

Operational integration of time dependent toxicity impact category in dynamic LCA

Allan Hayato Shimako^{a,b,c}, Ligia Tiruta-Barna^{a,b,c}, Aras Ahmadi^{a,b,c}

^a Université de Toulouse, INSA, UPS, INP, LISBP, 135 Avenue de Ranguel, F-31077 Toulouse, France

^b INRA, UMR792, Laboratoire d'Ingénierie des Systèmes Biologiques et des Procédés, F-31400 Toulouse, France

^c CNRS, UMR5504, F-31400 Toulouse, France

S1.	Compatibility of substances in ecoinvent 3.2 and USEtox [®] 2.0	2
S2.	Compatibility of compartments in ecoinvent 3.2 and USEtox [®] 2.0	4
S3.	Grape production : ecoinvent 3.2 dataset	5
S4.	Grape production : modified dataset.....	7
S5.	Conventional toxicity results for the testbed case “grape production” per substances, USEtox [™]	9
S6.	Parameters for dynamic LCA	30
S7.	Dynamic and conventional toxicity results	32

S1. Compatibility of substances in ecoinvent 3.2 and USEtox[®] 2.0

USEtox[®] 2.0 contains 27 inorganic substances but none match with the substances in ecoinvent dataset. In USEtox[®] 2.0 metals are presented with their oxidation state while in ecoinvent they are presented in their elemental form. SimaPro LCA software proposes an adaptation in which the substances from ecoinvent 3.2 database are correlated to the ionic form presented in USEtox[®] 2.0. This correspondence is presented in table S1.

Table S1 – Correspondence between inorganic substances presented in SimaPro and USEtox[®] 2.0, proposed by SimaPro LCA software

Name ecoinvent, SimaPro	Name Usetox [®] 2.0
Silver	Ag(I)
	Al(III)
Arsenic III	As(III)
Arsenic, ion	As(V)
Arsenic	As(V)
Barium	Ba(II)
Beryllium	Be(II)
Cadmium	Cd(II)
	Co(II)
Chromium III	Cr(III)
Chromium VI	Cr(VI)
	Cs(I)
Copper	Cu(II)
	Fe(II)
	Fe(III)
Mercury	Hg(II)
	Mn(II)
Molybdenum	Mo(VI)
Nickel	Ni(II)
Lead	Pb(II)
Antimony III	Sb(III)
Antimony V	Sb(V)
Antimony	Sb(V)
Antimony, ion	Sb(V)

	Se(IV)
	Sn(II)
	Sr(II)
Thallium	Tl(I)
Vanadium	V(V)
Zinc	Zn(II)

USEtox[®] 2.0 presents 3077 organic substances and 2880 match with the substances in ecoinvent dataset. As the name of substances might vary from one database to another, the correspondence between them was made by means of their CAS number.

S2. Compatibility of compartments in ecoinvent 3.2 and USEtox® 2.0

Compartments in ecoinvent database and USEtox® model are addressed differently. An adaptation has to be made in order to use ecoinvent 3.2 data in USEtox® 2.0 model.

Table S2 – Correspondence between compartments in ecoinvent 3.2 and USEtox® 2.

USEtox® 2 compartments	Ecoinvent 3 compartments
Urban air	Air emission, high population density/ air emission, unspecified (50%)
Rural air	Air emission, low population density / air emission, lower stratosphere & troposphere / air emission, low population density, long-term / air emission, unspecified (50%)
Freshwater	Water emission, river / water emission, lake / water emission, unspecified / water emission, river, long-term / water emission, ground water (only in human toxicity) / water emission, ground water long term (only in human toxicity)
Sea water	Water emission, ocean
Natural soil	Soil emission, forestry / soil emission, industrial / soil emission, unspecified / water emission, ground water (only in ecotoxicity) / water emission, ground water long-term (only in ecotoxicity)
Agricultural soil	Soil emission, agriculture

S3. Grape production : ecoinvent 3.2 dataset

Table S3 – Ecoinvent 3.2 dataset for the process “grape production”

	Value	Unit
Reference Products		
Grape	1	Kg
Emissions to Environment		
Compartment: air		
Ammonia	4.86E-05	Kg
Dinitrogen monoxide	3.91E-05	Kg
Nitrogen oxides	8.22E-06	Kg
Water	0.10372	m3
Compartment: soil		
Cadmium	5.21E-08	Kg
Chromium	-3.93E-07	Kg
Copper	-1.20E-06	Kg
Lead	5.87E-07	Kg
Nickel	-3.31E-08	Kg
Pesticides, unspecified	0.0005	Kg
Zinc	-8.14E-07	Kg
Compartment: water		
Nitrate	0.0026571	Kg
Phosphate	4.96E-07	Kg
Phosphorus	1.74E-06	Kg
Water	0.058384	m3
Water	0.014596	m3
Resources from Environment		
natural resource		
Energy, gross calorific value, in biomass	3.6698	MJ
Occupation, permanent crop, irrigated, intensive	0.333	m2*year
Transformation, from permanent crop, irrigated, intensive	0.333	m2
Transformation, to permanent crop, irrigated, intensive	0.333	m2
Processes from Technosphere		
ammonium nitrate, as N	0.002	Kg
electricity, low voltage	0.09	kWh
fertilising, by broadcaster	0.000733	Ha
Irrigation	0.1767	m3
pesticide, unspecified	0.0005	Kg
phosphate fertiliser, as P2O5	0.00133	Kg

potassium sulfate, as K ₂ O	0.00433	Kg
--	---------	----

Between the environmental interventions, it is noticed the presence of negative emissions. Nemecek et al. (2007) shows that the calculation of these emissions are based on the balance of all inputs (fertilizers, pesticides, seed and deposition) and outputs (exported biomass, leaching and erosion) related to the “agriculture soil” multiplied by the allocation factor. The final result of this calculation can lead to a negative value of emission to “agriculture soil”.

S4. Grape production : modified dataset

The modified data set was used in this work: pesticides were added as explained in the main document, and negative values (as mentioned here above) were set to zero.

Table S4 – Modified dataset for the process “grape production”

	Value	Unit
Reference Products		
Grape	1	Kg
Emissions to Environment		
Compartment: air		
Ammonia	4.86E-05	Kg
Dinitrogen monoxide	3.91E-05	Kg
Nitrogen oxides	8.22E-06	Kg
Water	0.10372	m3
Compartment: soil		
Cadmium	5.21E-08	Kg
Lead	5.87E-07	Kg
Copper	9.1E-06	Kg
Pesticides, unspecified	0.0005	Kg
Metalddehyde	0.0000059	Kg
Mancozeb	0.0000351	Kg
Glyphosate	0.0000672	Kg
Chlorothalonil	0.0000102	Kg
Aclonifen	0.0000058	Kg
Pendimethalin	0.0000066	Kg
Metolachlor	0.0000145	Kg
Isoproturon	0.0000124	Kg
Napropamide	0.0000046	Kg
Dimethenamide	0.0000055	Kg
Metamitron	0.0000039	Kg
Folpet	0.0000116	Kg
Compartment: water		
Nitrate	0.0026571	Kg
Phosphate	4.96E-07	Kg
Phosphorus	1.74E-06	Kg
Water	0.058384	m3
Water	0.014596	m3
Resources from Environment		

natural resource		
Energy, gross calorific value, in biomass	3.6698	MJ
Occupation, permanent crop, irrigated, intensive	0.333	m2*year
Transformation, from permanent crop, irrigated, intensive	0.333	m2
Transformation, to permanent crop, irrigated, intensive	0.333	m2
Processes from Technosphere		
ammonium nitrate, as N	0.002	Kg
electricity, low voltage	0.09	kWh
fertilising, by broadcaster	0.000733	Ha
Irrigation	0.1767	m3
phosphate fertiliser, as P2O5	0.00133	Kg
potassium sulfate, as K2O	0.00433	Kg
Metalddehyde	0.0000059	Kg
Mancozeb	0.0000351	Kg
Glyphosate	0.0000672	Kg
Chlorothalonil	0.0000102	Kg
Aclonifen	0.0000058	Kg
Pendimethalin	0.0000066	Kg
Metolachlor	0.0000145	Kg
Isoproturon	0.0000124	Kg
Napropamide	0.0000046	Kg
Dimethenamide	0.0000055	Kg
Metamitron	0.0000039	Kg
Folpet	0.0000116	Kg

S5. Conventional toxicity results for the testbed case “grape production” per substances, USEtox™

Table S5 – Conventional toxicity results per substance, obtained with USEtox® 2.0

Substance	Compart.	Sub-Compart.	Mass (kg)	Human non-can (cases)	Human cancer (cases)	Ecotoxicity (PAFm ³ day)
1-Butanol	Air	high. pop.	1.7E-12	0.0E+00	8.9E-20	2.2E-13
1-Butanol	Water	river	4.9E-09	0.0E+00	1.6E-16	2.2E-08
1-Pentanol	Air	high. pop.	1.1E-12	0.0E+00	0.0E+00	2.7E-13
1-Pentanol	Water	river	2.6E-12	0.0E+00	0.0E+00	3.2E-11
1-Propanol	Air	high. pop.	2.3E-09	0.0E+00	0.0E+00	2.2E-10
1-Propanol	Air	low. pop.	1.3E-16	0.0E+00	0.0E+00	1.2E-17
1-Propanol	Water	river	5.6E-12	0.0E+00	0.0E+00	1.3E-11
1,4-Butanediol	Air	high. pop.	4.9E-12	0.0E+00	0.0E+00	4.3E-12
1,4-Butanediol	Water	river	9.6E-12	0.0E+00	0.0E+00	7.0E-11
2-Methyl-1-propanol	Air	high. pop.	2.7E-12	0.0E+00	5.7E-20	5.6E-13
2-Methyl-1-propanol	Water	river	6.5E-12	0.0E+00	1.0E-19	4.2E-11
2-Methyl-4-chlorophenoxyacetic acid	Air	low. pop.	8.5E-14	0.0E+00	1.1E-18	6.5E-12
2-Methyl-4-chlorophenoxyacetic acid	Water	groundwater	1.3E-14	0.0E+00	3.2E-19	1.6E-12
2-Methyl-4-chlorophenoxyacetic acid	Water	river	1.9E-13	0.0E+00	4.7E-18	3.5E-10
2-Methyl-4-chlorophenoxyacetic acid	Soil	agricultural	6.1E-11	0.0E+00	1.5E-15	7.6E-09
2-Propanol	Air		1.0E-11	0.0E+00	0.0E+00	8.0E-13
2-Propanol	Air	high. pop.	9.8E-09	0.0E+00	0.0E+00	7.8E-10
2-Propanol	Air	low. pop.	2.0E-12	0.0E+00	0.0E+00	1.6E-13
2-Propanol	Water	river	1.9E-11	0.0E+00	0.0E+00	3.5E-11
2,4-D	Air	low. pop.	5.0E-11	0.0E+00	7.8E-17	1.6E-09
2,4-D	Soil	agricultural	4.5E-06	0.0E+00	4.6E-12	1.2E-04
2,4-D, dimethylamine salt	Air	low. pop.	4.1E-14	0.0E+00	0.0E+00	1.7E-11
4-Methyl-2-pentanol	Water	river	6.2E-18	0.0E+00	0.0E+00	5.4E-17
4-Methyl-2-pentanone	Air	low. pop.	4.5E-14	0.0E+00	8.8E-24	1.0E-15
4-Methyl-2-pentanone	Water		3.4E-11	0.0E+00	3.5E-20	9.9E-11

