Spatial and temporal variation of watertype-specific no-effect concentrations and risks of Cu, Ni and Zn

Supplementary Information

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Table S1 Cu, Ni and Zn NOEC lowest mean endpoint over taxa and species (ug total dissolved metal/l) and NOEC-range between brackets.

	Cu		Ni		Zn	
	Species name and number of data	**NOEC (µg/l)**	**Species name and number of data**	**NOEC (µg/l)**	**Species name and number of data**	**NOEC (µg/l)**
algae	Chlamydomonas reinhardtii (4)	101 (22-178)	Ankistodesmus falcatus (2)	33.8 (24.6-43.0)	Chlorella sp.(5)	114 (5.9-350)
	Chlorella vulgaris (17)	183 (31-510)	Chlamydomos sp (2)	17.9 (8.3-27.5)	Pseudokircheneriella subcapitata (30)	56.4 (4.0-358)
	Pseudokirchneriella subcapitata (12)	43.1 (15.7-164)	Chlorella sp. (2)	73.6(49.0-98.2)		
			Coelastrum microporum (4)	36.9 (15.6-70.0)		
			Desmodesmus spinosus (4)	28.3 (3.5-43.7)		
			Pediastrum duplex (2)	31.5 (23.5-39.5)		
			Pseudokircheneriella subcapitata (12)	107 (21.5-432)		
			Pseudokirchneriella sp. (2)	8.7 (3.5-13.8)		
			Scenedesmus accumitus (2)	7.7(3.1-12.3)		
crustacea	Ceriodaphnia dubia (14)	15.6 (4.0-122)	Alona affinis (2)	25.0 (25-25)	Ceriodaphnia dubia (8)	40.6 (25-100)
	Daphnia magna (9)	12.6 (12.6-181)	Ceriodaphnia dubia (10)	5.0 (2.8-15.3)	Daphnia longispina (2)	129 (91-209)
	Daphnia pulex (9)	18.2 (4-40)	Ceriodaphnia pulchella (4)	19.1 (9.9-28.2)	Daphnia magna (39)	105 (25-491)
	Gammarus pulex (1)	11.0	Ceriodaphnia quadrangula (8)	9.1 (2.0-34.9)	Hyalella azteca (1)	42.0
	Hyalella azteca (6)	54.3 (30-82)	Daphnia longispina (4)	27.8 (26.6-118)		
			Daphnia magna (32)	128 (50.5-389)		
			Hyalella azteca (1)	29.0		
			Peracantha truncata (4)	14.2 (2.5-25.8)		
			Simocephalus vetulus (8)	14.1(9.2-28.9)		
fish	Catostomus commersoni (2)	12.9 (12.9-12.9)	Brachydanio rerio (1)	40.0	Cottus bairdi (2)	99.50 (27-172)
	Esox lucius (2)	34.9 (34.9-34.9)	Oncorhynchus mykiss (5)	750 (265-1770)	Danio rerio (9)	1282 (180-2900)
	Ictalurus punctatus (2)	13.0 (13.0-13.0)			Jordanella floridae (2)	50.5 (26-75)
	Noemacheilus barbatulus (1)	120			Oncorhynchus mykiss (23)	286 (32-974)
	Oncorhynchus kisutch (5)	21.0 (18.0-28.0)			Phoxinus phoxinus (2)	50.0 (50.0-50.0)
	Oncorhynchus mykiss (7)	18.7 (2.2-45)			Pimephales promelas (1)	78.0
	Perca fluviatilis (2)	39.0 (39.0-188)			Salvelinus fontinalis (1)	534
	Pimephales notatus (3)	57.9 (44.0-71.8)			Salmo trutta (2)	154 (57-250)
	Pimephales promelas (12)	16.1 (4.8-6.06)				
	Salvelinus fontinalis (12)	14.0 (7.0-49.0)				

