FORMULARIUM GLOBOX 1.0

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Table 1: Overview of chemical-dependent symbols

Symbol	**Name**	**Unit**	**Diff.**	**Origin***	**Default**
GENERAL PROPERTY					
substype	type of substance	– (organic, metal, gas)	No	input	organic
PHYSICO-CHEMICAL PROPERTIES					
MOLW	molecular weight	kg*mol^-1	No	input (EU2 (III-75))	–
CHARGE	ionic charge of metal	– (integer)	No	metal: input (Morel & Hering (1993))	metal: 2
ACTCOEFF	activity coefficient of metal	–	No	metal: E	–
FREEION5seawater	fraction free ion of dissolved metal in sea water at a temperature of 5 degrees Celcius	–	Yes	metal: G1.3 (Byrne (1988))	**–**
FREEION25seawater	fraction free ion of dissolved metal in sea water at a temperature of 25 degrees Celcius	–	Yes	metal: G1.3 (Byrne (1988))	**–**
FREEIONseawater	fraction free ion of dissolved metal in sea water at environmental temperature	–	Yes	metal: E	**–**
H_0vapor	enthalpy of vaporization	J*mol^-1	No	organic: input (SB2 (24))	50E3
TEMPmelt	melting point	K	No	organic:	–

Symbol	Name	Unit	Diff.	Origin*	Default
				input (EU2 (III-75))	
TEMPtest	temperature at which vapour pressure and halflife times of organics are given	K	No	organic: input	298
VP_TEMPtest	vapour pressure at TEMPtest	Pa	No	organic: input (EU2 (III-75))	–
VP	vapour pressure at TEMP	Pa	Yes	organic: E	–
SOL	water solubility	mol*m^-3	Yes	organic: input	–
Kow	octanol-water partition coefficient	–	No	organic: input (EU2 (III-75))	–
PARTITION COEFFICIENTS					
HENRY	Henry's law constant	Pa*m^3*mol^-1	Yes	organic: input (EU2 (III-75))/E	–
K_airwater	air-water partition coefficient (dimensionless Henry's law constant)	–	Yes	organic: E; metal, gas: input	metal: 0 gas: ∝
Koc	organic carbon-water partition coefficient	m^3 water*kg-1 organic carbon	No	organic: input/E	
Kp_soil	solids-water partition coefficient in soil	m^3*kg^-1	Yes	organic: E; metal, gas: input	metal: 0 gas: 0
Kp_sed	solids-water part. coefficient in sediment	m^3*kg^-1	Yes	organic: E; metal, gas: input	metal: 0 gas: 0
Kp_susp	solids-water part. coefficient in	m^3*kg^-1	Yes	organic: E;	metal: 0

Symbol	Name	Unit	Diff.	Origin*	Default
	suspended matter			metal, gas: input	gas: 0
Kp_seased	solids-water part. coefficient in marine sediment	m^3*kg^-1	Yes	E	–
Kp_seasusp	solids-water part. coefficient in marine suspended matter	m^3*kg^-1	Yes	E	–
PARAMETERS FOR REGIONAL AND CONTINENTAL DISTRIBUTION					
Fass_aer	fraction of the chemical in air that is associated with aerosol particles	–	Yes	organic: E; metal, gas: input	metal: 0.95; gas: 0
SCAVratio	scavenging ratio of the chemical	–	Yes	E	–
K_soilwater	soil-water partition coefficient in standard soil	m water^3*m wet soil^-3	Yes	E	–
K_agrwater	soil-water partition coefficient in agricultural soil	m water^3*m wet soil^-3	Yes	E	–
K_nonagrwater	soil-water partition coefficient in non-agricultural soil	m^3 water*m^-3 wet soil	Yes	E	–
K_deepsoilwater	deep soil-water partition coefficient	m^3 water*m^-3 wet soil	Yes	E	–
K_sedwater	sediment-water partition coefficient	m^3 water*m^-3 wet sed	Yes	E	–
K_seasedseawater	marine sediment-water partition coefficient	m^3 water*m^-3 wet sed	Yes	E	–
K_airagr	partition coefficient between air and agricultural soil	m^3 wet soil*m^-3 air	Yes	E	–
K_airnonagr	partition coefficient between air and non-agricultural soil	m^3 wet soil*m^-3 air	Yes	E	–
K_leafair	partition coefficient between plant leaves and air	–	Yes	E	–
Fdiss_inlandwater	dissolved fraction in water column	–	Yes	E	–

Symbol	Name	Unit	Diff.	Origin*	Default
	of inland waters				
Fdiss_seawater	dissolved fraction in water column of seawater	–	Yes	E	
Fdiss_soil	fraction present in the water phase of (standard) soil	–	No	E	–
Fdiss_agr	fraction present in the water phase of agricultural soil	–	Yes	E	–
Fdiss_nonagr	fraction present in the water phase of non-agricultural soil	–	Yes	E	–
Fdiss_deepsoil	fraction present in the water phase of the deepsoil	–	No	E	–
Fdiss_sed	fraction present in the water phase of the sediment	–	No	E	–
Fdiss_seased	fraction present in the water phase of the marine sediment	–	No	E	–
Faer_sed	fraction of sediment compartment that is aerated	m^3 aer sed*m^-3 sed	No	EU2 (III-84)	0.1
Faer_seased	fraction of sea sediment compartment that is aerated	m^3 aer seased*m^-3 seased	No		0.1
SALINITYcorr	correction for salinity dependence of degradation rates	-	No		0.3
INTERMEDIA TRANSFER PARAMETERS					
DIFF_air_lake	diffusive mass flow from air to lake water	m^3 air*s^-1	Yes	E	–
DIFF_lake_air	diffusive mass flow from lake water to air	m^3 water*s^-1	Yes	E	–
DIFF_air_saltlake	diffusive mass flow from air to saltlake water	m^3 air*s^-1	Yes	E	–

Symbol	Name	Unit	Diff.	Origin*	Default
DIFF_saltlake_air	diffusive mass flow from saltlake water to air	m^3 water*s^-1	Yes	E	–
DIFF_air_seawater	diffusive mass flow from air to seawater	m^3 air*s^-1	Yes	E	–
DIFF_seawater_air	diffusive mass flow from seawater to air	m^3 seawater*s^-1	Yes	E	–
DIFF_air_nat	diffusive mass flow from air to natural soil	m^3 air*s^-1	Yes	E	–
DIFF_nat_air	diffusive mass flow from natural soil to air	m^3 nat*s^-1	Yes	E	–
DIFF_air_agr	diffusive mass flow from air to agricultural soil	m^3 air*s^-1	Yes	E	–
DIFF_agr_air	diffusive mass flow from agriculatural soil to air	m^3 agr*s^-1	Yes	E	–
DIFF_air_urb	diffusive mass flow from air to urban soil	m^3 air*s^-1	Yes	E	–
DIFF_urb_air	diffusive mass flow from urban soil to air	m^3 urb*s^-1	Yes	E	–
DIFF_lake_lakesed	diffusive mass flow from lake water to lake sediment	m^3 water*s^-1	Yes	E	–
DIFF_lakesed_lake	diffusive mass flow from lake sediment to lake water	m^3 sed*s^-1	Yes	E	–
DIFF_saltlake_saltlakesed	diffusive mass flow from saltlake water to saltlake sediment	m^3 water*s^-1	Yes	E	–
DIFF_saltlakesed_saltlake	diffusive mass flow from saltlake sediment to saltlake water	m^3 sed*s^-1	Yes	E	–
DIFF_seawater_seased	diffusive mass flow from seawater to sea sediment	m^3 seawater*s^-1	Yes	E	–
DIFF_seased_seawater	diffusive mass flow from sea sediment to seawater	m^3 seased*s^-1	Yes	E	–

Symbol	Name	Unit	Diff.	Origin*	Default
ADV_air_lake	advective mass flow from air to lake water	m^3 air*s^-1	Yes	E	–
ADV_air_saltlake	advective mass flow from air to saltlake water	m^3 air*s^-1	Yes	E	–
ADV_air_seawater	advective mass flow fromair to seawater	m^3 air*s^-1	Yes	E	–
ADV_air_nat	advective mass flow from air to natural soil	m^3 air*s^-1	Yes	E	–
ADV_air_agr	advective mass flow from air to agricultural soil	m^3 air*s^-1	Yes	E	–
ADV_air_urb	advective mass flow from air to urban soil	m^3 air*s^-1	Yes	E	–
ADV_nat_river	advective mass flow from natural soil to river water	m^3 nat*s^-1	Yes	E	–
ADV_agr_river	advective mass flow from agricultural soil to river water	m^3 agr*s^-1	Yes	E	–
ADV_urb_river	advective mass flow from urban soil to river water	m^3 urb*s^-1	Yes	E	–
ADV_nat_groundwater	advective mass flow from natural soil to groundwater	m^3 nat*s^-1	Yes	E	–
ADV_agr_groundwater	advective mass flow from agricultural soil to groundwater	m^3 agr*s^-1	Yes	E	–
ADV_urb_groundwater	advective mass flow from urban soil to groundwater	m^3 urb*s^-1	Yes	E	–
ADV_river_lake	advective mass flow from river water to lake water	m^3 water*s^-1	Yes	E	–
ADV_river_saltlake	advective mass flow from river water to saltlake water	m^3 water*s^-1	Yes	E	–