Acenaphthene	Air		9.9E-15	8.2E-21	2.9E-22	3.7E-14
Acenaphthene	Air	high. pop.	7.8E-16	1.2E-21	4.3E-23	3.0E-15
Acenaphthene	Air	low. pop.	3.4E-12	3.6E-19	1.3E-20	1.3E-11
Acenaphthene	Water	ocean	2.1E-13	1.4E-19	5.1E-21	2.0E-13
Acenaphthene	Water	river	3.6E-12	1.2E-17	4.1E-19	7.1E-09
Acenaphthylene	Air		3.1E-13	1.3E-19	0.0E+00	0.0E+00
Acenaphthylene	Water	ocean	1.3E-14	8.3E-21	0.0E+00	0.0E+00
Acenaphthylene	Water	river	2.2E-13	6.6E-19	0.0E+00	0.0E+00
Acephate	Air	low. pop.	5.3E-12	5.9E-19	1.6E-15	1.5E-10
Acephate	Soil	agricultural	4.9E-10	1.8E-17	5.0E-14	2.2E-08
Acetaldehyde	Air		1.8E-08	1.7E-15	8.9E-15	5.6E-09
Acetaldehyde	Air	high. pop.	6.7E-08	1.2E-14	6.2E-14	2.0E-08
Acetaldehyde	Air	low. pop.	3.2E-09	2.7E-17	1.4E-16	1.0E-09
Acetaldehyde	Water	river	1.6E-07	8.1E-15	4.1E-14	4.0E-06
Acetamide	Air	low. pop.	1.3E-12	6.9E-19	0.0E+00	7.6E-13
Acetamide	Soil	agricultural	7.1E-11	2.0E-17	0.0E+00	6.3E-11
Acetic acid	Air		2.2E-07	0.0E+00	0.0E+00	5.9E-07
Acetic acid	Air	high. pop.	3.1E-07	0.0E+00	0.0E+00	9.1E-07
Acetic acid	Air	low. pop.	4.6E-08	0.0E+00	0.0E+00	1.0E-07
Acetic acid	Water	river	1.7E-06	0.0E+00	0.0E+00	8.7E-05
Acetochlor	Soil	agricultural	1.0E-09	0.0E+00	0.0E+00	1.0E-06
Acetone	Air		2.9E-09	0.0E+00	1.4E-17	1.5E-10
Acetone	Air	high. pop.	4.5E-08	0.0E+00	3.8E-16	2.4E-09
Acetone	Air	low. pop.	5.5E-08	0.0E+00	8.7E-17	2.9E-09
Acetone	Water		8.0E-11	0.0E+00	2.9E-19	5.8E-11
Acetone	Water	river	2.2E-08	0.0E+00	8.2E-17	1.6E-08
Acetonitrile	Air	low. pop.	5.0E-10	0.0E+00	8.0E-18	2.3E-10
Acetonitrile	Water	river	1.1E-12	0.0E+00	3.7E-20	6.3E-12
Acetyl chloride	Water	river	2.0E-12	0.0E+00	0.0E+00	1.4E-10
Acifluorfen	Air	low. pop.	7.3E-13	3.1E-18	0.0E+00	0.0E+00
Acifluorfen	Soil	agricultural	3.1E-14	1.6E-19	0.0E+00	0.0E+00
Aclonifen	Soil	agricultural	5.8E-06	0.0E+00	0.0E+00	3.5E-02
Acrolein	Air		3.8E-09	0.0E+00	2.7E-12	4.2E-07
Acrolein	Air	high. pop.	5.9E-11	0.0E+00	8.2E-14	6.5E-09
Acrolein	Air	low. pop.	1.9E-09	0.0E+00	9.7E-14	2.2E-07
Acrylic acid	Air	high. pop.	9.2E-13	0.0E+00	8.7E-17	1.2E-11
Alachlor	Air	low. pop.	5.1E-12	0.0E+00	0.0E+00	4.2E-09
Alachlor	Soil	agricultural	1.6E-10	0.0E+00	0.0E+00	2.2E-07

Aldicarb	Soil	agricultural	1.3E-09	0.0E+00	5.4E-15	8.1E-07
Aldrin	Soil	agricultural	8.0E-09	5.5E-13	1.7E-12	3.0E-06
Allyl chloride	Water		1.1E-10	0.0E+00	4.3E-17	6.6E-09
Alpha-cypermethrin	Soil	agricultural	2.5E-12	0.0E+00	1.7E-19	1.2E-08
Ametryn	Soil	agricultural	5.1E-11	0.0E+00	0.0E+00	9.1E-08
Amitraz	Soil	agricultural	6.7E-11	0.0E+00	3.4E-18	9.4E-12
Aniline	Air	high. pop.	2.9E-11	1.0E-18	5.1E-17	1.2E-10
Aniline	Water	river	7.0E-11	4.4E-18	2.2E-16	4.1E-08
Anthranilic acid	Air	high. pop.	1.2E-12	0.0E+00	0.0E+00	0.0E+00
Anthraquinone	Soil	agricultural	1.5E-11	0.0E+00	0.0E+00	4.9E-11
Asulam	Soil	agricultural	1.3E-12	0.0E+00	1.3E-19	1.5E-11
Atrazine	Air	low. pop.	4.4E-12	8.4E-18	9.8E-18	7.7E-09
Atrazine	Water	groundwater	2.0E-12	7.4E-18	8.6E-18	6.9E-09
Atrazine	Water	river	7.7E-15	2.9E-20	3.3E-20	6.8E-10
Atrazine	Soil	agricultural	4.2E-09	3.4E-15	3.9E-15	1.5E-05
Azinphos-methyl	Soil	agricultural	2.8E-12	0.0E+00	6.4E-18	2.0E-08
Azoxystrobin	Air	low. pop.	2.4E-12	0.0E+00	0.0E+00	2.9E-08
Azoxystrobin	Soil	agricultural	3.2E-11	0.0E+00	0.0E+00	5.0E-07
Benfluralin	Soil	agricultural	3.4E-10	0.0E+00	1.7E-17	3.7E-09
Benomyl	Soil	agricultural	7.8E-13	0.0E+00	2.8E-20	6.2E-10
Bentazone	Air	low. pop.	2.2E-12	0.0E+00	9.3E-19	7.3E-12
Bentazone	Water	groundwater	7.3E-14	0.0E+00	8.9E-20	1.1E-12
Bentazone	Water	river	4.5E-17	0.0E+00	5.5E-23	9.1E-15
Bentazone	Soil	agricultural	4.4E-12	0.0E+00	2.3E-18	6.7E-11
Benzaldehyde	Air		2.9E-09	5.1E-17	6.7E-17	9.8E-09
Benzaldehyde	Air	high. pop.	2.9E-11	9.7E-19	1.3E-18	9.8E-11
Benzaldehyde	Air	low. pop.	5.2E-10	1.1E-18	1.4E-18	1.8E-09
Benzene	Air		2.5E-07	6.4E-14	1.6E-14	1.3E-08
Benzene	Air	high. pop.	3.4E-07	1.5E-13	3.8E-14	1.8E-08
Benzene	Air	low. pop.	1.5E-06	1.3E-13	3.3E-14	8.2E-08
Benzene	Air	stratosphere + troposphere	3.4E-13	2.8E-20	7.2E-21	1.8E-14
Benzene	Water		1.3E-08	1.8E-15	4.5E-16	3.4E-07
Benzene	Water	ocean	5.8E-09	2.1E-16	5.2E-17	1.3E-10
Benzene	Water	river	4.9E-07	6.5E-14	1.6E-14	1.2E-05
Benzene, 1-methyl-2-nitro-	Air	high. pop.	1.4E-12	1.1E-17	0.0E+00	2.9E-11
Benzene, 1,2-dichloro-	Air	high. pop.	8.1E-12	0.0E+00	4.2E-19	1.8E-11
Benzene, 1,2-dichloro-	Water	river	2.2E-07	0.0E+00	7.3E-15	5.0E-05
Benzene, chloro-	Water	river	3.1E-07	1.6E-14	1.6E-14	5.1E-05

Benzene, ethyl-	Air		3.0E-13	9.7E-20	1.6E-21	8.2E-15
Benzene, ethyl-	Air	high. pop.	1.7E-08	1.0E-14	1.7E-16	4.8E-10
Benzene, ethyl-	Air	low. pop.	6.5E-10	3.0E-17	5.3E-19	1.8E-11
Benzene, ethyl-	Water		7.5E-10	3.3E-17	1.1E-17	5.4E-08
Benzene, ethyl-	Water	ocean	8.0E-10	8.2E-18	1.0E-18	4.8E-12
Benzene, ethyl-	Water	river	1.4E-08	6.0E-16	2.1E-16	9.8E-07
Benzene, hexachloro-	Air		2.1E-11	1.5E-15	5.1E-16	1.1E-08
Benzene, hexachloro-	Air	high. pop.	4.7E-14	3.5E-18	1.2E-18	2.5E-11
Benzene, hexachloro-	Air	low. pop.	3.4E-20	2.3E-24	8.0E-25	1.8E-17
Benzene, pentachloro-	Air	high. pop.	1.2E-13	0.0E+00	3.2E-18	3.3E-11
Benzene, pentachloronitro-	Soil	agricultural	2.9E-11	7.4E-17	3.3E-16	1.1E-08
Benzo(a)anthracene	Air		5.9E-15	2.3E-18	0.0E+00	4.7E-11
Benzo(a)pyrene	Air		5.2E-11	2.1E-13	0.0E+00	8.1E-09
Benzo(a)pyrene	Air	high. pop.	1.6E-10	7.2E-13	0.0E+00	3.6E-08
Benzo(a)pyrene	Air	low. pop.	9.9E-09	3.6E-11	0.0E+00	8.5E-07
Benzo(b)fluoranthene	Air		7.0E-15	6.7E-18	0.0E+00	0.0E+00
Benzo(g,h,i)perylene	Air		4.3E-16	1.4E-20	0.0E+00	0.0E+00
Benzo(k)fluoranthene	Air		5.0E-15	2.2E-18	0.0E+00	0.0E+00
Bifenox	Soil	agricultural	4.0E-12	0.0E+00	0.0E+00	4.2E-10
Bifenthrin	Soil	agricultural	3.8E-12	0.0E+00	5.1E-19	5.2E-09
Bitertanol	Soil	agricultural	1.6E-12	0.0E+00	1.5E-18	8.9E-11
Bromacil	Soil	agricultural	5.1E-10	0.0E+00	0.0E+00	4.0E-07
Bromoxynil	Air	low. pop.	4.9E-14	0.0E+00	4.4E-20	3.3E-11
Bromoxynil	Water	groundwater	2.9E-13	0.0E+00	9.3E-19	5.6E-11
Bromoxynil	Water	river	1.2E-15	0.0E+00	3.8E-21	1.9E-11
Bromoxynil	Soil	agricultural	3.1E-11	0.0E+00	1.4E-17	6.1E-09
Bromuconazole	Soil	agricultural	1.8E-14	0.0E+00	0.0E+00	7.2E-11
Butadiene	Air		7.5E-13	4.3E-19	6.4E-19	0.0E+00
Butadiene	Air	high. pop.	4.2E-13	4.8E-19	7.1E-19	0.0E+00
Butadiene	Air	low. pop.	8.7E-14	1.4E-21	2.1E-21	0.0E+00
Butadiene	Air	stratosphere + troposphere	3.2E-13	5.2E-21	7.8E-21	0.0E+00
Butyl acetate	Water	river	6.4E-09	0.0E+00	0.0E+00	9.0E-08
Butyric acid, 4-(2,4-dichlorophenoxy)-	Air	low. pop.	2.5E-13	0.0E+00	2.3E-19	8.4E-12

Butyric acid, 4-(2,4-dichlorophenoxy)-	Soil	agricultural	4.2E-12	0.0E+00	2.5E-18	1.4E-10
Butyrolactone	Air	high. pop.	2.0E-12	0.0E+00	0.0E+00	6.5E-11
Butyrolactone	Water	river	4.7E-12	0.0E+00	0.0E+00	7.3E-10
Captan	Soil	agricultural	1.5E-09	5.2E-18	5.5E-17	5.9E-07
Carbaryl	Air	low. pop.	6.2E-13	1.0E-18	7.5E-19	4.5E-10
Carbaryl	Water	groundwater	2.3E-16	1.6E-21	1.2E-21	1.7E-13
Carbaryl	Water	river	2.9E-18	2.0E-23	1.5E-23	1.3E-13
Carbaryl	Soil	agricultural	9.9E-12	5.5E-18	4.1E-18	7.2E-09
Carbendazim	Soil	agricultural	1.5E-09	0.0E+00	1.8E-16	2.6E-05
Carbetamide	Soil	agricultural	3.4E-08	0.0E+00	0.0E+00	1.4E-06
Carbofuran	Soil	agricultural	4.6E-10	0.0E+00	4.2E-15	2.7E-06
Carbon disulfide	Air		1.3E-15	0.0E+00	7.0E-21	1.0E-16
Carbon disulfide	Air	high. pop.	6.2E-10	0.0E+00	5.2E-15	4.6E-11
Carbon disulfide	Air	low. pop.	5.8E-07	0.0E+00	1.2E-12	4.3E-08
Carbon disulfide	Water	river	1.1E-07	0.0E+00	2.1E-13	6.8E-06
Carfentrazone-ethyl	Air	low. pop.	6.7E-14	0.0E+00	0.0E+00	3.7E-10
Carfentrazone-ethyl	Soil	agricultural	1.5E-13	0.0E+00	0.0E+00	7.1E-12
Chloramine	Air	high. pop.	2.0E-09	0.0E+00	4.1E-15	2.5E-05
Chloramine	Water	river	1.8E-08	0.0E+00	9.5E-15	1.3E-03
Chlorfenvinphos	Soil	agricultural	2.1E-11	0.0E+00	4.5E-15	1.1E-07
Chloridazon	Soil	agricultural	1.6E-12	0.0E+00	0.0E+00	9.5E-10
Chlormequat	Soil	agricultural	1.4E-05	0.0E+00	5.9E-12	0.0E+00
Chloroacetic acid	Air	high. pop.	9.4E-08	0.0E+00	0.0E+00	3.5E-05
Chloroacetic acid	Water	river	3.1E-06	0.0E+00	0.0E+00	9.0E-03
Chloroform	Air		6.1E-16	1.2E-22	6.8E-22	1.5E-16
Chloroform	Air	high. pop.	7.8E-10	2.1E-16	1.2E-15	1.9E-10
Chloroform	Air	low. pop.	6.0E-10	7.7E-17	4.4E-16	1.5E-10
Chloroform	Water	river	2.5E-12	5.4E-19	2.1E-18	4.0E-11
Chlorosulfonic acid	Air		1.9E-14	0.0E+00	0.0E+00	1.5E-12
Chlorosulfonic acid	Air	high. pop.	1.6E-12	0.0E+00	0.0E+00	1.3E-10
Chlorosulfonic acid	Water	river	3.9E-12	0.0E+00	0.0E+00	2.3E-09
Chlorothalonil	Soil	agricultural	1.0E-05	4.3E-14	1.3E-12	7.3E-02
Chlorpyrifos	Air	low. pop.	2.4E-11	0.0E+00	8.0E-17	2.7E-07
Chlorpyrifos	Soil	agricultural	1.2E-09	0.0E+00	8.9E-15	6.4E-06
Chlorsulfuron	Soil	agricultural	2.5E-14	0.0E+00	2.3E-20	3.5E-11
Chlortoluron	Soil	agricultural	8.2E-06	0.0E+00	0.0E+00	1.5E-03
Choline chloride	Soil	agricultural	3.4E-12	0.0E+00	0.0E+00	8.3E-12
Chrysene	Air		6.4E-16	3.1E-20	0.0E+00	0.0E+00

