midstream	1.50	0.51	1.02	0.40	1.00	18.76	0.60
S12	Downstream	1.50	0.37	1.02	0.40	1.00	23.69	0.60

Table S4: Result of pesticide properties based leaching indices classification

No	Pesticide	LEACH	M. LEACH	GUS	Hornsby	LIX	LIN	GLI
1	Fipronil	High leaching potential	Low leaching potential	Transition	Moderate leaching potential	Transition	Non-leachable	Medium leaching potential
2	Sulfosulfuron	High leaching potential	High leaching potential	Highly leachable	High leaching potential	Leachable	Potentially leachable	High leaching potential
3	Metsulfuron methyl	High leaching potential	High leaching potential	Highly leachable	Moderate leaching potential	Leachable	Potentially leachable	High leaching potential
4	Chlorpyrifos	Low leaching potential	Low leaching potential	Non-leachable	Moderate leaching potential	Transition	Non-leachable	Low leaching potential
5	Malathion	Low leaching potential	Low leaching potential	Non-leachable	Low leaching potential	Non-leachable	Potentially leachable	Medium leaching potential
6	Chlorpyrifos	Low leaching potential	Low leaching potential	Non-leachable	Moderate leaching potential	Transition	Non-leachable	Low leaching potential
7	Carbendazim	High leaching potential	High leaching potential	Transition	Moderate leaching potential	Transition	Non-leachable	High leaching potential
8	Mancozeb (manzeb)	Low leaching potential	Low leaching potential	Non-leachable	Low leaching potential	Non-leachable	Non-leachable	Low leaching potential
9	Glyphosate	High leaching potential	High leaching potential	Non-leachable	Low leaching potential	Transition	Potentially leachable	High leaching potential
10	Dimethoate	High leaching potential	High leaching potential	Non-leachable	Moderate leaching potential	Transition	Potentially leachable	High leaching potential
11	Imidacloprid	High leaching potential	High leaching potential	Highly leachable	Moderate leaching potential	Leachable	Potentially leachable	High leaching potential
12	Mancozeb	Low leaching potential	Low leaching potential	Non-leachable	Low leaching potential	Non-leachable	Non-leachable	Low leaching potential

13	Lambda-cyhalothrin	Low leaching potential	Low leaching potential	Non-leachable	Low leaching potential	Non-leachable	Non-leachable	Low leaching potential
14	Malathion	Low leaching potential	Low leaching potential	Non-leachable	Low leaching potential	Non-leachable	Non-leachable	Low leaching potential
15	Thiophanate-methyl	High leaching potential	Low leaching potential	Non-leachable	Low leaching potential	Transition	Potentially leachable	Medium leaching potential
16	Pendimethalin	Low leaching potential	Low leaching potential	Non-leachable	Moderate leaching potential	Transition	Non-leachable	Low leaching potential
17	Thiram	Low leaching potential	Low leaching potential	Non-leachable	Low leaching potential	Non-leachable	Non-leachable	Medium leaching potential
18	Atrazine	High leaching potential	High leaching potential	Highly leachable	Moderate leaching potential	Leachable	Potentially leachable	High leaching potential
19	Carbofuran	High leaching potential	High leaching potential	Highly leachable	Moderate leaching potential	Leachable	Potentially leachable	High leaching potential
20	Propiconazole	High leaching potential	High leaching potential	Transition	Moderate leaching potential	Transition	Non-leachable	High leaching potential
21	Metribuzin	High leaching potential	High leaching potential	Transition	Moderate leaching potential	Transition	Non-leachable	High leaching potential