Symbol	Name	Unit	Diff.	Origin*	Default
ADV_river_river	advective mass flow from river water in one country to river water in another country	m^3 water*s^-1	Yes	E	–
ADV_river_seawater	advective mass flow from river water to sea water	m^3 river*s^-1	Yes	E	–
ADV_river_agr	advective mass flow from river water to agricultural soil	m^3 river*s^-1	Yes	E	
ADV_lake_river	advective mass flow from lake water to river water	m^3 water*s^-1	Yes	E	–
ADV_river_outside	advective mass flow from sediment to outside	m^3 sed*s^-1	Yes	E	–
ADV_lake_lakesed	advective mass flow from lake water to lake sediment	m^3 water*s^-1	Yes	E	–
ADV_lake_outside	advective mass flow from lake water to outside	m^3 water*s^-1	Yes	E	–
ADV_lakesed_outside	advective mass flow from sediment to outside	m^3 sed*s^-1	Yes	E	–
ADV_saltlake_saltlakesed	advective mass flow from saltlake water to saltlake sediment	m^3 water*s^-1	Yes	E	–
ADV_saltlakesed_saltlake	advective mass flow from saltlake sediment to saltlake water	m^3 sed*s^-1	Yes	E	–
ADV_saltlakesed_outside	advective mass flow from saltlake sediment to outside	m^3 sed*s^-1	Yes	E	–
ADV_groundwater_agr	advective mass flow from groundwater to agricultural soil	m^3 groundwater*s^-1	Yes	E	–
ADV_groundwater_river	advective mass flow from groundwater to river water	m^3 groundwater*s^-1	Yes	E	–
ADV_groundwater_groundwater	advective mass flow from groundwater in one country to groundwater in another country	m^3 groundwater*s^-1	Yes	E	–

Symbol	Name	Unit	Diff.	Origin*	Default
ADV_groundwater_seawater	advective mass flow from groundwater to seawater	m^3 groundwater*s^-1	Yes	E	–
ADV_seawater_seawater	advective mass flow from seawater in one sea to seawater in another sea	m^3 seawater*s^-1	Yes	E	–
ADV_seawater_seased	advective mass flow from seawater to sea sediment	m^3 seawater*s^-1	Yes	E	–
ADV_seased_seawater	advective mass flow from sea sediment to seawater	m^3 seased*s^-1	Yes	E	–
ADV_seawater_outside	advective mass flow from seawater to outside	m^3 seawater*s^-1	Yes	E	–
ADV_seased_outside	advective mass flow from sea sediment to outside	m^3 seased*s^-1	Yes	E	–
EXPOSURE DATA					
BCF_fish	bioconcentration factor from fresh water to fish	(mg chem*kg^-1 wet fish)/(mg chem*m^-3 water)	No	organic:E or input metal, gas: input	gas: 0
BCFsoil_leafcrops	bioconcentration factor from soil to leaf crops	(mg chem*kg^-1 wet leaf crops)/(mg chem*kg wet soil^-1)	No	organic:E or input metal, gas: input	gas: 0
BCFair_leafcrops	bioconcentration factor from air to leaf crops	(mg chem*kg^-1 wet leaf crops)/(mg chem*m^-3 air)	No	organic, metal: E or input gas: input	gas: 0
BCF_rootcrops	bioconcentration factor from soil to root crops	(mg chem* kg^-1 wet root crops)/(mg chem*kg^-1 wet	No	organic:E or input metal, gas: input	gas: 0

Symbol	Name	Unit	Diff.	Origin*	Default
		soil)			
BCF_meat	BCF from daily intake of cattle to cattle meat	(mg chem*kg^-1 meat)/(mg chem*d^-1)	No	organic:E or input metal, gas: input	gas: 0
BCF_milk	BCF from daily intake of cattle to milk	(mg chem*kg^-1 milk)/(mg chem*d^-1)	No	organic:E or input metal, gas: input	gas: 0
F_resp	respirable fraction of inhaled substance	–	No	input/EU2 (III-137)	1
BIO_inh	bioavailability for inhalation	–	No	input/EU2 (III-137)	0.75
BIO_oral	bioavailability for oral exposure	–	No	input/EU2 (III-137)	1
DISAPPEARANCE RATES					
DT50photo_air	half-life for photodegradation in air	s	No	organic, gas: input	organic: 160*24*3600 gas, metal: ∝
DT50bio_freshwater_TEMPtest	half-life for biodegradation in water at TEMPtest	s	No	organic: input/E gas: input	gas, metal: ∝
DT50bio_freshwater	half-life for biodegradation in rivers and freshwater lakes	s	Yes	E	
DT50bio_saltlake	half-life for biodegradation in saltlakes	s	Yes	E	E
DT50bio_seawater_TEMPtest	half-life for biodegradation in seawater at TEMPtest	s	No	organic: input/E gas: input	gas, metal: ∝
DT50bio_seawater	half-life for biodegradation in	s	Yes	E	

Symbol	Name	Unit	Diff.	Origin*	Default
	seawater				
DT50abio_sed	half-life for abiotic degradation in sediment	s	No	organic, gas: input	∝
DT50aerbio_sed_TEMPtest	half-life for aerobic biodegradation in sediment at TEMPtest	s	No	organic: input/E gas: input	gas, metal: ∝
DT50aerbio_sed	half-life for aerobic biodegradation in sediment	s	Yes	E	
DT50anaerbio_sed	half-life for anaerobic biodegradation in sediment	s	No	organic, gas: input	∝
DT50abio_saltlakesed	half-life for abiotic degradation in saltlake sediment	s	No	organic, gas: input	
DT50aerbio_saltlakesed	half-life for aerobic biodegradation in saltlake sediment	s	No	organic: input or E gas: input	gas, metal: ∝
DT50anaerbio_saltlakesed	half-life for anaerobic biodegradation in saltlake sediment	s	No	organic, gas: input	∝
DT50abio_seased	half-life for abiotic degradation in sea sediment	s	No	organic, gas: input or E	
DT50aerbio_seased_TEMPtest	half-life for aerobic biodegradation in water at TEMPtest	s	No	organic: input/E gas: input	gas, metal: ∝
DT50aerbio_seased	half-life for aerobic biodegradation in sea sediment	s	No	organic: input or E gas: input	gas, metal: ∝
DT50anaerbio_seased	half-life for anaerobic biodegradation in sea sediment	s	No	organic, gas: input	∝
DT50abio_soil	half-life for abiotic degradation in soil	s	No	organic, gas: input	∝
DT50bio_soil_TEMPtest	half-life for biodegradation in	s	No	organic:	gas, metal: ∝

Symbol	Name	Unit	Diff.	Origin*	Default
	(standard) soil at TEMPtest			input/E gas: input	
DT50bio_soil	half-life for biodegradation in (standard) soil	s	Yes	organic: input/E gas: input	gas, metal: ∝
DT50bio_agr	half-life for biodegradation in agricultural soil	s	Yes	organic: input/E gas: input	gas, metal: ∝
DT50bio_nonagr	half-life for biodegradation in non-agricultural soil	s	Yes	organic: input/E gas: input	gas, metal: ∝
DT50hydro_water_TEMPtest	half-life for hydrolysis in water at TEMPtest	s	No	organic, gas: input	∝
DT50hydro_water	half-life for hydrolysis in water	s	Yes	E	
DT50photo_water	half-life for photolysis in water	s	No	organic, gas: input	∝
readily_biodegradable	result of OECD/EU standardised biodegradability tests	(yes/no)	No	input	'no'
fulfilling_10d_window	result of OECD/EU standardised biodegradability tests	(yes/no)	No	input	'no'
inherently_biodegradable	result of OECD/EU standardised biodegradability tests	(yes/no)	No	input	'yes'
krad_OH	specific degradation rate constant for reaction with OH-radicals	s^-1	No	organic, gas: input or E metal: 0	–
kdeg_air	pseudo first rate constant for degradation in air	s^-1	Yes	input or E	–
kbio_freshwater	pseudo first order rate constant for biodegradation in rivers and freshwater lakes	s^-1	Yes	E	–