Clethodim	Air	low. pop.	3.6E-12	0.0E+00	0.0E+00	4.9E-11
Clethodim	Soil	agricultural	8.1E-12	0.0E+00	0.0E+00	1.7E-11
Clodinafop-propargyl	Soil	agricultural	3.7E-13	0.0E+00	0.0E+00	1.2E-12
Clomazone	Soil	agricultural	8.7E-10	0.0E+00	0.0E+00	2.5E-07
Clopyralid	Soil	agricultural	2.1E-11	0.0E+00	0.0E+00	9.4E-10
Cloquintocet-mexyl	Soil	agricultural	8.9E-14	0.0E+00	0.0E+00	4.6E-13
Cumene	Air		5.5E-17	0.0E+00	5.9E-25	4.3E-18
Cumene	Air	high. pop.	3.0E-08	0.0E+00	6.0E-16	2.5E-09
Cumene	Air	low. pop.	3.4E-11	0.0E+00	5.8E-20	2.5E-12
Cumene	Water	river	7.3E-08	0.0E+00	8.7E-16	2.0E-05
Cyclohexane	Air	high. pop.	3.7E-12	0.0E+00	7.8E-20	2.1E-15
Cycloxydim	Soil	agricultural	1.9E-15	0.0E+00	0.0E+00	7.9E-16
Cyfluthrin	Air	low. pop.	1.3E-13	0.0E+00	2.1E-19	1.1E-06
Cyfluthrin	Soil	agricultural	6.0E-12	0.0E+00	3.0E-19	1.5E-07
Cymoxanil	Soil	agricultural	7.4E-11	0.0E+00	0.0E+00	5.7E-09
Cypermethrin	Air	low. pop.	3.1E-13	0.0E+00	3.0E-19	1.5E-07
Cypermethrin	Soil	agricultural	1.8E-09	0.0E+00	2.3E-16	2.4E-05
Cyproconazole	Soil	agricultural	1.5E-12	0.0E+00	0.0E+00	3.5E-10
Cyprodinil	Soil	agricultural	2.0E-10	0.0E+00	0.0E+00	4.4E-08
Deltamethrin	Soil	agricultural	3.7E-11	0.0E+00	7.6E-18	2.7E-08
Diazinon	Soil	agricultural	2.4E-10	0.0E+00	7.5E-15	3.8E-07
Dibenz(a,h)anthracene	Air		3.3E-15	1.8E-17	0.0E+00	2.5E-13
Dicamba	Air	low. pop.	1.3E-12	0.0E+00	2.1E-18	9.3E-11
Dicamba	Water	groundwater	2.1E-13	0.0E+00	4.9E-19	5.9E-12
Dicamba	Water	river	8.5E-16	0.0E+00	2.0E-21	1.6E-12
Dicamba	Soil	agricultural	4.3E-11	0.0E+00	6.5E-18	1.2E-09
Dichlorprop	Air	low. pop.	5.9E-14	0.0E+00	0.0E+00	7.0E-13
Dichlorprop	Water	groundwater	6.1E-14	0.0E+00	0.0E+00	6.8E-13
Dichlorprop	Water	river	2.6E-16	0.0E+00	0.0E+00	1.1E-13
Dichlorprop	Soil	agricultural	2.5E-12	0.0E+00	0.0E+00	2.7E-11
Diclofop-methyl	Soil	agricultural	2.4E-11	0.0E+00	0.0E+00	9.9E-10
Diclotophos	Soil	agricultural	7.0E-11	0.0E+00	1.6E-15	1.0E-07
Diethyl ether	Air	high. pop.	2.5E-14	0.0E+00	3.1E-22	4.6E-17
Diethylamine	Air	high. pop.	2.7E-09	0.0E+00	0.0E+00	5.9E-09
Diethylamine	Water	river	6.6E-09	0.0E+00	0.0E+00	7.2E-07
Diethylene glycol	Air	high. pop.	2.8E-13	1.3E-20	0.0E+00	1.5E-14
Difenoconazole	Soil	agricultural	3.5E-10	0.0E+00	0.0E+00	5.2E-07
Diflubenzuron	Air	low. pop.	6.7E-14	0.0E+00	8.1E-20	1.2E-08
Diflubenzuron	Soil	agricultural	3.1E-09	0.0E+00	3.0E-17	4.5E-06
Diflufenican	Soil	agricultural	6.6E-11	0.0E+00	0.0E+00	1.6E-09

Dimethachlor	Soil	agricultural	2.1E-09	0.0E+00	0.0E+00	2.8E-07
Dimethenamid	Air	low. pop.	5.8E-14	0.0E+00	0.0E+00	8.8E-11
Dimethenamid	Water	groundwater	2.0E-14	0.0E+00	0.0E+00	1.2E-10
Dimethenamid	Water	river	2.6E-16	0.0E+00	0.0E+00	3.6E-11
Dimethenamid	Soil	agricultural	5.5E-06	0.0E+00	0.0E+00	3.1E-02
Dimethoate	Soil	agricultural	1.5E-10	0.0E+00	1.9E-16	1.9E-07
Dimethomorph	Soil	agricultural	5.6E-11	0.0E+00	0.0E+00	8.3E-09
Dimethyl malonate	Air	high. pop.	1.6E-12	0.0E+00	0.0E+00	2.7E-11
Dimethylamine	Air	high. pop.	2.1E-13	0.0E+00	0.0E+00	7.7E-13
Dimethylamine	Water	river	1.4E-08	0.0E+00	0.0E+00	2.3E-06
Dioxin, 2,3,7,8 Tetrachlorodibenzo -p-	Air		6.1E-14	2.3E-12	0.0E+00	1.9E-08
Dioxin, 2,3,7,8 Tetrachlorodibenzo -p-	Air	high. pop.	8.6E-15	3.4E-13	0.0E+00	2.9E-09
Dioxin, 2,3,7,8 Tetrachlorodibenzo -p-	Air	low. pop.	1.4E-14	5.4E-13	0.0E+00	4.2E-09
Dioxin, 2,3,7,8 Tetrachlorodibenzo -p-	Air	low. pop., long-term	4.6E-19	1.7E-17	0.0E+00	1.4E-13
Dipropylamine	Air	high. pop.	8.0E-12	0.0E+00	0.0E+00	1.1E-10
Dipropylamine	Water	river	1.9E-11	0.0E+00	0.0E+00	1.3E-08
Dipropylthiocarbam ic acid S-ethyl ester	Soil	agricultural	1.1E-10	0.0E+00	1.1E-16	2.2E-09
Diquat	Soil	agricultural	2.2E-11	0.0E+00	4.6E-16	1.1E-07
Diquat dibromide	Soil	agricultural	2.9E-11	0.0E+00	1.2E-15	2.2E-06
Dithianone	Soil	agricultural	2.2E-10	0.0E+00	2.6E-16	3.2E-07
Diuron	Soil	agricultural	1.0E-09	0.0E+00	3.8E-15	4.7E-06
Endosulfan	Soil	agricultural	6.4E-10	0.0E+00	8.2E-16	5.2E-07
Endothall	Soil	agricultural	2.2E-11	0.0E+00	5.1E-18	3.2E-10
Epoxiconazole	Soil	agricultural	4.1E-12	0.0E+00	0.0E+00	4.4E-09
Esfenvalerate	Air	low. pop.	7.6E-13	0.0E+00	0.0E+00	2.0E-07
Esfenvalerate	Soil	agricultural	1.6E-12	0.0E+00	0.0E+00	6.6E-08
Ethalfuralin	Soil	agricultural	7.1E-10	0.0E+00	0.0E+00	2.7E-07
Ethane, 1,1,1- trichloro-, HCFC- 140	Air		1.1E-15	0.0E+00	1.8E-23	2.1E-16
Ethane, 1,1,1- trichloro-, HCFC- 140	Air	low. pop.	1.2E-10	0.0E+00	1.8E-18	2.3E-11
Ethane, 1,1,1- trichloro-, HCFC- 140	Water	river	6.6E-17	0.0E+00	9.9E-25	5.5E-16
Ethane, 1,1,1,2-	Air		1.3E-09	1.5E-17	5.4E-18	0.0E+0

tetrafluoro-, HFC-134a						0
Ethane, 1,1,1,2-tetrafluoro-, HFC-134a	Air	high. pop.	1.7E-10	2.1E-18	7.6E-19	0.0E+00
Ethane, 1,1,1,2-tetrafluoro-, HFC-134a	Air	low. pop.	4.4E-10	4.9E-18	1.8E-18	0.0E+00
Ethane, 1,1,2-trichloro-1,2,2-trifluoro-, CFC-113	Air		2.1E-10	0.0E+00	7.7E-19	0.0E+00
Ethane, 1,1,2-trichloro-1,2,2-trifluoro-, CFC-113	Air	high. pop.	4.4E-14	0.0E+00	2.2E-22	0.0E+00
Ethane, 1,1,2-trichloro-1,2,2-trifluoro-, CFC-113	Air	low. pop., long-term	2.4E-11	0.0E+00	5.6E-20	0.0E+00
Ethane, 1,2-dichloro-	Air		1.8E-14	6.3E-21	0.0E+00	2.3E-15
Ethane, 1,2-dichloro-	Air	high. pop.	9.5E-08	4.9E-14	0.0E+00	1.2E-08
Ethane, 1,2-dichloro-	Air	low. pop.	2.5E-10	4.2E-17	0.0E+00	3.0E-11
Ethane, 1,2-dichloro-	Water	river	1.0E-07	7.3E-14	0.0E+00	6.1E-07
Ethane, 2-chloro-1,1,1,2-tetrafluoro-, HCFC-124	Air		2.1E-10	0.0E+00	0.0E+00	0.0E+00
Ethanol	Air		1.5E-12	3.0E-21	0.0E+00	2.2E-13
Ethanol	Air	high. pop.	5.5E-08	2.0E-16	0.0E+00	8.5E-09
Ethanol	Air	low. pop.	1.2E-08	7.0E-18	0.0E+00	1.9E-09
Ethanol	Water		2.9E-14	6.5E-23	0.0E+00	7.8E-14
Ethanol	Water	river	1.3E-08	2.9E-17	0.0E+00	3.5E-08
Ethene, chloro-	Air		4.1E-16	1.1E-21	3.8E-22	0.0E+00
Ethene, chloro-	Air	high. pop.	3.3E-08	1.7E-13	5.7E-14	0.0E+00
Ethene, chloro-	Water	river	3.9E-10	3.3E-16	1.0E-15	0.0E+00
Ethene, tetrachloro-	Air		9.0E-13	2.5E-19	9.5E-19	5.8E-13
Ethene, tetrachloro-	Air	high. pop.	1.3E-10	5.0E-17	1.9E-16	8.5E-11
Ethene, tetrachloro-	Air	low. pop.	2.7E-10	4.7E-17	1.8E-16	1.7E-10
Ethephon	Air	low. pop.	2.2E-18	0.0E+00	2.0E-23	2.4E-16
Ethephon	Water	groundwater	1.5E-19	0.0E+00	7.5E-25	1.5E-17
Ethephon	Water	river	8.9E-22	0.0E+00	4.5E-27	1.2E-18
Ethephon	Soil	agricultural	2.3E-10	0.0E+00	2.2E-16	2.4E-08
Ethofumesate	Soil	agricultural	5.9E-10	0.0E+00	0.0E+00	9.2E-08