Continuation of Table S1

	Cu		Ni		Zn	
	Species name and number of data	**NOEC (µg/l)**	**Species name and number of data**	**NOEC (µg/l)**	**Species name and number of data**	**NOEC (µg/l)**
other taxa	Brachionus calyciflorus(rotifer) (4)	47.5 (8.2-103)	Bufo terrestris (toad) (5)	640 (640-1360)	Anuraeopsis fissa (rotifer) (1)	50.0
	Campeloma decisum (mollusc) (2)	8.0 (8.0-8.0)	Gastrophryne carolensis(toad) (5)	80.0 (70.0-450)	Brachionus rubens (rotifer) (1)	50.0
	Chironomus riparius (insect) (1)	16.9	Hydra littoralis (hydrozoa) (1)	60.0	Dreissena polymorpha (mollusc) (1)	382
	Clistoronia magnifica (insect) (2)	10.7 (8.3-13.0)	Xenopus laevis(frog) (6)	88.2 (84.5-4790)	Ephoron virgo (insect) (1)	718
	Dreissenia polymorpha (bivalve) (2)	18.5 (16.0-21.0)			Potamopyrgus jenkinsi (mollusc) (1)	72
	Juga plicifera (mollusc) (1)	6.0				
	Lemna minor L.(plant) (1)	30.0				
	Paratanytarsus parthenogeneticus (insect) (2)	40.0				
	Villosa iris (bivalve) (1)	19.1				

.Between brackets: number of data. NOECs are lowest endpoint means per species. Summarized from [1-3]

Table S2 Overview biotic ligand binding constants. Me = metal

BLM	Algae			Crustacea			Fish		
	Cu	Ni[4]	Zn	Cu[5]	Ni[4]	Zn[6]	Cu[7]	Ni[4]	Zn[8]
logK BL-Me		4.0		8.02	4.0	5.3	8.02	4.0	5.5
logK BL-MeOH		-		8.02	-	-	7.32	-	-
logK BL-MeCO3				7.44	-	-	7.01	-	-
logK BL-H	n.a.	5.9	n.a.	6.67	5.9	5.8	5.4	6.8	6.3
logK BL-Ca		2.1		-	3.1	3.2	3.47	3.7	3.6
logK BL-Mg		3.3		-	3.3	2.7	3.58	4.0	3.1
logK BL-Na		-		2.91	-	1.9	3.19	-	2.4
Regression	Cu[9]	Ni	Zn[10]	Cu	Ni	Zn	Cu	Ni	Zn
Slope	-1.140	n.r.	-0.754	n.r.	n.r.	n.r.	n.r.	n.r.	n.r.
Intercept	-0.812		-1.294						

n.a.= not available

n.r. = not relevant since a full BLM is available

Stability constants fit in general BLM equations (see paper, methods section)

Regressions are used if BLM are not available in the following general formulae:

$$Intrinsic\ Sensitivity = NOEC / (10^{Slope*\ pH.Test+Intercept})$$

$$Environmental\ Moderator <- 10^{Slope*\ pH.sample+\ Intercept}$$

$$NOEC_{sample} = IntrinsicSensitivity \times EnvironmentalModerator$$

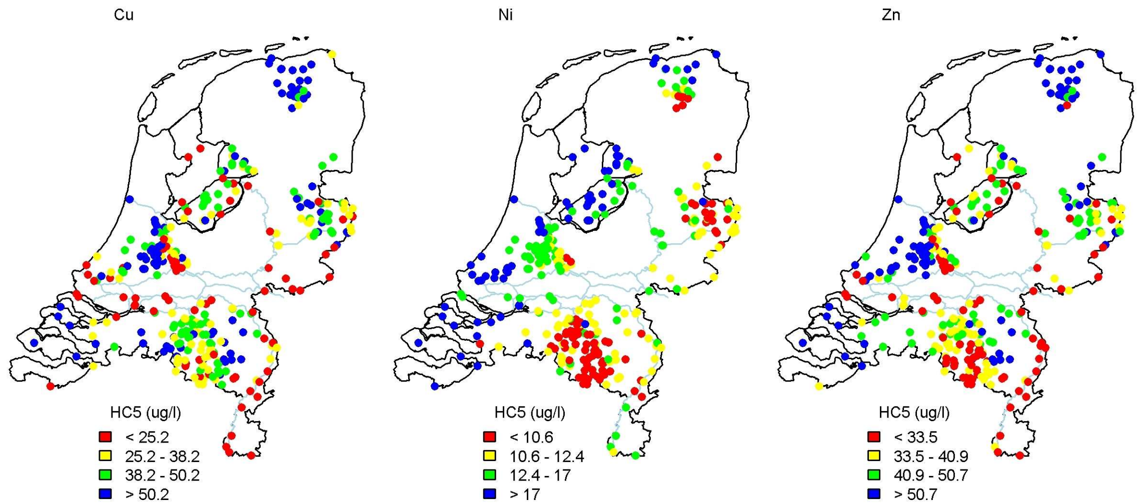

Figure S1 Spatial variation of site-specific annual average HC5.