Symbol	Name	Unit	Diff.	Origin*	Default
kbio_saltlake	pseudo first order rate constant for biodegradation in saltlakes	s^-1	Yes	E	–
kbio_seawater	pseudo first order rate constant for marine biodegradation	s^-1	Yes	E	–
khydro_inlandwater	pseudo first order rate constant for hydrolysis in inland water	s^-1	Yes	E	–
khydro_seawater	pseudo first order rate constant for hydrolysis in seawater	s^-1	Yes	E	–
kphoto_water	pseudo first order rate constant for photolysis in surface water	s^-1	No	E	–
kdeg_freshwater	pseudo first order degradation rate constant in inland waters	s^-1	No	E	–
kdeg_saltlake	pseudo first order degradation rate constant in inland waters	s^-1	No	E	–
kdeg_seawater	pseudo first order degradation rate constant in sea water	s^-1	Yes	E	–
kaerbio_sed	pseudo first order for aerobic biodegradation rate constant in sediment	s^-1	No	E	
kaerbio_saltlakesed	pseudo first order for aerobic biodegradation rate constant in saltlake sediment	s^-1	No	E	
kaerbio_seased	pseudo first order for aerobic biodegradation rate constant in sea sediment	s^-1	No	E	
kanaerbio_sed	pseudo first order for anaerobic biodegradation rate constant in sediment	s^-1	No	E	
kanaerbio_saltlakesed	pseudo first order for anaerobic biodegradation rate constant in	s^-1	No	E	

Symbol	Name	Unit	Diff.	Origin*	Default
	slatlake sediment				
kanaerbio_seased	pseudo first order for anaerobic biodegradation rate constant in sea sediment	s^-1	No	E	
kabio_sed	pseudo first order for abiotic degradation rate constant in sediment	s^-1	No	E	
kabio_saltlakesed	pseudo first order for abiotic degradation rate constant in saltlake sediment	s^-1	No	E	
kabio_seased	pseudo first order for abiotic degradation rate constant in sea sediment	s^-1	Yes	E	
kdeg_sed	pseudo first order degradation rate constant in sediment	s^-1	No	E	–
kdeg_saltlakesed	pseudo first order degradation rate constant in marine sediment	s^-1	No	E	–
kdeg_seased	pseudo first order degradation rate constant in marine sediment	s^-1	No	E	–
kbio_agr	pseudo first order biodegradation rate constant in agricultural soil	s^-1	Yes	E	
kbio_nonagr	pseudo first order biodegradation rate constant in non-agricultural soil	s^-1	Yes	E	
kabio_soil	pseudo first order abiotic degradation rate constant in soil	s^-1	No	E	
kdeg_agr	pseudo first order degradation rate constant in agricultural soil	s^-1	Yes	E	–
kdeg_nonagr	pseudo first order degradation rate constant in non-agricultural soil	s^-1	Yes	E	–
PURFsurfacew	purification factor for surface water	–	No	E	–

Symbol	Name	Unit	Diff.	Origin*	Default
PURFgroundw	purification factor for groundwater	–	No	E	–
PURFsys1	purification factor for system 1	–	No	E	–
PURFsys2	purification factor for system 2	–	No	E	–
fac1a	Kow-dependent partial purification factor for system 1	–	No	E	–
fac1b	Henry-coefficient-dependent partial purification factor for system 1	–	No	E	–
fac1c	aerobic-degradation-half-life-dependent partial purification factor for system 1	–	No	E	–
fac2a	Kow-dependent partial purification factor for system 2	–	No	E	–
fac2b	Henry-coefficient-dependent partial purification factor for system 2	–	No	E	–
fac2c	aerobic-degradation-half-life-dependent partial purification factor for system 2	–	No	E	–

*Legend: D = chemical data set; E = GLOBOX equation (in formularium); G1.1 = GLOBACK part 1, sheet 'countries'; G1.2 = GLOBACK part 1, sheet 'seas'; U1 = USES 1.0 (+ page number); U2 = USES 2.0 (+ page number); EU1 = EUSES 1.00 (+ page number); EU II = EUSES 2.0 (+ page number); SB2 = SimpleBox 2.0 (+ page number); input = to be provided by the user; references: sea reference list below.

Table 2: Overview of chemical-independent symbols

Symbol	Name	Unit	Diff.	Origin*	Default
MEDIA CHARACTERISTICS					
RHO_air	density of air	kg air*m^-3 air	No	EU2 (III-76)	1.3
RHO_water	density of water	kg water*m^-3 water	No	EU2 (III-76)	1000
RHO_solid	density of solid phase	kg solid*m^-3 solid	No	EU2 (III-76)	2500
RHO_soil	wet bulk density of (standard) soil	kg wet soil*m^-3 soil	Yes	E	–
RHO_agr	wet bulk density of agricultural soil	kg wet soil*m^-3 soil	Yes	E	–
RHO_nonagr	wet bulk density of non-agricultural soil	kg wet soil*m^-3 soil	Yes	E	–
Fair_soil	volume fraction of air in (standard) soil	m^3 air*m^-3 soil	No	EU2 (III-76)	0.2
Fair_agr	volume fraction of air in agricultural soil	m^3 air*m^-3 soil	Yes	G1.1	–
Fair_nonagr	volume fraction of air in natural soil	m^3 air*m^-3 soil	Yes	G1.1	–
Fwater_soil	volume fraction of porewater in (standard) soil	m^3 water*m^-3 soil	No	EU2 (III-76)	0.2
Fwater_agr	volume fraction of porewater in agricultural soil	m^3 water*m^-3 soil	Yes	G1.1	–
Fwater_nonagr	volume fraction of porewater in non-agricultural soil	m^3 water*m^-3 soil	Yes	G1.1	–
Fwater_deepsoil	volume fraction of porewater in deep soil	m^3 water*m^-3 soil	No	GLOBOX assumption	0.2
Fwater_sed	volume fraction of porewater in	m^3 water*m^-3	No	EU2 (III-76)	0.8

Symbol	Name	Unit	Diff.	Origin*	Default
	sediment	sed			
Fwater_susp	volume fraction of water in suspended matter	m^3 water*m^-3 susp	No	EU2 (III-76)	0.9
Fwater_bio	volume fraction of water in aquatic biota	m^3 water*m^-3 biota	No	U1 (297)	0.95
Fsolid_soil	volume fraction of solids in (standard) soil	m^3 solids*m^-3 soil	No	EU2 (III-76)	0.6
Fsolid_agr	volume fraction of solids in agricultural soil	m^3 solids*m^-3 soil	Yes	E	–
Fsolid_nonagr	volume fraction of solids in non-agricultural soil	m^3 solids*m^-3 soil	Yes	E	–
Fsolid_deepsoil	volume fraction of solids in deep soil	m^3 solids*m^-3 soil	No	E	–
Fsolid_sed	volumefraction solids in sediment	m^3 solids*m^-3 sed	No	E	–
Fsolid_susp	volumefraction solids in suspended matter in fresh water	m^3 solids*m^-3 susp	No	E	–
Fsolid_runoff	volume fraction solids in soil runoff water	m^3 solids*m^-3 water	Yes	G1.1	–
Foc_soil	weight fraction organic carbon in soil	kg oc*kg^-1 solid	Yes	G1.1	–
Foc_sed	weight fraction organic carbon in freshwater sediment	kg oc*kg^-1 solid	Yes	G1.1	–
Foc_seased	weight fraction organic carbon in marine sediment	kg oc*kg^-1 solid	Yes	G1.2	–
Foc_susp	weight fraction organic carbon in suspended matter	kg oc*kg^-1 solid	Yes	land: G1.1	–
Foc_seasusp	weight fraction organic carbon in marine suspended matter	kg oc*kg^-1 solid	Yes	G1.2	–
OHCONC_air	concentration of hydroxyl	molecules*m^-3	Yes	land: G1.1	–

Symbol	Name	Unit	Diff.	Origin*	Default
	radicals in air			seas: G1.2	
OHCONCref_air	concentration of hydroxyl radicals in air	molecules*m^-3	No	value for Europe	10.5E11
BIOCONC_water	concentration of biota in inland water	kg wwt*m^-3	No	EU2 III-99	0.001
SUSPFRACTION_inlandwater	volume fraction of suspended matter in river and lake water	–	Yes	G1.1	–
SUSPCONC_inlandwater	concentration of suspended matter in river and lake water	kg solids*m^-3 water	Yes	E	–
SUSPFRACTION_seawater	volume fraction of suspended matter in seawater	–	Yes	G1.2	–
SUSPCONC_seawater	concentration of suspende matter in sea water	kg solids*m^-3 water	Yes	E	–
SURFaer	specific surface area of aerosol particles	m^2*m^-3	No	EU2 III-76	5.88E–4
CONjunge	constant of Junge equation	Pa*m	No	Noordijk & De Leeuw, 1991	0.17
COLLECTeff	aerosol collection efficiency	–	No	EU2 III-99	2E5
RESTIME_lake	residence time of water in freshwater lakes	s	Yes	G1.1; Shiklomanov ’03	
EVAPrate_lake	evaporation rate from freshwater lakes and salt lakes	m*s-1	Yes	G1.1	–
EVAP_lake	evaporation of water from freshwater lakes	m^3*s-1	Yes	E	–
EVAP_saltlake	evaporation of water from salt lakes	m^3*s-1	Yes	G1.1	–
RAINDIRECT_lake	direct precipitation on lake surface	m^3*s-1	Yes	E	–