Ethoprop	Soil	agricultural	2.7E-11	0.0E+00	1.1E-14	3.7E-07
Ethyl acetate	Air	high. pop.	4.5E-08	0.0E+00	3.6E-16	4.1E-09
Ethyl acetate	Water	river	1.2E-10	0.0E+00	3.1E-19	3.6E-10
Ethylamine	Air	high. pop.	6.7E-12	0.0E+00	0.0E+00	9.7E-12
Ethylamine	Water	river	1.6E-11	0.0E+00	0.0E+00	8.4E-10
Ethylene diamine	Air	high. pop.	1.8E-08	0.0E+00	0.0E+00	1.7E-07
Ethylene diamine	Water	river	4.4E-08	0.0E+00	0.0E+00	1.7E-05
Ethylene oxide	Air		7.4E-12	4.7E-18	0.0E+00	4.8E-12
Ethylene oxide	Air	high. pop.	1.5E-10	1.5E-16	0.0E+00	9.5E-11
Ethylene oxide	Air	low. pop.	8.4E-13	2.1E-19	0.0E+00	5.5E-13
Ethylene oxide	Air	stratosphere + troposphere	3.1E-12	7.7E-19	0.0E+00	2.0E-12
Ethylene oxide	Water	river	3.3E-08	2.9E-14	0.0E+00	3.7E-07
Fenamiphos	Soil	agricultural	2.8E-10	0.0E+00	2.8E-16	2.1E-07
Fenbuconazole	Soil	agricultural	1.3E-13	0.0E+00	1.5E-19	3.1E-10
Fenoxaprop-P ethyl ester	Soil	agricultural	1.1E-12	0.0E+00	0.0E+00	5.5E-13
Fenoxaprop ethyl ester	Soil	agricultural	2.0E-12	0.0E+00	0.0E+00	1.1E-11
Fenoxycarb	Soil	agricultural	1.6E-11	0.0E+00	0.0E+00	8.2E-10
Fenpiclonil	Soil	agricultural	1.8E-11	0.0E+00	0.0E+00	4.3E-08
Fentin hydroxide	Soil	agricultural	4.6E-12	0.0E+00	2.5E-16	5.6E-06
Fipronil	Soil	agricultural	4.2E-10	0.0E+00	9.8E-15	7.2E-06
Fluazifop-p-butyl	Air	low. pop.	1.4E-12	0.0E+00	0.0E+00	3.4E-10
Fludioxonil	Soil	agricultural	3.4E-11	0.0E+00	0.0E+00	8.6E-09
Flufenacet	Air	low. pop.	5.3E-13	0.0E+00	0.0E+00	1.8E-09
Flufenacet	Soil	agricultural	1.6E-11	0.0E+00	0.0E+00	5.7E-08
Flumetsulam	Air	low. pop.	1.3E-13	0.0E+00	0.0E+00	3.5E-10
Flumetsulam	Soil	agricultural	5.9E-12	0.0E+00	0.0E+00	1.8E-08
Flumiclorac-pentyl	Air	low. pop.	2.1E-13	0.0E+00	0.0E+00	1.5E-10
Flumiclorac-pentyl	Soil	agricultural	9.2E-15	0.0E+00	0.0E+00	8.7E-14
Flumioxazin	Air	low. pop.	2.2E-12	0.0E+00	0.0E+00	5.3E-09
Flumioxazin	Soil	agricultural	2.8E-12	0.0E+00	0.0E+00	4.0E-08
Fluoranthene	Air		5.4E-14	2.9E-19	1.4E-20	3.6E-11
Fluorene	Air		4.9E-14	7.6E-20	3.7E-21	7.6E-13
Fluroxypyr	Soil	agricultural	1.9E-12	0.0E+00	0.0E+00	9.0E-10
Flutolanil	Soil	agricultural	5.2E-12	0.0E+00	4.6E-18	1.8E-09
Folpet	Soil	agricultural	1.2E-05	3.7E-14	1.3E-13	3.9E-02
Fomesafen	Air	low. pop.	8.0E-12	9.9E-17	0.0E+00	4.4E-10
Fomesafen	Soil	agricultural	1.8E-11	2.2E-16	0.0E+00	1.3E-09
Formaldehyde	Air		4.6E-08	6.0E-13	7.7E-15	7.7E-07
Formaldehyde	Air	high. pop.	1.7E-07	4.3E-12	4.5E-14	3.1E-06

Formaldehyde	Air	low. pop.	9.3E-08	1.1E-13	6.8E-15	1.5E-06
Formaldehyde	Air	stratosphere + troposphere	2.7E-12	3.1E-18	2.0E-19	4.2E-11
Formaldehyde	Water		8.5E-09	1.2E-15	2.7E-15	2.5E-06
Formaldehyde	Water	river	1.4E-07	1.9E-14	4.3E-14	3.9E-05
Formamide	Air	high. pop.	2.0E-12	0.0E+00	0.0E+00	3.0E-12
Formamide	Water	river	4.7E-12	0.0E+00	0.0E+00	3.3E-11
Formic acid	Air	high. pop.	5.3E-11	0.0E+00	0.0E+00	1.5E-10
Formic acid	Air	low. pop.	3.1E-09	0.0E+00	0.0E+00	6.7E-09
Formic acid	Water	river	1.4E-12	0.0E+00	0.0E+00	6.2E-11
Fosetyl-aluminium	Soil	agricultural	1.3E-09	9.8E-20	5.7E-20	2.8E-09
Furan	Air		8.8E-17	2.8E-21	3.2E-22	2.2E-19
Furan	Air	low. pop.	1.3E-08	1.8E-14	2.0E-15	3.5E-11
Glufosinate ammonium	Soil	agricultural	6.1E-11	0.0E+00	3.5E-18	2.5E-10
Glutaraldehyde	Water	ocean	1.8E-10	0.0E+00	0.0E+00	1.7E-11
Glyphosate	Air	low. pop.	1.6E-09	0.0E+00	6.4E-17	1.6E-08
Glyphosate	Water	groundwater	5.0E-12	0.0E+00	8.0E-19	3.6E-10
Glyphosate	Water	river	2.6E-14	0.0E+00	4.1E-21	8.3E-12
Glyphosate	Soil	agricultural	6.7E-05	0.0E+00	7.8E-12	4.8E-03
Glyphosate	Soil	industrial	2.0E-09	0.0E+00	7.0E-17	1.4E-07
Heptane	Air		6.3E-10	0.0E+00	0.0E+00	9.2E-15
Heptane	Air	high. pop.	1.6E-07	0.0E+00	0.0E+00	4.0E-12
Hexane	Air		7.0E-16	6.7E-25	9.1E-23	9.4E-20
Hexane	Air	high. pop.	4.1E-07	7.2E-16	9.8E-14	8.6E-11
Hexane	Air	low. pop.	2.7E-07	4.2E-17	5.8E-15	1.6E-11
Hexazinone	Soil	agricultural	4.7E-11	0.0E+00	4.6E-17	1.2E-06
Hydramethylnon	Soil	agricultural	1.1E-12	0.0E+00	9.4E-19	2.0E-12
Imazamox	Air	low. pop.	3.2E-13	0.0E+00	0.0E+00	1.5E-10
Imazamox	Soil	agricultural	2.4E-12	0.0E+00	0.0E+00	1.3E-09
Imazapyr	Soil	agricultural	8.4E-14	0.0E+00	0.0E+00	6.9E-14
Imazethapyr	Air	low. pop.	2.1E-12	0.0E+00	4.9E-19	2.5E-10
Imazethapyr	Soil	agricultural	6.3E-12	0.0E+00	9.5E-19	9.7E-10
Imidacloprid	Soil	agricultural	2.6E-06	0.0E+00	5.2E-12	3.2E-03
Indeno(1,2,3-cd)pyrene	Air		1.3E-15	5.4E-19	0.0E+00	0.0E+00
Ioxynil	Soil	agricultural	1.1E-10	0.0E+00	0.0E+00	1.5E-08
Iprodione	Soil	agricultural	1.4E-09	0.0E+00	1.4E-15	3.3E-06
Isoprene	Air		1.2E-15	8.1E-23	0.0E+00	5.3E-20
Isoprene	Air	low. pop.	4.5E-11	6.4E-20	0.0E+00	1.5E-15
Isopropylamine	Air	high. pop.	3.3E-12	0.0E+00	0.0E+00	1.3E-11
Isopropylamine	Water	river	8.0E-12	0.0E+00	0.0E+00	1.3E-09

Isoproturon	Soil	agricultural	1.2E-05	0.0E+00	0.0E+00	1.5E-02
Isoxaflutole	Soil	agricultural	1.0E-11	0.0E+00	0.0E+00	1.7E-09
Kresoxim-methyl	Soil	agricultural	9.9E-13	0.0E+00	3.2E-20	9.5E-10
Lambda-cyhalothrin	Air	low. pop.	7.0E-20	0.0E+00	0.0E+00	5.9E-14
Lambda-cyhalothrin	Water	groundwater	3.6E-23	0.0E+00	0.0E+00	3.3E-19
Lambda-cyhalothrin	Water	river	8.9E-26	0.0E+00	0.0E+00	1.2E-17
Lambda-cyhalothrin	Soil	agricultural	1.1E-10	0.0E+00	0.0E+00	9.7E-07
Lenacil	Soil	agricultural	2.4E-11	0.0E+00	0.0E+00	9.3E-08
Linuron	Soil	agricultural	2.9E-09	0.0E+00	2.4E-14	1.4E-05
m-Xylene	Air		2.1E-09	0.0E+00	0.0E+00	3.8E-11
m-Xylene	Air	high. pop.	1.5E-08	0.0E+00	0.0E+00	2.8E-10
m-Xylene	Air	low. pop.	9.4E-13	0.0E+00	0.0E+00	1.7E-14
m-Xylene	Water		2.4E-10	0.0E+00	0.0E+00	2.9E-08
m-Xylene	Water	river	2.3E-08	0.0E+00	0.0E+00	2.7E-06
Malathion	Soil	agricultural	4.1E-11	0.0E+00	7.5E-20	2.8E-09
Maleic hydrazide	Soil	agricultural	2.9E-11	0.0E+00	4.1E-19	3.0E-10
Mancozeb	Soil	agricultural	3.5E-05	0.0E+00	7.3E-12	6.9E-02
Maneb	Soil	agricultural	6.7E-13	1.6E-20	5.5E-20	7.1E-10
Mcpa - sodium salt	Soil	agricultural	5.3E-06	0.0E+00	0.0E+00	1.7E-04
MCPB	Air	low. pop.	8.1E-14	0.0E+00	4.7E-20	2.7E-12
MCPB	Water	groundwater	8.6E-16	0.0E+00	1.5E-21	2.0E-14
MCPB	Water	river	1.9E-13	0.0E+00	3.2E-19	3.6E-10
MCPB	Soil	agricultural	2.1E-11	0.0E+00	3.6E-18	4.8E-10
Mepiquat chloride	Soil	agricultural	2.5E-11	0.0E+00	7.8E-23	7.4E-13
Metalaxil	Soil	agricultural	1.6E-11	0.0E+00	6.2E-18	2.8E-09
Metalaxyl-M	Soil	agricultural	2.1E-10	0.0E+00	0.0E+00	7.3E-08
Metam-sodium dihydrate	Soil	agricultural	1.7E-05	0.0E+00	0.0E+00	1.5E-01
Metamitron	Soil	agricultural	3.9E-06	0.0E+00	0.0E+00	3.6E-05
Metazachlor	Soil	agricultural	5.0E-06	0.0E+00	0.0E+00	2.1E-04
Methane, bromo-, Halon 1001	Air		1.7E-15	0.0E+00	1.4E-19	1.8E-14
Methane, chlorodifluoro-, HCFC-22	Air		1.3E-15	0.0E+00	1.1E-23	0.0E+00
Methane, chlorodifluoro-, HCFC-22	Air	high. pop.	1.9E-09	0.0E+00	1.7E-17	0.0E+00
Methane, chlorodifluoro-, HCFC-22	Air	low. pop.	4.6E-09	0.0E+00	3.7E-17	0.0E+00
Methane, dichloro-,	Air		5.9E-11	3.3E-18	3.9E-17	4.9E-12