Table S5: Briggs RF leaching and LPI classification for 9 different senarios

Pesticide	**S1**	**S2**	**S3**	**S4**	**S5**	**S6**	**S7**	**S8**	**S9**	**S10**	**S11**	**S12**
Carbofuran	L	L	L	L	L	L	L	L	L	L	L	L
Malathion	V L	V L	V L	V L	V L	V L	V L	V L	V L	V L	V L	V L
Atrazine	V L	V L	V L	V L	V L	V L	V L	V L	V L	V L	V L	V L
Carbendazim	M	M	L	M	M	M	L	M	M	M	L	M
Chlorpyrifos	V L	V L	V L	V L	V L	V L	V L	V L	V L	V L	V L	V L
Dimethoate	H	H	H	H	H	H	H	H	H	H	H	H
Fipronil	V L	V L	V L	V L	V L	V L	V L	V L	V L	V L	V L	V L
Glyphosate	VH	VH	VH	VH	VH	VH	VH	VH	VH	VH	VH	VH
Imidacloprid	H	H	H	H	H	H	H	H	H	H	H	H
Lambda-cyhalothrin	V L	V L	V L	V L	V L	V L	V L	V L	V L	V L	V L	V L
Malathion	V L	V L	V L	V L	V L	V L	V L	V L	V L	V L	V L	V L
Mancozeb	V L	V L	V L	V L	V L	V L	V L	V L	V L	V L	V L	V L
Metribuzin	L	L	L	L	L	L	L	L	L	L	L	L
Metsulfuron methyl	VH	VH	VH	VH	VH	VH	VH	VH	VH	VH	VH	VH
Monocrotophos	VH	VH	VH	VH	VH	VH	VH	VH	VH	VH	VH	VH
Pendimethalin	V L	V L	V L	V L	V L	V L	V L	V L	V L	V L	V L	V L

Propiconazole	V L	V L	V L	V L	V L	V L	V L	V L	V L	V L	V L	V L
Sulfosulfuron	VH	VH	VH	VH	VH	VH	VH	VH	VH	VH	VH	VH
Thiophanate-methyl	M	M	M	M	M	M	M	M	M	M	M	M
Thiram	L	L	L	L	L	L	L	L	L	L	L	L
Zineb	M	M	M	M	M	M	M	M	M	M	M	M
Leaching Potential Index (LPI)												
Carbofuran	V L	V L	V L	V L	V L	V L	V L	V L	V L	V L	V L	V L
Malathion	V L	V L	V L	V L	V L	V L	V L	V L	V L	V L	V L	V L
Atrazine	V L	V L	V L	V L	V L	V L	V L	V L	V L	V L	V L	V L
Carbendazim	V L	V L	V L	V L	V L	V L	V L	V L	V L	V L	V L	V L
Chlorpyrifos	V L	V L	V L	V L	V L	V L	V L	V L	V L	V L	V L	V L
Dimethoate	V L	V L	V L	V L	V L	V L	V L	V L	V L	V L	V L	L
Fipronil	V L	V L	V L	V L	V L	V L	V L	V L	V L	V L	V L	V L
Glyphosate	V L	V L	V L	V L	V L	V L	V L	V L	V L	V L	V L	V L
Imidacloprid	V L	V L	V L	L	V L	V L	L	L	V L	L	M	H
Lambda-cyhalothrin	V L	V L	V L	V L	V L	V L	V L	V L	V L	V L	V L	V L
Malathion	V L	V L	V L	V L	V L	V L	V L	V L	V L	V L	V L	V L
Mancozeb	V L	V L	V L	V L	V L	V L	V L	V L	V L	V L	V L	V L
Metribuzin	V L	V L	V L	V L	V L	V L	V L	V L	V L	V L	L	L
Metsulfuron methyl	V L	V L	L	L	V L	L	L	M	L	M	H	VH
Monocrotophos	V L	L	L	M	V L	L	M	H	VL	H	VH	VH
Pendimethalin	V L	V L	V L	V L	V L	V L	V L	V L	V L	V L	V L	V L
Propiconazole	V L	V L	V L	V L	V L	V L	V L	V L	V L	V L	V L	V L
Sulfosulfuron	V L	V L	L	M	V L	L	M	H	L	M	VH	VH
Thiophanate-methyl	V L	V L	V L	V L	V L	V L	V L	V L	V L	V L	V L	V L
Thiram	V L	V L	V L	V L	V L	V L	V L	V L	V L	V L	V L	V L
Zineb	V L	V L	V L	V L	V L	V L	V L	V L	V L	V L	V L	V L

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