Symbol	Name	Unit	Diff.	Origin*	Default
RAINDIRECT_saltlake	precipitaion on saltlake surface	m^3*s-1	Yes	E	–
PLANT-SPECIFIC PARAMETERS					
Fwater_plant	volume fraction of water in plant tissue	m^3 water*m^-3 plant	No	EU2 III-129	0.65
Flipid_plant	volume fraction of lipids in plant tissue	m^3 lipids*m^-3 plant	No	EU2 III-129	0.01
Fair_plant	volume fraction of air in plant tissue	m^3 air*m^-3 plant	No	EU2 III-129	0.3
RHO_plant	bulk density of plant tissue	kg plant*m^-3 plant	No	EU2 III-129	700
AREA_plant	leaf surface area	m^2	No	EU2 III-129	5
g_plant	conductance	m*s^-1	No	EU2 III-129	0.001
V_leaf	shoot volume	m^3	No	EU2 III-129	0.002
Qtransp	transpiration stream	m^3*s^-1	No	EU2 III-129	1E-3/(24*3600)
b	correction exponent for differences between plant lipids and octanol	-	No	EU2 III-129	0.95
kgrowth_plant	growth-rate constant for dilution by growth	s^-1	No	EU2 III-129	0.035/(24*3600)
kmetab_plant	pseudo-first-order rate constant for metabolism in plants	s^-1	No	EU2 III-129	0
kphoto_plant	pseudo-first-order rate constant for photodegradatio in plants	s^-1	No	EU2 III-129	0
kelim_plant	pseudo-first-order rate constant for elimination in plants	s^-1	No	E	–
TSCF	transpiration-stream concentration factor	–	No	E	–
K_plantwater	plant-water partition coefficient	–	No	E	–
CLIMATIC PARAMETERS					
TEMP	average environmental	K	Yes	land: G1.1	–

Symbol	Name	Unit	Diff.	Origin*	Default
	temperature			seas: G1.2	
WINDSPEED	average wind speed 10 m above the surface	m*s^-1	Yes	land: G1.1	seas: 9
RAINRATE	average annual precipitation	m*s^-1	Yes	land: G1.1 seas: G1.2	–
RAINDAYS	average number of days per year with a rainfall of more than 1 mm	d*yr^-1	Yes	land: G1.1	seas: 250
Ftime_rain	fraction of time with precipitation #Olivier#	–	Yes	E	–
FROSTMONTHS	average number of months per year with an average temperature below zero	month*yr^-1	Yes	land: G1.1	seas: 0
Ftime_frost	fraction of time with temperatures below zero	–	Yes	land: E	–
DIMENSIONAL PARAMETERS					
SYSTEMAREA	total area of the system	m^2	Yes	land: G1.1 seas: G1.2	–
Farea_seaice	fraction of sea that is covered by ice	–	Yes	seas: G1.2	–
Farea_agr	fraction of area that is agricultural soil	–	Yes	land: G1.1	–
Farea_nat	fraction of area that is natural soil	–	Yes	land: G1.1	–
Farea_urb	fraction of area that is urban soil	–	Yes	land: G1.1	–
Friver_frozen	fraction of river water that is frozen	–	Yes	land: G1.1	
MIXDEPTH_lake	mixing depth of freshwater lakes	m	Yes	land: G1.1	–
MIXDEPTH_seawater	mixing depth of the sea compartment	m	Yes	seas: G1.2	–
TOTALDEPTH_lake	total depth of freshwater lakes	m	Yes	land: G1.1	–

Symbol	Name	Unit	Diff.	Origin*	Default
TOTALDEPTH_saltlake	total depth of saltlakes	m	Yes	land: G1.1	–
HEIGHT_air	atmospheric mixing height	m	Yes	land: G1.1 seas: G1.2	–
DEPTH_sed	mixing depth of the sediment compartment	m	No	EU2 III-100	0.03
DEPTH_agr	mixing depth of the compartment of agricultural soil	m	No	EU2 III-101	0.2
DEPTH_nonagr	mixing depth of the compartments of natural and urban soil	m	Yes	G1.1	–
DEPTH_groundwater	mixing depth of the compartment groundwater	m	No	GLOBOX assumption	100
AREA_lake	area of compartment lake	m^2	Yes	G1.1	
AREA_deeplake	area of freshwater lake that are not fully mixed	m^2	Yes	land: G1.1	
AREA_saltlake	area of compartment saltlake	m^2	Yes	G1.1	
AREA_lakesed	area of compartment lake sediment	m^2	Yes	G1.1	
AREA_saltlakesed	area of compartment saltlake sediment	m^2	Yes	E	
AREA_seased	area of compartment sea sediment	m^2	Yes	G1.2	
AREA_nat	area of compartment natural soil	m^2	Yes	E	
AREA_agr	area of compartment agricultural soil	m^2	Yes	E	
AREA_urb	area of compartment urban soil	m^2	Yes	E	
AREA_landice	area that is covered by ice	m^2	Yes	G1.1	–
V_air	volume of compartment air	m^3	Yes	E	
V_river	volume of compartment river	m^3	Yes	G1.1	
V_lake	volume of compartment	m^3	Yes	E	

Symbol	Name	Unit	Diff.	Origin*	Default
	freshwater lake				
V_saltlake	volume of compartment saltlake	m^3	Yes	E	
V_seawater	volume of compartment seawater	m^3	Yes	E	
V_lakesed	volume of compartment lake sediment	m^3	Yes	E	
V_saltlakesed	volume of compartment saltlake sediment	m^3	Yes	E	
V_seased	volume of compartment seasediment	m^3	Yes	E	
V_agr	volume of compartment agricultural soil	m^3	Yes	E	
V_nat	volume of compartment natural soil	m^3	Yes	E	
V_urb	volume of compartment urban soil	m^3	Yes	E	
V_groundwater	volume of compartment groundwater	m^3	Yes	E	
DISTRIBUTION PARAMETERS					
AEROSOLDEPRATE	deposition velocity of the aerosol particles	m*s^-1	Yes	land: G1.1 seas: G1.2	
GASABS_water	overall mass transfer coefficient for gas absorption across the air-water interface	m air*s^-1	Yes	E	
VOLAT_inlandwater	overall mass transfer coefficient for volatilisation across the air-water interface of inland water	m water*s^-1	Yes	E	
VOLAT_seawater	overall mass transfer coefficient for volatilisation across the air-water interface of sea water	m seawater*s^-1	Yes	E	
GASABS_nat	overall mass transfer coefficient	m air*s^-1	Yes	E	

Symbol	Name	Unit	Diff.	Origin*	Default
	for gas absorption across the interface between air and natural soil				
GASABS_agr	overall mass transfer coefficient for gas absorption across the interface between air and agricultural soil	m air*s^-1	Yes	E	
GASABS_urb	overall mass transfer coefficient for gas absorption across the interface between air and urban soil	m air*s^-1	Yes	E	
VOLAT_nat	overall mass transfer coefficient for volatilisation across the interface between air and natural soil	m soil*s^-1	Yes	E	
VOLAT_agr	overall mass transfer coefficient for volatilisation across the interface between air and agricultural soil	m soil*s^-1	Yes	E	
VOLAT_urb	overall mass transfer coefficient for volatilisation across the interface between air and urban soil	m soil*s^-1	Yes	E	
DRYDEP_aer	mass transfer coefficient for dry deposition of aerosol-associated chemical	m air*s^-1	Yes	E	
WASHOUT	mass transfer coefficient for wet atmospheric deposition	m water*s^-1	Yes	E	
LEACH_agr	mass transfer coefficient for leaching from agricultural soil	m soil*s^-1	Yes	E	

Symbol	Name	Unit	Diff.	Origin*	Default
LEACH_nonagr	mass transfer coefficient for for leaching from non-agricultural soil	m soil*s^-1	Yes	E	
ADSORB_sed	overall mass transfer coefficient for adsorption across the sediment-water interface	m water*s^-1	Yes	E	
ADSORB_seased	mass transfer coefficient for adsorption across the sea sediment-water interface	m seawater*s^-1	Yes	E	
DESORB_sed	mass transfer coefficient for desorption across the sediment-water interface	m sed*s^-1	Yes	E	
DESORB_seased	mass transfer coefficient for desorption across the sea sediment-water interface	m seased*s^-1	Yes	E	
PRODratesusp_inlandwater	rate of production of suspended matter in the water column of inland water per unit area	kg solid*m^2*s^-1	No	SB2 (54)	10/(1000*365*24*3600)
PRODratesusp_seawater	rate of production of suspended matter in the sea water column per unit area	kg solid*m^2*s^-1	No	SB2 (54)	1/(1000*365*24*3600)
PRODsusp_saltlake	rate of production of suspended matter in the water column of saltlakes	kg solid*s^-1	Yes	E	
PRODsusp_seawater	rate of production of suspended matter in the sea water column	kg solid*s^-1	Yes	E	
riverinflow_solid	inflow of suspended solids into the river compartment	kg solid*s^-1	Yes	E	
riveroutflow_solid	outflow of suspended solids out of the river compartment	kg solid*s^-1	Yes	E	