HCC-30						
Methane, dichloro-, HCC-30	Air	high. pop.	4.1E-11	3.3E-18	3.8E-17	3.5E-12
Methane, dichloro-, HCC-30	Air	low. pop.	1.8E-09	6.0E-17	7.0E-16	1.5E-10
Methane, dichloro-, HCC-30	Water	river	9.0E-09	3.8E-16	4.2E-15	5.0E-08
Methane, dichlorodifluoro-, CFC-12	Air		1.1E-15	0.0E+00	2.5E-22	0.0E+00
Methane, dichlorodifluoro-, CFC-12	Air	high. pop.	4.8E-10	0.0E+00	1.6E-16	0.0E+00
Methane, dichlorodifluoro-, CFC-12	Air	low. pop.	2.4E-13	0.0E+00	2.9E-20	0.0E+00
Methane, monochloro-, R-40	Air	low. pop.	3.3E-09	0.0E+00	1.2E-15	1.9E-10
Methane, tetrachloro-, CFC-10	Air		4.9E-13	1.7E-18	5.7E-18	2.2E-14
Methane, tetrachloro-, CFC-10	Air	high. pop.	4.2E-10	2.0E-15	6.6E-15	1.8E-11
Methane, trichlorofluoro-, CFC-11	Air	high. pop.	6.2E-13	0.0E+00	4.0E-20	0.0E+00
Methanol	Air		1.1E-07	0.0E+00	1.0E-15	2.1E-08
Methanol	Air	high. pop.	5.6E-07	0.0E+00	8.6E-15	1.1E-07
Methanol	Air	low. pop.	5.8E-08	0.0E+00	1.8E-16	1.1E-08
Methanol	Water		2.6E-09	0.0E+00	2.4E-17	5.9E-09
Methanol	Water	ocean	1.1E-09	0.0E+00	4.5E-20	2.6E-12
Methanol	Water	river	3.5E-08	0.0E+00	3.3E-16	8.0E-08
Methomyl	Air	low. pop.	7.6E-18	0.0E+00	5.3E-23	1.1E-14
Methomyl	Water	groundwater	1.2E-19	0.0E+00	1.4E-24	2.0E-16
Methomyl	Water	river	1.3E-21	0.0E+00	1.6E-26	3.8E-17
Methomyl	Soil	agricultural	2.4E-17	0.0E+00	6.7E-23	4.1E-14
Methoxyfenozide	Soil	agricultural	2.8E-11	0.0E+00	0.0E+00	2.7E-08
Methyl acetate	Air	high. pop.	1.5E-09	0.0E+00	0.0E+00	5.8E-10
Methyl acetate	Water	river	3.5E-09	0.0E+00	0.0E+00	2.7E-08
Methyl acrylate	Air	high. pop.	1.0E-12	0.0E+00	0.0E+00	2.8E-12
Methyl acrylate	Water	river	2.0E-11	0.0E+00	0.0E+00	6.4E-09
Methyl ethyl ketone	Air	high. pop.	4.5E-08	0.0E+00	5.1E-17	1.9E-09
Methyl ethyl ketone	Air	low. pop.	5.4E-13	0.0E+00	2.3E-22	2.3E-14
Methyl formate	Air	high. pop.	8.2E-13	0.0E+00	0.0E+00	3.1E-13
Methyl formate	Water	river	3.3E-13	0.0E+00	0.0E+00	2.7E-12
Methyl lactate	Air	high. pop.	6.9E-12	0.0E+00	0.0E+00	1.4E-11

Methylamine	Air	high. pop.	1.9E-12	0.0E+00	0.0E+00	4.9E-12
Methylamine	Water	river	4.6E-12	0.0E+00	0.0E+00	3.7E-10
Metiram	Soil	agricultural	7.8E-06	0.0E+00	9.8E-17	1.9E-07
Metolachlor	Air	low. pop.	1.7E-11	0.0E+00	4.6E-18	1.1E-08
Metolachlor	Water	groundwater	2.7E-13	0.0E+00	3.3E-19	3.3E-10
Metolachlor	Water	river	1.3E-15	0.0E+00	1.6E-21	8.5E-11
Metolachlor	Soil	agricultural	1.5E-05	0.0E+00	2.5E-12	1.8E-02
Metribuzin	Air	low. pop.	6.7E-12	0.0E+00	9.4E-18	2.2E-09
Metribuzin	Soil	agricultural	8.5E-11	0.0E+00	4.5E-17	5.9E-08
Metsulfuron-methyl	Soil	agricultural	3.6E-12	0.0E+00	2.8E-19	2.8E-09
Monocrotophos	Soil	agricultural	3.7E-10	0.0E+00	3.2E-14	2.9E-07
Monoethanolamine	Air	high. pop.	1.4E-08	0.0E+00	0.0E+00	2.3E-08
Monoethanolamine	Water		2.1E-11	0.0E+00	0.0E+00	1.3E-09
Monosodium acid methanearsonate	Soil	agricultural	3.6E-11	0.0E+00	0.0E+00	2.5E-09
Napropamide	Soil	agricultural	4.6E-06	0.0E+00	9.3E-13	5.5E-04
Nicosulfuron	Soil	agricultural	4.6E-12	0.0E+00	0.0E+00	3.0E-10
Nitrobenzene	Air	high. pop.	4.1E-11	5.7E-17	2.8E-16	3.1E-10
Nitrobenzene	Water	river	1.6E-10	1.3E-16	6.3E-16	2.0E-08
o-Xylene	Air		8.3E-10	0.0E+00	0.0E+00	2.6E-11
o-Xylene	Air	high. pop.	6.6E-12	0.0E+00	0.0E+00	2.0E-13
o-Xylene	Water		1.8E-10	0.0E+00	0.0E+00	1.6E-08
Orbencarb	Soil	agricultural	1.1E-10	0.0E+00	0.0E+00	2.7E-08
Oryzalin	Soil	agricultural	4.5E-11	0.0E+00	4.3E-17	3.9E-07
Oxamyl	Soil	agricultural	2.2E-11	0.0E+00	2.5E-17	4.5E-08
Oxydemeton methyl	Soil	agricultural	5.4E-13	0.0E+00	0.0E+00	2.1E-10
Paraquat	Air	low. pop.	4.3E-12	0.0E+00	2.1E-17	1.2E-08
Paraquat	Soil	agricultural	2.4E-11	0.0E+00	1.3E-17	1.3E-07
Parathion	Soil	agricultural	7.6E-11	0.0E+00	2.1E-16	1.5E-06
Parathion, methyl	Air	low. pop.	8.2E-13	0.0E+00	2.3E-18	3.2E-10
Parathion, methyl	Soil	agricultural	3.5E-14	0.0E+00	3.5E-20	6.0E-12
Pendimethalin	Air	low. pop.	4.5E-11	0.0E+00	5.5E-18	1.5E-07
Pendimethalin	Water	groundwater	2.8E-14	0.0E+00	1.6E-20	5.8E-11
Pendimethalin	Water	river	4.7E-17	0.0E+00	2.6E-23	2.0E-11
Pendimethalin	Soil	agricultural	6.6E-06	0.0E+00	2.4E-12	1.4E-02
Pentane	Air		2.5E-10	0.0E+00	0.0E+00	2.3E-12
Pentane	Air	high. pop.	9.2E-07	0.0E+00	0.0E+00	1.1E-08
Pentane	Air	low. pop.	5.0E-07	0.0E+00	0.0E+00	2.9E-09
Permethrin	Air	low. pop.	6.7E-13	0.0E+00	2.9E-19	6.0E-09
Permethrin	Soil	agricultural	2.8E-12	0.0E+00	1.2E-19	7.5E-10
Phenanthrene	Air		7.5E-13	2.6E-18	0.0E+00	8.3E-11

Phenmedipham	Soil	agricultural	4.5E-10	0.0E+00	6.7E-18	2.7E-08
Phenol	Air		1.4E-10	0.0E+00	7.5E-18	3.1E-09
Phenol	Air	high. pop.	2.3E-08	0.0E+00	2.0E-15	5.9E-07
Phenol	Air	low. pop.	1.3E-09	0.0E+00	2.2E-17	2.4E-08
Phenol	Water		4.4E-09	0.0E+00	6.2E-16	4.1E-06
Phenol	Water	ocean	1.1E-08	0.0E+00	4.8E-18	2.2E-10
Phenol	Water	river	8.8E-08	0.0E+00	1.2E-14	8.1E-05
Phenol, 2,4-dichloro-	Air		1.1E-13	0.0E+00	2.1E-18	1.1E-10
Phenol, 2,4-dichloro-	Air	high. pop.	3.1E-12	0.0E+00	7.8E-17	3.2E-09
Phenol, pentachloro-	Air		3.5E-11	2.9E-16	6.3E-16	2.0E-07
Phenol, pentachloro-	Air	high. pop.	3.6E-13	3.0E-18	6.6E-18	2.2E-09
Phenol, pentachloro-	Air	low. pop.	4.3E-09	3.5E-14	7.6E-14	2.1E-05
Phenol, pentachloro-	Soil		1.2E-12	8.5E-19	1.9E-18	3.5E-09
Phorate	Soil	agricultural	4.8E-11	0.0E+00	2.4E-15	5.0E-07
Phosmet	Soil	agricultural	5.3E-12	0.0E+00	2.6E-18	5.7E-08
Picloram	Soil	agricultural	3.1E-15	0.0E+00	8.7E-22	1.2E-12
Piperonyl butoxide	Soil	agricultural	7.5E-12	3.1E-19	1.2E-19	1.2E-10
Pirimicarb	Soil	agricultural	1.7E-10	0.0E+00	3.0E-17	6.8E-09
Polychlorinated biphenyls	Air		5.7E-11	4.5E-15	0.0E+00	1.0E-08
Polychlorinated biphenyls	Air	high. pop.	2.5E-14	2.0E-18	0.0E+00	4.6E-12
Polychlorinated biphenyls	Water		3.1E-14	4.5E-17	0.0E+00	2.3E-10
Prochloraz	Soil	agricultural	4.3E-06	4.4E-12	8.2E-12	4.2E-03
Procymidone	Soil	agricultural	3.4E-10	0.0E+00	9.8E-17	6.0E-09
Profenofos	Soil	agricultural	5.6E-11	0.0E+00	1.6E-16	1.6E-06
Prometryn	Soil	agricultural	3.0E-11	0.0E+00	1.0E-17	2.6E-07
Pronamide	Soil	agricultural	3.7E-06	5.8E-12	2.4E-12	9.7E-04
Propachlor	Soil	agricultural	1.7E-09	0.0E+00	5.9E-17	6.1E-07
Propanal	Air		3.9E-15	0.0E+00	0.0E+00	1.6E-15
Propanal	Air	high. pop.	6.1E-11	0.0E+00	0.0E+00	2.4E-11
Propanal	Air	low. pop.	1.4E-10	0.0E+00	0.0E+00	6.0E-11
Propanal	Water	river	3.0E-12	0.0E+00	0.0E+00	1.4E-10
Propargite	Soil	agricultural	1.5E-11	0.0E+00	4.0E-18	6.4E-10
Propene	Air		1.3E-10	0.0E+00	0.0E+00	0.0E+00
Propene	Air	high. pop.	1.4E-07	0.0E+00	0.0E+00	0.0E+00
Propene	Air	low. pop.	1.1E-08	0.0E+00	0.0E+00	0.0E+00