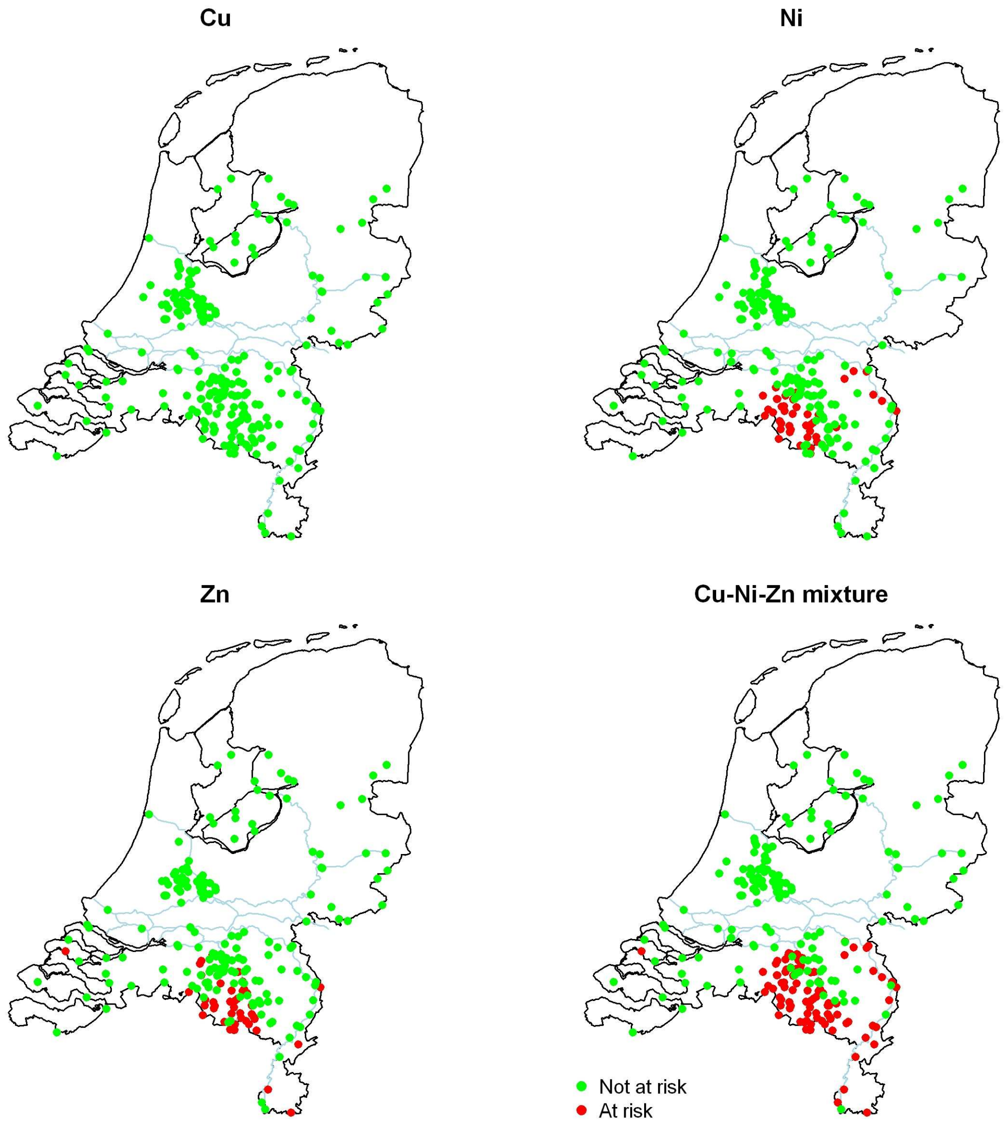

Figure S2 Overview sites at risk for single metals and Cu, Ni and Zn mixture (SumRCR). A site is considered to be at risk when RCR>1.

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