Symbol	Name	Unit	Diff.	Origin*	Default
NETsedrate_saltlake	net sedimentation rate in saltlakes	m sed*s^-1	Yes	E	
NETsedrate_seawater	net marine sedimentation rate	m sed*s^-1	Yes	E	
GROSSsedrate_saltlake	gross sedimentation rate in saltlakes	m sed*s^-1	Yes	E	
GROSSsedrate_seawater	gross marine sedimentation rate	m sed*s^-1	Yes	E	
sedrate_inlandwater	settling rate of suspended solids in inland water	m sed*s^-1	Yes	E	
sedrate_seawater	settling rate of suspended solids in sea water	m sed*s^-1	Yes	E	
RESUSPrate_saltlake	resuspension rate in saltlakes	m sed*s^-1	Yes	E	
RESUSPrate_seawater	resuspension rate in sea	m sed*s^-1	Yes	E	
SETTLvelocity_susp	settling velocity of the suspended particles in water	m water*s^-1	No	EU2 III-100	2.5/(24*3600)
MTC_seadeepsea		m seawater*s^-1	No	E	
Finf_soil	fraction of rain water that infiltrates into soil	–	Yes	E	
WATERrunoff	total water runoff from soil into the water compartment	m^3*s^-1	Yes	E	
EROSION_nat	erosion rate of natural soil	m soil*s^-1	Yes	E	
EROSION_agr	erosion rate of agricultural soil	m soil*s^-1	Yes	E	
EROSION_urb	erosion rate of urban soil	m soil*s^-1	Yes	E	
RUNOFF_nat	rainwater run-off from natural soil	m soil*s^-1	Yes	E	
RUNOFF_agr	rainwater run-off from agricultural soil	m soil*s^-1	Yes	E	
RUNOFF_urb	rainwater run-off from urban soil	m soil*s^-1	Yes	E	
kaw_air	partial mass transfer coef. at the air side of the air-water interface	m air*s^-1	Yes	EU2 III-108	

Symbol	Name	Unit	Diff.	Origin*	Default
kaw_water	partial mass transfer coef. at the water side of the air-water interface	m water*s^-1	Yes	EU2 III-108	
kasl_air	partial mass transfer coef. at the air-side of the air-soil interface	m air*s^-1	Yes	EU2 III-101	90.5/(24*3600)
kasl_soilair	partial mass transfer coef. at the soilair-side of the air-soil interface	m air*s^-1	Yes	G1.1	
kasl_soilwater	partial mass transfer coef. at the soilwater-side of the air-soil interface	m air*s^-1	No	EU1 III-40	5.56E-10
kws_water	partial mass transfer coeff. at the water-side of the sediment-water interface	m water*s^-1	No	EU1 III-40	0.01/3600
kws_sed	partial mass transfer coeff. at the porewater-side of the sediment-water interface	m porewater*s^-1	No	EU1 III-40	0.0001/3600
INTRAMEDIUM EXCHANGE PARAMETERS					
FLOW_river_river(i,j)	river flows from region i to region j	m^3 water*s^-1	Yes	land, to countries: G2.5 land, to regions: G2.6	
FLOW_groundwater_groundwater(i,j)	groundwater flows from region i to region j	m^3 water*s^-1	Yes	land: G2.8	
FLOW_seawater_seawater(i,j)	sea water flows from region i to region j	m^3 seawater*s^-1	Yes	seas: G2.9	
INTERMEDIUM EXCHANGE PARAMETERS					
FLOW_soil_groundwater	waterflows from soil to groundwater	m^3 water*s^-1	Yes	land: G1.1	

Symbol	Name	Unit	Diff.	Origin*	Default
FLOW_river_lake	waterflows from river to lake	m^3 water*s^-1	Yes	E	
FLOW_river_saltlake	waterflows from river to saltlake	m^3 water*s^-1	Yes	E	
FLOW_river_agr	waterflows from river to agricultural soil	m^3 water*s^-1	Yes	G1.1	
FLOW_river_seawater(i,j)	waterflows from river in region i to seawater in region j	m^3 water*s^-1	Yes	G1.1	
FLOW_lake_river	waterflows from lake to river	m^3 water*s^-1	Yes	E	
FLOW_groundwater_river	waterflows from groundwater to river	m^3 water*s^-1	Yes	land: G1.1	
FLOW_groundwater_agr	waterflows from groundwater to agricultural soil	m^3 water*s^-1	Yes	land: G1.1	
FLOW_groundwater_seawater(i,j)	waterflows from groundwater in regioni to seawater in region j	m^3 water*s^-1	Yes	land: G1.1	
EXPOSURE PARAMETERS					
ICdwt_soil	daily intake of soil by cattle	kg dry soil*d^-1	No	EU2 (III-134)	0.41
ICdwt_grass	daily intake of grass by cattle	kg dry plant*d^-1	No	EU2 (III-134)	16.9
IC_air	daily intake of air by cattle	m^3 air*d^-1	No	EU2 (III-134)	122
CONVgrass	conversion dry to fresh weight plants	kg fresh plant*kg^-1 dry plant	No	EU2 (III-134)	4
CONVagr	conversion dry to total agricultural soil	kg wet soil*kg ^-1 solid	Yes	E	
Fdrw_safe	fraction of drinking water that is safe	–	Yes	land: G1.1	
Fdrw_grw	fraction of safe drinking water that is groundwater	–	Yes	land: G1.1	
CATCH_seafish	production of marine fish	kg*s-1	Yes	seas: G1.2	

Symbol	Name	Unit	Diff.	Origin*	Default
IH_drw	daily intake of drinking water	m^3 drw*d^-1	Yes	land: G1.1	
IH_freshwaterfish	daily intake of freshwater fish	kg fresh[water] fish*d^-1	Yes	land: G1.1	1E–3
IH_seafish	daily intake of marine fish	kg marine fish*d^-1	Yes	land: G1.1	0.011
IH_leafcrops	daily intake of leaf crops	kg leaf crops*d^-1	Yes	land: G1.1	
IH_rootcrops	daily intake of root crops	kg root crops*d^-1	Yes	land: G1.1	
IH_meat	daily intake of meat	kg meat*d^-1	Yes	land: G1.1	
IH_dairy	daily intake of dairy products	kg dairy*d^-1	Yes	land: G1.1	
IH_air	daily ventilation rate	m^3 air*d^-1	Yes	land: G1.1	
PROD_freshwaterfish	production of freshwater fish	kg freshwater fish*d^-1	Yes	land: G1.1	
PROD_leafcrops	production of leaf crops [1.1.BW]	kg leaf crops*d^-1	Yes	land: G1.1	
PROD_rootcrops	production of root crops [1.1.BX]	kg root crops*d^-1	Yes	land: G1.1	
PROD_meat	production of meat [1.1.BY]	kg meat*d^-1	Yes	land: G1.1	
PROD_dairy	production of dairy [1.1.BZ]	kg dairy*d^-1	Yes	land: G1.1	
IMPORT_freshwaterfish	import of freshwater fish [1.1.CG]	kg freshwater fish*d^-1	Yes	land: G1.1	
IMPORT_leafcrops	import of leaf crops [1.1.CC]	kg leaf crops*d^-1	Yes	land: G1.1	
IMPORT_rootcrops	import of root crops [1.1.CD]	kg root crops*d^-1	Yes	land: G1.1	
IMPORT_meat	import of meat [1.1.CE	kg meat*d^-1	Yes	land: G1.1	
IMPORT_dairy	import of dairy [1.1.CF]	kg dairy*d^-1	Yes	land: G1.1	
EXPORT_freshwaterfish	export of freshwater fish [1.1.CM]	kg freshwater fish*d^-1	Yes	land: G1.1	
EXPORT_leafcrops	export of leaf crops [1.1.CI]	kg leaf crops*d^-1	Yes	land: G1.1	
EXPORT_rootcrops	export of root crops [1.1.CJ]	kg root crops*d^-1	Yes	land: G1.1	