						0
Propene	Water	river	8.2E-08	0.0E+00	0.0E+00	0.0E+00
Propiconazole	Air	low. pop.	7.9E-13	0.0E+00	1.0E-18	3.1E-10
Propiconazole	Water	groundwater	5.4E-16	0.0E+00	8.3E-21	2.7E-13
Propiconazole	Water	river	5.2E-20	0.0E+00	8.0E-25	1.2E-15
Propiconazole	Soil	agricultural	1.9E-11	0.0E+00	3.9E-17	9.5E-09
Propionic acid	Air		1.3E-12	0.0E+00	0.0E+00	8.9E-12
Propionic acid	Air	high. pop.	8.4E-09	0.0E+00	0.0E+00	6.0E-08
Propionic acid	Air	low. pop.	5.1E-09	0.0E+00	0.0E+00	3.3E-08
Propionic acid	Water	river	1.8E-08	0.0E+00	0.0E+00	1.3E-06
Propylamine	Air	high. pop.	7.3E-13	0.0E+00	0.0E+00	5.0E-13
Propylamine	Water	river	1.8E-12	0.0E+00	0.0E+00	4.7E-11
Propylene oxide	Air	high. pop.	3.9E-09	1.4E-15	2.6E-14	3.5E-09
Propylene oxide	Water	river	9.0E-09	2.1E-15	2.2E-14	1.4E-07
Prosulfuron	Soil	agricultural	7.9E-13	0.0E+00	0.0E+00	5.2E-09
Pymetrozine	Soil	agricultural	1.5E-12	0.0E+00	0.0E+00	3.2E-10
Pyrene	Air		3.9E-14	1.3E-19	1.1E-20	2.0E-10
Pyrethrin	Soil	agricultural	8.1E-12	0.0E+00	0.0E+00	2.0E-07
Pyrimethanil	Soil	agricultural	1.1E-10	0.0E+00	0.0E+00	5.1E-09
Pyriithiobac sodium salt	Soil	agricultural	2.0E-12	0.0E+00	0.0E+00	2.8E-09
Quizalofop ethyl ester	Air	low. pop.	2.5E-13	0.0E+00	3.9E-19	3.3E-10
Quizalofop ethyl ester	Soil	agricultural	4.3E-11	0.0E+00	1.7E-16	2.2E-08
Rimsulfuron	Soil	agricultural	2.8E-12	0.0E+00	0.0E+00	1.8E-09
Rotenone	Soil	agricultural	4.6E-12	0.0E+00	2.0E-18	5.3E-10
Sethoxydim	Air	low. pop.	5.4E-13	0.0E+00	4.3E-20	2.2E-11
Sethoxydim	Soil	agricultural	2.2E-10	0.0E+00	6.7E-18	1.8E-09
Simazine	Soil	agricultural	4.2E-11	0.0E+00	6.9E-16	4.4E-07
Sodium formate	Air	high. pop.	2.2E-11	0.0E+00	0.0E+00	1.0E-11
Sodium formate	Water	river	5.3E-11	0.0E+00	0.0E+00	1.2E-10
Styrene	Air		1.2E-09	6.0E-16	1.2E-16	1.6E-11
Styrene	Air	high. pop.	2.6E-10	2.7E-16	5.3E-17	4.0E-12
Styrene	Air	low. pop.	2.1E-10	3.4E-18	6.7E-19	2.7E-12
Sulfentrazone	Air	low. pop.	5.1E-12	0.0E+00	0.0E+00	2.6E-08
Sulfentrazone	Soil	agricultural	2.9E-11	0.0E+00	0.0E+00	3.1E-07
Sulfosulfuron	Soil	agricultural	3.7E-14	0.0E+00	0.0E+00	4.4E-11
Sulfuric acid	Air		1.3E-10	0.0E+00	0.0E+00	6.2E-09
Sulfuric acid	Air	high. pop.	5.2E-11	0.0E+00	0.0E+00	2.6E-09
Sulfuric acid	Air	low. pop.	7.5E-09	0.0E+00	0.0E+00	3.5E-07
Sulfuric acid	Soil	agricultural	5.4E-09	0.0E+00	0.0E+00	3.0E-07

t-Butyl methyl ether	Air	high. pop.	4.9E-10	5.2E-17	8.7E-18	1.2E-11
t-Butyl methyl ether	Water	ocean	3.4E-11	9.3E-20	1.6E-20	1.7E-13
t-Butyl methyl ether	Water	river	2.0E-11	2.7E-19	8.7E-20	5.6E-11
t-Butylamine	Air	high. pop.	2.8E-12	0.0E+00	0.0E+00	2.6E-11
t-Butylamine	Water	river	6.6E-12	0.0E+00	0.0E+00	1.7E-09
Tebupirimphos	Soil	agricultural	1.8E-11	0.0E+00	0.0E+00	4.1E-07
Teflubenzuron	Soil	agricultural	1.3E-12	0.0E+00	6.1E-18	1.2E-09
Tefluthrin	Air	low. pop.	1.5E-14	0.0E+00	0.0E+00	4.3E-11
Tefluthrin	Water	groundwater	7.3E-20	0.0E+00	0.0E+00	3.2E-17
Tefluthrin	Water	river	1.0E-22	0.0E+00	0.0E+00	5.2E-16
Tefluthrin	Soil	agricultural	1.4E-11	0.0E+00	0.0E+00	6.2E-09
Terbacil	Soil	agricultural	6.0E-10	0.0E+00	2.5E-15	1.9E-06
Terbufos	Soil	agricultural	5.3E-11	0.0E+00	1.8E-14	3.3E-07
Thiazole, 2-(thiocyanatemetethylthio)benzo-	Soil	agricultural	4.5E-10	0.0E+00	0.0E+00	2.2E-07
Thidiazuron	Soil	agricultural	3.5E-12	0.0E+00	0.0E+00	3.3E-09
Thifensulfuron-methyl	Soil	agricultural	4.0E-14	0.0E+00	5.9E-20	2.1E-10
Thiodicarb	Air	low. pop.	2.6E-13	0.0E+00	7.5E-20	3.2E-10
Thiodicarb	Soil	agricultural	1.1E-14	0.0E+00	1.5E-21	1.3E-11
Thiram	Soil	agricultural	2.8E-06	0.0E+00	2.2E-13	9.1E-03
Toluene	Air		3.5E-07	1.6E-18	1.8E-14	4.4E-09
Toluene	Air	high. pop.	1.5E-07	6.9E-19	1.4E-14	1.9E-09
Toluene	Air	low. pop.	1.2E-07	5.4E-19	9.5E-16	1.4E-09
Toluene	Water		1.3E-08	1.7E-17	1.5E-16	2.9E-07
Toluene	Water	ocean	1.2E-08	2.4E-19	2.3E-17	3.4E-11
Toluene	Water	river	8.9E-08	1.2E-16	1.0E-15	2.0E-06
Toluene, 2-chloro-	Air	high. pop.	2.9E-11	0.0E+00	1.1E-17	4.6E-12
Toluene, 2-chloro-	Water	river	6.4E-11	0.0E+00	8.5E-18	4.7E-09
Triadimenol	Soil	agricultural	3.0E-13	0.0E+00	2.2E-19	5.5E-11
Triallate	Soil	agricultural	8.4E-14	0.0E+00	3.6E-19	5.7E-12
Triasulfuron	Soil	agricultural	2.5E-14	0.0E+00	1.9E-19	2.9E-11
Tribenuron-methyl	Soil	agricultural	8.8E-13	0.0E+00	1.1E-18	2.0E-11
Tribufos	Soil	agricultural	3.3E-11	0.0E+00	1.9E-15	2.3E-09
Trichlorfon	Soil	agricultural	2.3E-14	0.0E+00	4.0E-20	2.8E-10
Triclopyr	Soil	agricultural	9.1E-11	0.0E+00	0.0E+00	4.0E-08
Triethylene glycol	Water		3.8E-11	0.0E+00	0.0E+00	1.5E-11
Triethylene glycol	Water	ocean	1.2E-09	0.0E+00	0.0E+00	2.5E-17
Triethylene glycol	Water	river	3.8E-11	0.0E+00	0.0E+00	1.5E-11
Trifluralin	Air	low. pop.	7.4E-11	7.8E-18	7.7E-17	1.5E-08
Trifluralin	Soil	agricultural	1.7E-08	5.7E-15	5.6E-14	2.6E-06

Triforine	Soil	agricultural	1.4E-11	0.0E+00	3.7E-18	1.9E-09
Trimethylamine	Air	high. pop.	7.6E-13	0.0E+00	0.0E+00	1.1E-12
Trimethylamine	Water	river	1.8E-12	0.0E+00	0.0E+00	1.2E-10
Trinexapac-ethyl	Soil	agricultural	3.2E-11	0.0E+00	0.0E+00	1.6E-09
Urea	Water	river	3.6E-12	0.0E+00	0.0E+00	3.7E-11
Vinclozolin	Soil	agricultural	1.1E-10	0.0E+00	1.2E-16	2.2E-08
Xylene	Air		2.1E-07	9.9E-16	2.3E-14	2.3E-09
Xylene	Air	high. pop.	9.3E-08	8.4E-16	2.0E-14	1.0E-09
Xylene	Air	low. pop.	5.6E-07	2.5E-16	5.7E-15	6.0E-09
Xylene	Water		6.4E-09	1.2E-17	7.7E-17	2.0E-07
Xylene	Water	ocean	7.3E-09	9.3E-19	1.7E-17	1.7E-11
Xylene	Water	river	5.4E-08	9.8E-17	6.5E-16	1.7E-06
Antimony	Soil	agricultural	9.5E-14	0.0E+00	4.5E-17	9.1E-09
Antimony	Soil		5.2E-12	0.0E+00	2.2E-15	5.0E-07
Antimony	Water	river	2.3E-08	0.0E+00	2.0E-11	4.4E-03
Antimony	Water	groundwater , long-term	1.4E-07	0.0E+00	1.1E-10	1.3E-02
Antimony	Water	groundwater	1.7E-09	0.0E+00	1.5E-12	1.7E-04
Antimony	Water		9.0E-11	0.0E+00	7.6E-14	1.7E-05
Antimony	Air	low. pop., long-term	2.3E-11	0.0E+00	1.4E-14	1.6E-06
Antimony	Air	low. pop.	4.7E-09	0.0E+00	2.8E-12	3.1E-04
Antimony	Air	high. pop.	2.3E-10	0.0E+00	1.4E-13	1.6E-05
Antimony	Air		4.5E-08	0.0E+00	2.8E-11	3.0E-03
Arsenic	Soil	industrial	1.5E-10	1.7E-13	1.3E-11	3.2E-06
Arsenic	Soil	agricultural	6.3E-10	9.6E-13	7.1E-11	1.3E-05
Arsenic	Soil		1.3E-11	1.5E-14	1.1E-12	2.7E-07
Arsenic	Water	river	2.3E-08	5.0E-11	3.7E-09	9.3E-04
Arsenic	Water	ocean	1.8E-09	6.0E-12	4.4E-10	2.5E-22
Arsenic	Water	groundwater , long-term	4.4E-07	9.6E-10	7.1E-08	9.4E-03
Arsenic	Water	groundwater	1.0E-08	2.2E-11	1.6E-09	2.2E-04
Arsenic	Water		2.2E-09	4.9E-12	3.6E-10	9.1E-05
Arsenic	Air	low. pop., long-term	1.4E-09	2.7E-12	2.0E-10	2.0E-05
Arsenic	Air	low. pop.	3.8E-08	7.6E-11	5.6E-09	5.7E-04
Arsenic	Air	high. pop.	3.9E-09	8.3E-12	5.6E-10	5.8E-05
Arsenic	Air		6.4E-11	1.3E-13	9.2E-12	9.5E-07
Barium	Soil	industrial	1.9E-07	0.0E+00	2.5E-10	3.0E-03
Barium	Soil	agricultural	9.3E-12	0.0E+00	1.2E-14	1.5E-07
Barium	Soil		3.3E-10	0.0E+00	4.3E-13	5.2E-06
Barium	Water	river	5.0E-07	0.0E+00	1.3E-09	1.6E-02
Barium	Water	ocean	2.9E-08	0.0E+00	7.5E-11	2.9E-20