Symbol	Name	Unit	Diff.	Origin*	Default
EXPORT_meat	export of meat [1.1.CK]	kg meat*d^-1	Yes	land: G1.1	
EXPORT_dairy	export of dairy [1.1.CL]	kg dairy*d^-1	Yes	land: G1.1	
DOSE_air	human dose, caused by inhalation	kg chem*kg^-1 BW*d^-1	Yes	E	
DOSE_drw	human dose, caused by intake of drinking water	kg chem*kg^-1 BW*d^-1	Yes	E	
DOSE_leafcrops	human dose, caused by intake of leaf crops	kg chem*kg^-1 BW*d^-1	Yes	E	
DOSE_rootcrops	human dose, caused by intake of root crops	kg chem*kg^-1 BW*d^-1	Yes	E	
DOSE_freswaterfish	human dose, caused by intake of freshwater fish	kg chem*kg^-1 BW*d^-1	Yes	E	
DOSE_seafish	human dose, caused by intake of marine fish	kg chem*kg^-1 BW*d^-1	Yes	E	
DOSE_meat	human dose, caused by intake of meat, meat products and eggs	kg chem*kg^-1 BW*d^-1	Yes	E	
DOSE_dairy	human dose, caused by intake of dairy products	kg chem*kg^-1 BW*d^-1	Yes	E	
DOSE_totaloral	total human dose, caused by oral intake	kg chem*kg^-1 BW*d^-1	Yes	E	
DOSE_total	total human dose	kg chem*kg^-1 BW*d^-1	Yes	E	
INTAKE_drw[NIEUW]	intake through drinking water	kg chem*d^-1	No	E	
INTAKE_leafcrops	intake through leaf crops	kg chem*d^-1	No	E	
INTAKE_rootcrops	intake through root crops	kg chem*d^-1	No	E	
INTAKE_freshwaterfish	intake through freshwater fish	kg chem*d^-1	No	E	
INTAKE_seafish	intake through marine fish	kg chem*d^-1	No	E	
INTAKE_meat	intake through meat, meat products and eggs	kg chem*d^-1	No	E	
INTAKE_dairy	intake through dairy products	kg chem*d^-1	No	E	

Symbol	Name	Unit	Diff.	Origin*	Default
INTAKE_totaloral	intake through oral intake	kg chem*d^-1	No	E	
INTAKE_air	intake through inhalation	kg chem*d^-1	No	E	
INTAKE_total	intake through oral intake and inhalation	kg chem*d^-1	No	E	
iF	intake fraction	–	Yes	E	
iFtot	total intake fraction	–	No	E	
BW	average human body weight [1.1.BL]	kg	Yes	G1.1	
Npop	population [1.1.BI]	–	Yes	land: G1.1	
BORDER					
BORDERLENGTH	length of boundary with neighbouring countries or seas [2.2; 2.3; 2.4]	m	Yes	land/land: G2.2 sea/sea: G2.3 land/sea: G2.4	
BORDERHEIGHT_air(i,j)	height of air mixing layer at boundarybetween region i and j	m	Yes	E	
BORDERWINDSPEED	windspeed at border between region i and j	m*s^-1	Yes	E	
EMISSION					
to_air	emission to air	kg chem*s^-1	Yes	input	0
to_nat	emission to natural soil	kg chem*s^-1	Yes	input	0
to_agr	emission to agricultural soil	kg chem*s^-1	Yes	input	0
to_urb	emission to urban soil	kg chem*s^-1	Yes	input	0
to_river	emission to river water	kg chem*s^-1	Yes	input	0
to_lake	emission to lake water	kg chem*s^-1	Yes	input	0
to_saltlake	emission to saltlake water	kg chem*s^-1	Yes	input	0
to_seawater	emission to seawater	kg chem*s^-1	Yes	input	0
BALANCE EQUATIONS					

Symbol	Name	Unit	Diff.	Origin*	Default
V(i)	volume of regcomp i	m^3	Yes	E	
ADV(i,j)	advective mass flow from regcomp i to regcomp j (within one region)	m^3*s^-1	Yes	E	
DIFF(i,j)	diffusive mass flow from regcomp i to regcomp j within one region, or within one compartment	m^3*s^-1	Yes	E	
kdeg(i)	pseudo first rate constant for degradation in regcomp i	s^-1	Yes	E	
ADV_outside(i)	advective mass flow from regcomp i to outside	m^3*s^-1	Yes	E	
EMIS(i)	emission flow to regcomp i	kg*s^-1	Yes	E	
Abig(i,j)	fate matrix	m^3*s^-1	Yes	E	
CONC(i)	steady-state concentration in regcomp i	kg*m^-3	Yes	E	
MASS(i)	steady-state mass amount in regcomp i	kg	Yes	E	
CONCENTRATIONS					
C_air	concentration of the chemical in air	kg chem*m^-3	Yes	E	
C_river	concentration of the chemical in river water	kg chem*m^-3	Yes	E	
C_lake	concentration of the chemical in lake water	kg chem*m^-3	Yes	E	
C_lakesed	concentration of the chemical in lake sediment	kg chem*m^-3	Yes	E	
C_saltlake	concentration of the chemical in saltlake water	kg chem*m^-3	Yes	E	
C_saltlakesed	concentration of the chemical in	kg chem*m^-3	Yes	E	

Symbol	Name	Unit	Diff.	Origin*	Default
	saltlake sediment				
C_seawater	concentration of the chemical in sea water	kg chem*m^-3	Yes	E	
C_seased	concentration of the chemical in seawater sediment	kg chem*m^-3	Yes	E	
C_nat	concentration of the chemical in natural soil	kg chem*m^-3	Yes	E	
C_agr	concentration of the chemical in agricultural soil	kg chem*m^-3	Yes	E	
C_urb	concentration of the chemical in urban soil	kg chem*m^-3	Yes	E	
C_groundwater	concentration of the chemical in ground water	kg chem*m^-3	Yes	E	
C_drw	concentration of the chemical in drinking water	kg chem*m^-3	Yes	E	
C_purfsurfacew	concentration of the chemical in purified drinking water from surface water	kg chem*m^-3	Yes	E	
C_purfgroundw	concentration of the chemical in purified drinking water from groundwater	kg chem*m^-3	Yes	E	
C_leafcrops	concentration of the chemical in locally produced leaf crops	kg chem*m^-3	Yes	E	
C_leafcropsimp	concentration of the chemical in imported leaf crops	kg chem*m^-3	No	E	
C_rootcrops	concentration of the chemical in locally produced root crops	kg chem*m^-3	Yes	E	
C_rootcropsimp	concentration of the chemical in imported root crops	kg chem*m^-3	No	E	
C_freshwaterfish	concentration of the chemical in	kg chem*m^-3	Yes	E	

Symbol	Name	Unit	Diff.	Origin*	Default
	locally caught freshwater fish				
C_freshwaterfishimp	concentration of the chemical in imported freshwater fish	kg chem*m^-3	No	E	
C_seafish	concentration of the chemical in marine fish	kg chem*m^-3	Yes	E	
C_seafishaverage	concentration of the chemical in average marine fish	kg chem*m^-3	No	E	
C_grass	concentration of the chemical in grass	kg chem*m^-3	Yes	E	
C_meat	concentration of the chemical in locally produced meat	kg chem*m^-3	Yes	E	
C_meatimp	concentration of the chemical in imported meat	kg chem*m^-3	No	E	
C_dairy	concentration of the chemical in locally produced dairy products	kg chem*m^-3	Yes	E	
C_dairyimp	concentration of the chemical in imported dairy products	kg chem*m^-3	No	E	
CHARACTERISATION FACTOR CALCULATIONS					
RCRtox_river	Risk Characterisation Ratio for aquatic ecotoxicity in rivers	–	Yes	E	
RCRtox_lake	Risk Characterisation Ratio for aquatic ecotoxicity in freshwater lakes	–	Yes	E	
RCRtox_saltlake	Risk Characterisation Ratio for aquatic ecotoxicity in saltlakes	–	Yes	E	
RCRtox_seawater	Risk Characterisation Ratio for marine ecotoxicity	–	Yes	E	
RCRtox_soil	Risk Characterisation Ratio for terrestrial ecotoxicity	–	Yes	E	
RCRtox_lakesed	Risk Characterisation Ratio for	–	Yes	E	

Symbol	Name	Unit	Diff.	Origin*	Default
	freshwater lake sediment ecotoxicity				
RCRtox_saltlakesed	Risk Characterisation Ratio for saltlake sediment ecotoxicity	–	Yes	E	
RCRtox_seased	Risk Characterisation Ratio for marine sediment ecotoxicity	–	Yes	E	
RCRtox_humnoncarc	Risk Characterisation Ratio for human toxicity for noncarcinogenic human toxicity	–	Yes	E	
RCRtox_humcarc	Risk Characterisation Ratio for human toxicity for carcinogenic human toxicity	–	Yes	E	
SFtox_river	sensitivity factor of region = fraction of freshwater river volume in region sensitive for aquatic ecotoxicity of this substance	–	Yes	input	1
SFtox_lake	sensitivity factor of region = fraction of freshwater lake volume in region sensitive for aquatic ecotoxicity of this substance	–	Yes	input	1
SFtox_saltlake	sensitivity factor of region = fraction of saltlake volume in region sensitive for aquatic ecotoxicity of this substance	–	Yes	input	1
SFtox_seawater	sensitivity factor of region = fraction of seawater volume in region sensitive for marine ecotoxicity of this substance	–	Yes	input	1

Symbol	Name	Unit	Diff.	Origin*	Default
SFtox_soil	sensitivity factor of region = fraction of soil volume in region sensitive for terrestrial ecotoxicity of this substance	–	Yes	input	1
SFtox_lakesed	sensitivity factor of region = fraction of lake sediment volume in region sensitive for sediment ecotoxicity of this substance	–	Yes	input	1
SFtox_saltlakesed	sensitivity factor of region = fraction of saltlake sediment volume in region sensitive for sediment ecotoxicity of this substance	–	Yes	input	1
SFtox_seased	sensitivity factor of region = fraction of marine sediment volume in region sensitive for sediment ecotoxicity of this substance	–	Yes	input	1
TFtox_river	threshold factor of region = fraction of freshwater river volume in region where threshold for aquatic ecotoxicity of this substance is exceeded	–	Yes	input	1
TFtox_lake	threshold factor of region = fraction of freshwater lake volume in region where threshold for aquatic ecotoxicity of this substance is exceeded	–	Yes	input	1
TFtox_saltlake	threshold factor of region = fraction of saltlake volume in	–	Yes	input	1

Symbol	Name	Unit	Diff.	Origin*	Default
	region sensitive where threshold for ecotoxicity of this substance is exceeded				
TFtox_seawater	threshold factor of region = fraction of seawater volume in region where threshold marine ecotoxicity of this substance is exceeded	–	Yes	input	1
TFtox_nat	threshold factor of region = fraction of natural soil volume in region where threshold for terrestrial ecotoxicity of this substance is exceeded	–	Yes	input	1
TFtox_agr	threshold factor of region = fraction of agricultural soil volume in region where threshold for terrestrial ecotoxicity of this substance is exceeded	–	Yes	input	1
TFtox_urb	threshold factor of region = fraction of urban soil volume in region where threshold for terrestrial ecotoxicity of this substance is exceeded	–	Yes	input	1
TFtox_lakesed	threshold factor of region = fraction of lake sediment volume in region where threshold for sediment ecotoxicity of this substance is exceeded	–	Yes	input	1
TFtox_saltlakesed	threshold factor of region = fraction of saltlake sediment	–	Yes	input	1

Symbol	Name	Unit	Diff.	Origin*	Default
	volume in region where threshold for sediment ecotoxicity of this substance is exceeded				
TFtox_seased	threshold factor of region = fraction of marine sediment volume in region where threshold for sediment ecotoxicity of this substance is exceeded	–	Yes	input	1
TFtox_humnoncarc	threshold factor of region = fraction of humans in region where threshold for human toxicity of this noncarcinogenic substance is exceeded	–	Yes	input	1
IPICRtox_river	Integrated Potential Impact Characterisation Ratio for aquatic ecotoxicity in rivers	–	No		
IPICRtox_lake	Integrated Potential Impact Characterisation Ratio for aquatic ecotoxicity in lakes	–	No		
IPICRtox_saltlake	Integrated Potential Impact Characterisation Ratio for aquatic ecotoxicity in saltlakes	–	No		
IPICRtox_seawater	Integrated Potential Impact Characterisation Ratio for marine ecotoxicity	–	No		
IPICRtox_soil	Integrated Potential Impact Characterisation Ratio for terrestrial ecotoxicity	–	No		
IPICRtox_lakesed	Integrated Potential Impact Characterisation Ratio for	–	No		

Symbol	Name	Unit	Diff.	Origin*	Default
	sediment ecotoxicity in lake sediment				
IPICRtox_saltlakesed	Integrated Potential Impact Characterisation Ratio for sediment ecotoxicity in saltlake sediment	–	No		
IPICRtox_seased	Integrated Potential Impact Characterisation Ratio for sediment ecotoxicity in marine sediment	–	No		
IPICRtox_humnoncarc	Integrated Potential Impact Characterisation Ratio for noncarcinogenic human toxicity	–	No		
IPICRtox_humcarc	Integrated Potential Impact Characterisation Ratio for for carcinogenic human toxicity	–	No		
IAICRtox_river	Integrated Actual Impact Characterisation Ratio for aquatic ecotoxicity in rivers	–	No		
IAICRtox_lake	Integrated Actual Impact Characterisation Ratio for aquatic ecotoxicity in lakes	–	No		
IAICRtox_saltlake	Integrated Actual Impact Characterisation Ratio for aquatic ecotoxicity in saltlakes	–	No		
IAICRtox_seawater	Integrated Actual Impact Characterisation Ratio for marine ecotoxicity	–	No		
IAICRtox_soil	Integrated Actual Impact Characterisation Ratio for	–	No		

Symbol	Name	Unit	Diff.	Origin*	Default
	terrestrial ecotoxicity				
IAICRtox_lakesed	Integrated Actual Impact Characterisation Ratio for sediment ecotoxicity in lake sediment	–	No		
IAICRtox_saltlakesed	Integrated Actual Impact Characterisation Ratio for sediment ecotoxicity in saltlake sediment	–	No		
IAICRtox_seased	Integrated Actual Impact Characterisation Ratio for sediment ecotoxicity in marine sediment	–	No		
IAICRtox_humnoncarc	Integrated Actual Impact Characterisation Ratio for noncarcinogenic human toxicity	–	No		
IAICRtox_humcarc	Integrated Actual Impact Characterisation Ratio for carcinogenic human toxicity	–	No		
CFtoxpot_river	characterisation factor for potential toxic impact on river ecosystems	–	No	E	
CFtoxpot_lake	characterisation factor for potential toxic impact on lake ecosystems	–	No	E	
CFtoxpot_saltlake	characterisation factor for potential toxic impact on saltlake ecosystems	–	No	E	
CFtoxpot_seawater	characterisation factor for potential toxic impact on marine	–	No	E	

Symbol	Name	Unit	Diff.	Origin*	Default
	ecosystems				
CFtoxpot_soil	characterisation factor for potential toxic impact on terrestrial ecosystems	–	No	E	
CFtoxpot_lakesed	characterisation factor for potential toxic impact on lake sediment ecosystems	–	No	E	
CFtoxpot_saltlakesed	characterisation factor for potential toxic impact on saltlake sediment ecosystems	–	No	E	
CFtoxpot_seased	characterisation factor for potential toxic impact on marine sediment ecosystems	–	No	E	
CFtoxpot_humnoncarc	characterisation factor for noncarcinogenic toxicity to humans	–	No	E	
CFtoxpot_humcarc	characterisation factor for carcinogenic toxicity to humans	–	No	E	
CFtoxact_river	characterisation factor for actual toxic impact on river ecosystems	–	No	E	
CFtoxact_lake	characterisation factor for actual toxic impact on lake ecosystems	–	No	E	
CFtoxact_saltlake	characterisation factor for actual toxic impact on saltlake ecosystems	–	No	E	
CFtoxact_seawater	characterisation factor for actual toxic impact on marine ecosystems	–	No	E	
CFtoxact_soil	characterisation factor for actual toxic impact on terrestrial	–	No	E	

Symbol	Name	Unit	Diff.	Origin*	Default
	ecosystems				
CFtoxact_lakesed	characterisation factor for actual toxic impact on lake sediment ecosystems	–	No	E	
CFtoxact_saltlakesed	characterisation factor for actual toxic impact on saltlake sediment ecosystems	–	No	E	
CFtoxact_seased	characterisation factor for actual toxic impact on marine sediment ecosystems	–	No	E	
CFtoxact_humnoncarc	characterisation factor for actual noncarcinogenic toxic impact on humans	–	No	E	
CFtoxact_humcarc	characterisation factor for actual carcinogenic toxic impact on humans	–	No	E	
EFFECT_aquatox	effect factor for aquatic ecotoxicity	m^3*kg^-1	No	input	
EFFECT_marinetox	effect factor for marine ecotoxicity	m^3*kg^-1	No	input	
EFFECT_terrtox	effect factor for terrestrial ecotoxicity	kg^-1*kg^-1	No	input	
EFFECT_sedtox	effect factor for freshwater sediment ecotoxicity	kg^-1*kg^-1	No	input	
EFFECT_seasedtox	effect factor for seawater sediment ecotoxicity	kg^-1*kg^-1	No	input	
EFFECThum_noncarc	effect factor for human toxicity by noncarcinogenics	yr*kg^-1	No	input	
EFFECThum_carc	effect factor for human toxicity by carcinogenics	yr*kg^-1	No	input	

Symbol	Name	Unit	Diff.	Origin*	Default
MISCELLANEOUS					
Rgas	gas constant	J*mol^-1*K^-1	No	EU2 (III-76)	8.3144

*Legend: D = chemical data set; E = GLOBOX equation (in formularium); G1.1 = GLOBACK part 1, sheet 'countries'; G1.2 = GLOBACK part 1, sheet 'seas'; U1 = USES 1.0 (+ page number); U2 = USES 2.0 (+ page number); EU1 = EUSES 1.00 (+ page number); EU II = EUSES 2.0 (+ page number); SB2 = SimpleBox 2.0 (+ page number); input = to be provided by the user; references: sea reference list below.