Barium	Water	groundwater , long-term	2.0E-06	0.0E+00	5.1E-09	3.1E-02
Barium	Water	groundwater	3.1E-09	0.0E+00	8.1E-12	4.9E-05
Barium	Water		2.3E-06	0.0E+00	6.0E-09	7.2E-02
Barium	Air	low. pop., long-term	1.5E-09	0.0E+00	2.6E-12	1.7E-05
Barium	Air	low. pop.	4.3E-08	0.0E+00	7.5E-11	4.8E-04
Barium	Air	high. pop.	1.1E-08	0.0E+00	1.9E-11	1.2E-04
Barium	Air		1.8E-08	0.0E+00	3.0E-11	2.0E-04
Beryllium	Water	river	7.8E-12	3.9E-37	2.1E-18	1.1E-07
Beryllium	Water	groundwater , long-term	1.2E-07	6.2E-33	3.3E-14	9.4E-04
Beryllium	Water	groundwater	3.3E-10	1.6E-35	8.8E-17	2.5E-06
Beryllium	Water		8.0E-11	4.0E-36	2.1E-17	1.1E-06
Beryllium	Air	low. pop., long-term	3.3E-11	3.1E-16	2.3E-13	1.7E-07
Beryllium	Air	low. pop.	1.5E-10	1.4E-15	1.0E-12	7.7E-07
Beryllium	Air	high. pop.	1.2E-10	1.3E-14	9.8E-12	6.1E-07
Beryllium	Air		4.1E-12	2.5E-16	1.9E-13	2.1E-08
Cadmium	Soil	industrial	3.8E-12	1.7E-16	4.5E-14	4.5E-06
Cadmium	Soil	agricultural	5.3E-08	4.9E-11	1.3E-08	6.2E-02
Cadmium	Soil		1.2E-11	5.4E-16	1.5E-13	1.4E-05
Cadmium	Water	river	5.3E-09	4.6E-13	1.2E-10	1.2E-02
Cadmium	Water	ocean	6.9E-10	6.6E-14	1.8E-11	4.4E-21
Cadmium	Water	groundwater , long-term	1.7E-07	1.5E-11	3.9E-09	2.0E-01
Cadmium	Water	groundwater	5.0E-10	4.4E-14	1.2E-11	5.9E-04
Cadmium	Water		9.4E-10	8.1E-14	2.2E-11	2.2E-03
Cadmium	Air	stratosphere + troposphere	1.7E-16	5.6E-20	1.5E-17	1.4E-10
Cadmium	Air	low. pop., long-term	3.5E-11	1.2E-14	3.1E-12	2.9E-05
Cadmium	Air	low. pop.	1.1E-08	3.6E-12	9.5E-10	8.9E-03
Cadmium	Air	high. pop.	2.7E-09	1.1E-12	2.3E-10	2.2E-03
Cadmium	Air		1.7E-10	6.4E-14	1.5E-11	1.4E-04
Chromium VI	Soil		6.7E-08	3.5E-09	7.8E-12	3.5E-03
Chromium VI	Water	river	1.3E-07	1.4E-08	3.1E-11	1.4E-02
Chromium VI	Water	groundwater , long-term	9.5E-07	9.7E-08	2.2E-10	5.0E-02
Chromium VI	Water	groundwater	4.1E-09	4.2E-10	9.5E-13	2.2E-04
Chromium VI	Water		5.1E-10	5.3E-11	1.2E-13	5.4E-05
Chromium VI	Air	low. pop., long-term	1.7E-10	1.4E-11	4.1E-14	6.2E-06
Chromium VI	Air	low. pop.	8.5E-09	7.0E-10	2.1E-12	3.1E-04

Chromium VI	Air	high. pop.	1.7E-10	1.4E-11	1.6E-13	6.3E-06
Chromium VI	Air		2.6E-12	2.1E-13	1.5E-15	9.7E-08
Copper	Soil	industrial	5.7E-10	0.0E+00	4.2E-17	3.0E-03
Copper	Soil	agricultural		0.0E+00	1.0E-09	4.8E+0 1
Copper	Soil		4.2E-08	0.0E+00	3.2E-15	2.2E-01
Copper	Water	river	3.2E-08	0.0E+00	4.6E-15	3.2E-01
Copper	Water	ocean	1.2E-09	0.0E+00	7.6E-17	5.0E-23
Copper	Water	groundwater , long-term	2.4E-05	0.0E+00	3.4E-12	1.3E+0 2
Copper	Water	groundwater	3.8E-09	0.0E+00	5.4E-16	2.0E-02
Copper	Water		8.1E-09	0.0E+00	1.2E-15	8.1E-02
Copper	Air	stratosphere + troposphere	2.9E-14	0.0E+00	9.8E-19	1.1E-07
Copper	Air	low. pop., long-term	2.2E-09	0.0E+00	7.5E-14	8.0E-03
Copper	Air	low. pop.	1.1E-07	0.0E+00	3.8E-12	4.1E-01
Copper	Air	high. pop.	1.1E-08	0.0E+00	3.6E-13	3.9E-02
Copper	Air		2.5E-08	0.0E+00	8.5E-13	9.2E-02
Lead	Soil	industrial	1.7E-10	1.5E-17	5.3E-15	7.0E-08
Lead	Soil	agricultural	5.9E-07	9.0E-11	3.2E-08	2.4E-04
Lead	Soil		4.6E-10	4.0E-17	1.4E-14	1.9E-07
Lead	Water	river	3.0E-08	4.4E-15	1.6E-12	2.1E-05
Lead	Water	ocean	1.9E-09	1.5E-16	5.2E-14	1.3E-27
Lead	Water	groundwater , long-term	2.8E-07	4.1E-14	1.4E-11	1.1E-04
Lead	Water	groundwater	7.6E-10	1.1E-16	3.9E-14	3.1E-07
Lead	Water		8.1E-09	1.2E-15	4.2E-13	5.6E-06
Lead	Air	stratosphere + troposphere	3.4E-16	1.6E-20	5.5E-18	9.6E-14
Lead	Air	low. pop., long-term	2.3E-09	1.1E-13	3.7E-11	6.5E-07
Lead	Air	low. pop.	1.2E-07	5.5E-12	2.0E-09	3.4E-05
Lead	Air	high. pop.	1.7E-08	7.7E-13	2.7E-10	4.9E-06
Lead	Air		2.5E-08	1.1E-12	4.0E-10	7.0E-06
Mercury	Soil	industrial	7.6E-13	1.1E-16	1.2E-14	1.2E-08
Mercury	Soil	agricultural	4.2E-11	1.5E-12	1.8E-10	6.6E-07
Mercury	Water	river	4.6E-09	8.9E-13	1.1E-10	1.0E-04
Mercury	Water	ocean	1.1E-11	4.8E-15	5.7E-13	1.0E-26
Mercury	Water	groundwater , long-term	1.9E-08	3.7E-12	4.4E-10	3.0E-04
Mercury	Water	groundwater	4.6E-11	8.9E-15	1.1E-12	7.1E-07

Mercury	Water		9.2E-11	1.8E-14	2.1E-12	2.0E-06
Mercury	Air	stratosphere + troposphere	1.2E-18	1.3E-20	1.6E-18	1.3E-14
Mercury	Air	low. pop., long-term	1.8E-11	2.0E-13	2.3E-11	1.9E-07
Mercury	Air	low. pop.	3.4E-09	3.8E-11	4.5E-09	3.7E-05
Mercury	Air	high. pop.	4.2E-10	4.4E-12	5.2E-10	4.4E-06
Mercury	Air		2.8E-09	3.0E-11	3.5E-09	2.9E-05
Molybdenum	Soil	agricultural	3.3E-11	0.0E+00	2.9E-13	4.9E-09
Molybdenum	Soil		7.3E-12	0.0E+00	5.0E-16	1.1E-09
Molybdenum	Water	river	6.5E-09	0.0E+00	8.7E-13	1.9E-06
Molybdenum	Water	ocean	5.1E-11	0.0E+00	5.7E-15	1.3E-26
Molybdenum	Water	groundwater , long-term	4.1E-07	0.0E+00	5.5E-11	6.1E-05
Molybdenum	Water	groundwater	1.5E-08	0.0E+00	2.1E-12	2.3E-06
Molybdenum	Water		1.8E-10	0.0E+00	2.5E-14	5.4E-08
Molybdenum	Air	low. pop., long-term	4.5E-10	0.0E+00	1.2E-12	4.7E-08
Molybdenum	Air	low. pop.	1.1E-09	0.0E+00	2.8E-12	1.1E-07
Molybdenum	Air	high. pop.	2.1E-09	0.0E+00	5.4E-12	2.2E-07
Molybdenum	Air		4.5E-09	0.0E+00	1.2E-11	4.7E-07
Nickel	Soil	industrial	5.7E-11	1.5E-14	8.2E-16	8.9E-06
Nickel	Soil	agricultural	8.7E-10	4.2E-13	2.3E-14	1.3E-04
Nickel	Soil		7.8E-11	2.0E-14	1.1E-15	1.2E-05
Nickel	Water	river	2.6E-08	1.3E-11	7.2E-13	7.7E-03
Nickel	Water	ocean	1.4E-09	6.9E-13	3.9E-14	1.5E-21
Nickel	Water	groundwater , long-term	7.9E-06	3.9E-09	2.2E-10	1.2E+0 0
Nickel	Water	groundwater	1.9E-08	9.2E-12	5.2E-13	2.9E-03
Nickel	Water		9.2E-09	4.5E-12	2.5E-13	2.8E-03
Nickel	Air	stratosphere + troposphere	1.2E-15	4.8E-19	2.7E-20	1.3E-10
Nickel	Air	low. pop., long-term	4.8E-10	1.9E-13	1.1E-14	5.1E-05
Nickel	Air	low. pop.	8.3E-08	3.3E-11	1.9E-12	9.0E-03
Nickel	Air	high. pop.	6.8E-08	2.7E-11	1.5E-12	7.3E-03
Nickel	Air		1.5E-09	6.2E-13	3.5E-14	1.7E-04
Silver	Soil	agricultural	5.3E-19	0.0E+00	6.0E-20	5.4E-14
Silver	Soil		2.6E-13	0.0E+00	7.2E-17	2.6E-08
Silver	Water	river	4.9E-10	0.0E+00	2.6E-13	9.6E-05
Silver	Water	ocean	2.0E-11	0.0E+00	1.2E-14	3.7E-25
Silver	Water	groundwater , long-term	9.4E-09	0.0E+00	5.0E-12	9.5E-04

Silver	Water	groundwater	2.0E-10	0.0E+00	1.0E-13	2.0E-05
Silver	Water		1.7E-08	0.0E+00	8.9E-12	3.2E-03
Silver	Air	low. pop., long-term	3.9E-11	0.0E+00	1.3E-12	2.7E-06
Silver	Air	low. pop.	6.9E-13	0.0E+00	2.4E-14	4.9E-08
Silver	Air	high. pop.	1.4E-10	0.0E+00	4.7E-12	1.0E-05
Silver	Air		2.1E-13	0.0E+00	7.0E-15	1.5E-08
Thallium	Water	river	2.6E-10	0.0E+00	1.4E-11	9.1E-06
Thallium	Water	groundwater , long-term	1.7E-08	0.0E+00	9.4E-10	3.0E-04
Thallium	Water	groundwater	2.9E-11	0.0E+00	1.6E-12	5.1E-07
Thallium	Water		1.9E-11	0.0E+00	1.1E-12	6.8E-07
Thallium	Air	low. pop.	2.1E-12	0.0E+00	8.3E-14	2.6E-08
Thallium	Air	high. pop.	1.4E-10	0.0E+00	5.4E-12	1.7E-06
Thallium	Air		1.6E-11	0.0E+00	6.3E-13	2.0E-07
Vanadium	Soil	agricultural	3.3E-10	0.0E+00	4.3E-13	1.9E-05
Vanadium	Soil		2.6E-12	0.0E+00	3.2E-15	1.5E-07
Vanadium	Water	river	5.0E-09	0.0E+00	1.2E-11	5.6E-04
Vanadium	Water	ocean	1.6E-10	0.0E+00	4.7E-13	1.7E-22
Vanadium	Water	groundwater , long-term	4.9E-07	0.0E+00	1.2E-09	2.9E-02
Vanadium	Water	groundwater	9.3E-10	0.0E+00	2.2E-12	5.4E-05
Vanadium	Water		2.2E-10	0.0E+00	5.2E-13	2.5E-05
Vanadium	Air	low. pop., long-term	1.6E-09	0.0E+00	3.0E-12	6.5E-05
Vanadium	Air	low. pop.	1.2E-08	0.0E+00	2.3E-11	5.1E-04
Vanadium	Air	high. pop.	2.4E-07	0.0E+00	4.3E-10	9.7E-03
Vanadium	Air		5.5E-10	0.0E+00	1.0E-12	2.3E-05
Zinc	Soil	industrial	6.0E-09	0.0E+00	3.4E-12	4.4E-04
Zinc	Soil	agricultural	1.1E-06	0.0E+00	2.2E-08	8.0E-02
Zinc	Soil		2.0E-08	0.0E+00	1.1E-11	1.4E-03
Zinc	Water	river	5.2E-07	0.0E+00	5.4E-10	7.0E-02
Zinc	Water	ocean	7.9E-08	0.0E+00	9.5E-11	1.8E-20
Zinc	Water	groundwater , long-term	1.4E-05	0.0E+00	1.4E-08	1.0E+00
Zinc	Water	groundwater	5.0E-08	0.0E+00	5.1E-11	3.7E-03
Zinc	Water		1.8E-08	0.0E+00	1.9E-11	2.4E-03
Zinc	Air	stratosphere + troposphere	1.7E-14	0.0E+00	1.1E-16	8.6E-10
Zinc	Air	low. pop., long-term	1.7E-09	0.0E+00	1.1E-11	8.5E-05
Zinc	Air	low. pop.	1.9E-07	0.0E+00	1.2E-09	9.5E-03
Zinc	Air	high. pop.	2.7E-08	0.0E+00	1.7E-10	1.4E-03
Zinc	Air		5.1E-08	0.0E+00	3.3E-10	2.6E-03

S6. Parameters for dynamic LCA

Table S6. Parameters requested by the dynamic LCI model (from Tiruta-Barna et al., 2016)

	Parameter	Name	Significance
Process model (specific for process i)	$\alpha(t)$	Production function	Describes the time shape of the activity (e.g. continuous, constant, discontinuous...)
	$\beta(t)$	Environmental intervention function	Describe the time shape of the emissions/resource consumptions. Usually linked to $\alpha(t)$
	r	Production period	Time between the earliest input (raw material) and the latest output of the activity
	T	Representative period	Life time of the main infrastructure (material support) related to the activity
	t_0	Start date of the analysis	Arbitrary or calendar dependent
Supply model (process link i-j)	δ	Delay	Storage time, no activity takes place
	τ	Supply period	Supply frequency for intermittent supply; $\tau=T$ for continuous supply

Table S7– Temporal parameters for dynamic LCI calculation (related to the functional unit, 1 kg of grape).

Process	T (years)	r (days)	τ (days)	α (kg.day ⁻¹)	β (kg.day ⁻¹)
Grape production	25	365	365	$x := t - \text{trunc}(t) ;$ $\text{if}(x < 4/12, 0,$ $\text{if}(x < 10/12, (12/5)$ $/25, 0))$	<u>Pesticides</u> $x := t - \text{trunc}(t) ;$ $b^1 * (1/10) * \text{if}(x < 4/12, 0, \text{if}(x < 11/$ $12, \text{if}((x * 12 -$ $\text{trunc}(x * 12)) < 0.25, 6.855, 0), 0)$ $)$ $\left\{ \begin{array}{l} 0, \quad \text{month} < 4 \\ b^1 * 0.6855, \quad 4 \leq \text{month} < 11 \\ \quad \quad \quad \text{and week} = 1 \\ 0, \quad \quad \quad \text{month} \geq 11 \end{array} \right.$
					<u>N₂O</u> 1/25
Pesticides production	50	1	182.5	1/50	1/50
Fertilizers production	50	1	182.5	1/50	1/50
Irrigation	1	1	0	1	1
Electricity production	30	365	365	$x := t - \text{trunc}(t) ;$ $\text{if}(x < 10/12, 0, 6)$	$x := t - \text{trunc}(t) ; \text{if}(x < 10/12, 0,$ $6)$ $\left\{ \begin{array}{l} 0, \quad \text{month} < 10 \\ 6, \quad \text{month} \geq 10 \end{array} \right.$
Fertilising, by	1	365	365	$x := t - \text{trunc}(t) ;$ $\text{if}(x < 5/12, 0,$	$x := t - \text{trunc}(t) ; \text{if}(x < 5/12, 0,$ $\text{if}(x < 5.25/12, 24, \text{if}(x < 8/12, 0, \text{if}($

broadcaster				if($x < 5.25/12, 24, i$ f($x < 8/12, 0, i$ f($x < 8$.25,24,0))))	$x < 8.25, 24, 0$))) $\begin{cases} 0, & month < 5 \\ 24, & 5 \leq month < 5.25 \\ 0, & 5.25 \leq month < 8 \\ 24, & 8 \leq month < 8.25 \\ 0, & month \geq 8.25 \end{cases}$
-------------	--	--	--	---	---

¹ b represents the values of pesticides emissions for the “grape production” dataset, obtained from the matrix of environmental interventions (SimaPro/ecoinvent)

Table S8 – Supply parameters for the dynamic LCI model (related to the functional unit, 1 kg of grape).

Producer	Consumer	Continuous	Supply model	
			a = see ²	δ =60 days
Pesticides	Grape production	No	a = see ²	δ =60 days
Fertilizers	Grape production	No	a = see ²	δ =60 days
Irrigation	Grape production	No	a = -0.177	δ = 0 days
Electricity	Grape production	No	a = -0.090	δ = 0 days
Fertilising, by broadcaster	Grape production	No	a = 7.33×10^{-4}	δ = 0 days

² represents the demand of pesticides or fertilizers by the foreground process (from technological matrix extracted from SimaPro/ecoinvent for the testbed case). Values can be found in the dataset presented in S4.

S7. Dynamic and conventional toxicity results

Toxicity results of Prochloraz and Copper for the testbed case of production of 1 kg of grape

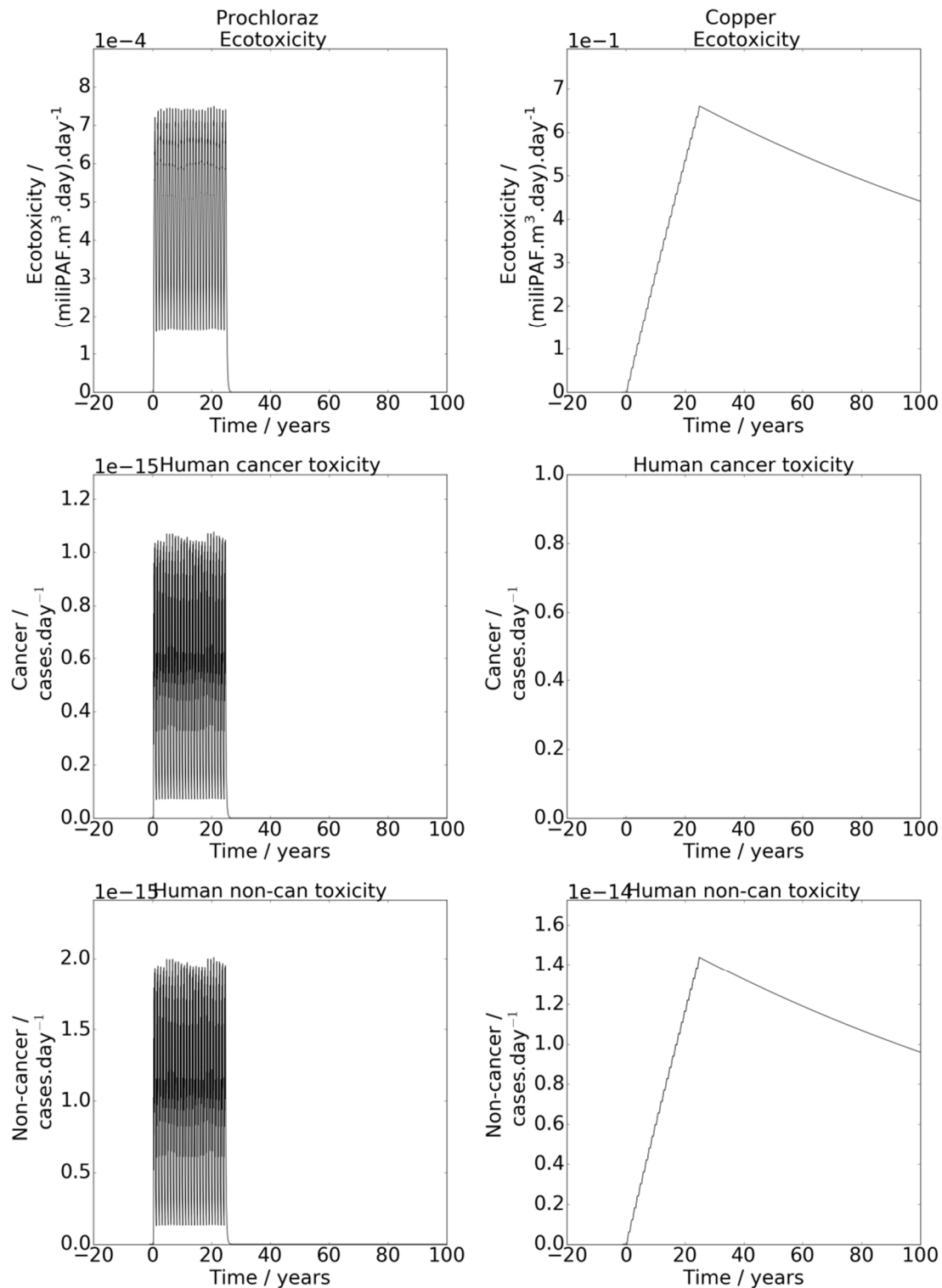


Figure S1 – Current Ecotoxicity $n_{eco}(t)$ (A), cancer (B) and non-cancer (C) human toxicity $n_{human}(t)$ of Prochloraz for the production of 1 kg of grapes

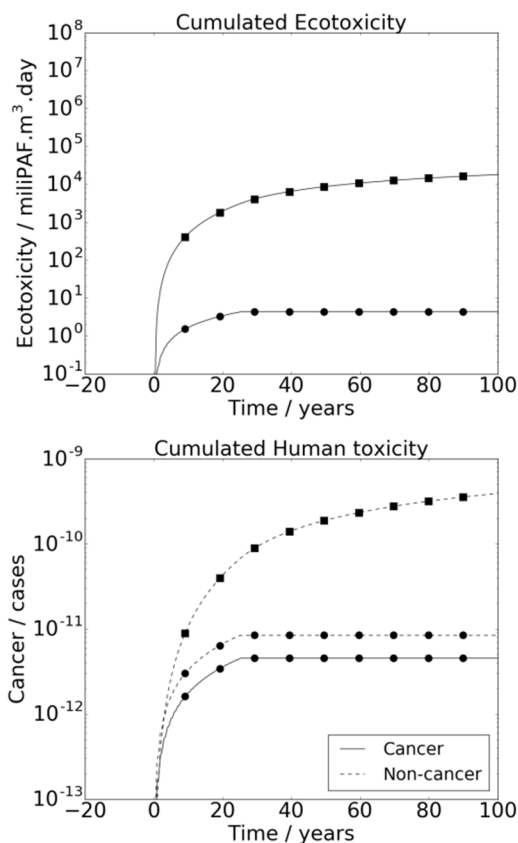


Figure S2 – Cumulated dynamic ecotoxicity $n_{eco,cumul}$ (A) and human toxicity $n_{human,cumul}$ (B) of prochloraz (●) and copper (■) for the production of 1 kg of grapes.

Contribution of individual pesticides to total toxicity impacts

Table S9 – Contribution of organic pesticides on dynamic and conventional toxicity impacts. Results for human toxicity (Cancer and Non-cancer) and ecotoxicity (Eco) impacts for the production of 1 kg of grape. The values for dynamic approach represent cumulated (eco)toxicity at 100 years.

Substance	Dynamic (100 years)			Conventional		
	Cancer	Non-cancer	Eco	Cancer	Non-cancer	Eco
Folpet	0.0%	0.0%	0.2%	0.0%	0.0%	0.0%
Thiram	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
Imidacloprid	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
Napropamide	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
Chlorothalonil	0.0%	0.0%	0.3%	0.0%	0.0%	0.1%
Pronamide	0.1%	0.0%	0.0%	0.0%	0.0%	0.0%
Pendimethalin	0.0%	0.0%	0.1%	0.0%	0.0%	0.0%
Metolachlor	0.0%	0.0%	0.1%	0.0%	0.0%	0.0%
Prochloraz	0.1%	0.0%	0.0%	0.0%	0.0%	0.0%
Mancozeb	0.0%	0.0%	0.3%	0.0%	0.0%	0.1%

Metiram	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
MCPB	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
Glyphosate	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
Chlormequat	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
2,4-D	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
Metam-sodium dihydrate	0.0%	0.0%	0.7%	0.0%	0.0%	0.1%
Chlortoluron	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
Isoproturon	0.0%	0.0%	0.1%	0.0%	0.0%	0.0%
Metamitron	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
Metazachlor	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
Aclonifen	0.0%	0.0%	0.1%	0.0%	0.0%	0.0%
Dimethenamid	0.0%	0.0%	0.1%	0.0%	0.0%	0.0%

References

- Nemecek T. & Kägi T. (2007) Life Cycle Inventories of Swiss and European Agricultural Production Systems. Final report ecoinvent V2.0 No. 15a. Agroscope Reckenholz-Taenikon Research Station ART, Swiss Centre for Life Cycle Inventories, Zurich and Dübendorf, CH, retrieved from: www.ecoinvent.ch
- Wernet, G., Bauer, C., Steubing, B., Reinhard, J., Moreno-Ruiz, E., and Weidema, B. (2016) The ecoinvent database version 3 (part I): overview and methodology. *The International Journal of Life Cycle Assessment*, [online] 21(9), pp.1218–1230. Available at: <<http://link.springer.com/10.1007/s11367-016-1087-8>> [Accessed 09 01 2017].