Table Basis media characteristics

	Equation	Reference*
MEDIA CHARACTERISTICS		
	L: Fsolid_agr = 1-Fwater_agr-Fair_agr	U1 (75)
	L: Fsolid_nonagr = 1-Fwater_nonagr-Fair_nonagr	U1 (75)
	Fsolid_deepsoil = 1-Fwater_deepsoil	
	Fsolid_sed = 1-Fwater_sed	U1 (75)
	Fsolid_susp = 1-Fwater_susp	U1 (75)
	L: RHO_soil = Fair_soil*RHO_air+Fwater_soil*RHO_water+Fsolid_soil*RHO_solid	EU2 (III-77)
	L: RHO_agr = Fair_agr*RHO_air+Fwater_agr*RHO_water+Fsolid_agr*RHO_solid	EU2 (III-77)
	L: RHO_nonagr = Fair_nonagr*RHO_air+Fwater_nonagr*RHO_water+Fsolid_nonagr*RHO_solid	EU2 (III-77)

Table 3: Overview of chemical-dependent equations

Number	Equation	Reference*
PHYSICO-CHEMICAL PARAMETERS		
	metal: CHARGE = 1: ACTCOEFF = 10^-0.15	Morel &

Number	Equation	Reference*
	metal: CHARGE = 2: ACTCOEFF = 10^-0.58 metal: CHARGE = 3: ACTCOEFF = 10^-1.31 metal: CHARGE ≥ 4: ACTCOEFF = 10^-2.34	Hering (1993) (based on ionic strenth sea water = 0.7 (Van Breemen, 1972))
	S: metal: FREEIONseawater = FREEION25seawater+(TEMP-(273+5))*(FREEION5seawater-FREEION25seawater)/20	
	organic: $VP=VP\_TEMPtest\times e^{\left(\frac{H0vapor}{Rgas}\left(\frac{1}{TEMPtest}-\frac{1}{TEMP}\right)\right)}$ [VP, VP_TEMPtest, H0vapor, TEMPtest, TEMP]	SB2 (24)
	organic: SOL>0: HENRY unknown: HENRY = VP_TVP/SOL	EU2 (III-78)
	organic: $Koc=\frac{1.26\times Kow^{0.81}}{1000}$ [Koc, Kow]	EU2 (III-80)
	organic: K_airwater = HENRY/(Rgas*TEMP)	EU2 (III-78)
	L: organic: Kp_soil = Foc_soil* Koc	EU2 (III-81)
PARTITIONING PARAMETERS		
	organic: TEMPmelt<=TEMP: $Fass\_aer=\frac{CONjunge\times SURFaer}{VP+CONjunge\times SURFaer}$ [Fass_aer, CONjunge, SURFaer, VP] organic: TEMPmelt>TEMP: $Fass\_aer=\frac{CONjunge\times SURFaer}{VP\times e^{6.79\times\left(1-\frac{TEMPmelt}{TEMP}\right)}+CONjunge\times SURFaer}$	EU2 (III-78)

Number	Equation	Reference*
	[Fass_aer, CONjunge, SURFaer, VP, TEMPmelt, TEMP]	
	organic: SCAVratio = ((1-Fass_aer)/K_airwater)+Fass_aer*COLLECTeff metal, gas: SCAVratio = Fass_aer*COLLECTeff	SB2 (30)
	L: organic: Kp_susp = Foc_susp* Koc	EU2 (III-81)
	S: organic: Kp_seasusp = Foc_seasusp* Koc S: metal, gas: Kp_seasusp = Kp_susp	
	L: organic: Kp_sed = Foc_sed* Koc	EU2 (III-81)
	S: organic: Kp_seased = Foc_seased* Koc S: metal, gas: Kp_seased = Kp_sed	
	L: K_sedwater = Fwater_sed+Fsolid_sed*Kp_sed*RHO_solid	SB2 (31)
	S: K_seasedseawater = Fwater_sed+Fsolid_sed*Kp_seased*RHO_solid	
	L: K_soilwater = Fair_soil*K_airwater + Fwater_soil+ Fsolid_soil*Kp_soil*RHO_solid	EU2 (III-83)
	L: K_agrwater = Fair_agr*K_airwater + Fwater_agr+ Fsolid_agr*Kp_soil*RHO_solid	EU2 (III-83)
	K_nonagrwater = Fair_nonagr*K_airwater + Fwater_nonagr+ Fsolid_nonagr*Kp_soil*RHO_solid	-
	K_deepsoilwater = Fwater_deepsoil + Fsolid_deepsoil*Kp_soil*RHO_solid	
	L: AREA_agr>0: K_airagr = K_airwater/K_agrwater	
	L: K_airnonagr = K_airwater/K_nonagrwater	
	organic: K_plantwater=Fwater_plant+Flipid_plant*Kow [b]	EU2 (III-130)
	L: organic: K_leafair = Fair_plant+(K_plantwater/K_airwater)	EU2 (III-131)
BIOCONCENTRATION PARAMETERS		
	L: organic: BCF_rootcrops unknown: BCF_rootcrops = (K_plantwater/RHO_plant)/(K_agrwater/RHO_agr) L: gas: BCF_rootcrops unknown: BCF_rootcrops = 0	EU2 (III-130; III-107)

Number	Equation	Reference*
	organic: $TSCF=0.784\times e^{-(\log(Kow)-1.78)^2/2.44}$	EU2 (III-130)
	kelim_plant = kmetab_plant+kphoto_plant	EU2 (III-131)
	L: organic: BCFsoil_leafcrops unknown: $BCFsoil\_leafcrops=\frac{RHO\_agr\times TSCF\times Qtransp}{\left(\frac{AREAplant\times g\_plant}{K\_leafair\times V\_leaf}+kelim\_plant+kgrowth\_plant\right)\times RHO\_plant\times V\_leaf\times K\_agrwater}$ [BCFsoil_leafcrops, RHO_agr, TSCF, Qtransp, AREA_plant, g_plant, K_leafair, V_leaf, kelim_plant, kgrowth_plant, RHO_plant, K_agrwater]	EU2 (III-131-132; III-107)
	L: organic: BCFair_leafcrops unknown: $BCFair\_leafcrops=\frac{1-Fass\_aer}{\frac{1}{K\_leafair}+\frac{(kelim\_plant+kgrowth\_plant)\times V\_leaf}{g\_plant\times AREA\_plant}\times RHO\_plant}$ L: metal: BCFair_leafcrops unknown: BCFair_leafcrops = (1-Fass_aer)/((kelim_plant+kgrowth_plant)*V_leaf/(g_plant*AREA_plant))*RHO_plant) $BCFair\_leafcrops=\frac{1-Fass\_aer}{\frac{(kelim\_plant+kgrowth\_plant)\times V\_leaf}{g\_plant\times AREA\_plant}\times RHO\_plant}$ [BCFair_leafcrops, Fass_aer, K_leafair, kelim_plant, kgrowth_plant, V_leaf, g_plant, AREA_plant, *RHO_plant]	EU2 (III-131-132; III-107)
	organic: BCF_fish unknown: log(Kow)<=6: $BCF\_fish=10^{0.85\times\log(Kow)-0.7-3}$ [BCF_fish, Kow] organic: BCF_fish unknown: log(Kow)>6: $BCF\_fish=10^{-0.2\times(\log(Kow))^2+2.74\times\log(Kow)-4.72-3}$ [BCF_fish, Kow]	EU2 (III-122)
	organic: BCF_meat unknown: $BCF\_meat=10^{-7.6+\log(Kow)}$ [BCF_meat, Kow]	EU2 (III-134)
	organic: BCF_milk unknown: $BCF\_milk=10^{-8.1+\log(Kow)}$	EU2 (III-

Number	Equation	Reference*
	[BCF_milk, Kow]	134)
FRACTIONATION PARAMETERS		
	L: SUSPCONC_inlandwater = SUSPFRACTION_inlandwater*Fsolid_susp*RHO_solid	
	S: SUSPCONC_seawater = SUSPFRACTION_seawater*Fsolid_susp*RHO_solid	
	L: organic, metal: $\text{Fdiss\_inlandwater} = \dfrac{1}{1+\text{Kp\_susp}\times\text{SUSPCONC\_inlandwater}+\dfrac{\text{BCF\_fish}}{1\text{-Fwater\_bio}}\times\text{BIOCONC\_water}}$ [Fdiss_inlandwater, Kp_susp, SUSPCONC_inlandwater, BCF_fish, Fwater_bio, BIOCONC_water] L: gas: Fdiss_inlandwater = 1	SB2 (32)
	S: organic, metal: $\text{Fdiss\_seawater} = \dfrac{1}{1+\text{Kp\_seasusp}\times\text{SUSPCONC\_seawater}+\dfrac{\text{BCF\_fish}}{1-\text{Fwater\_bio}}\times\text{BIOCONC\_water}}$ [Fdiss_seawater, Kp_seasusp, SUSPCONC_seawater, BCF_fish, Fwater_bio, BIOCONC_water] S: gas: Fdiss_ seawater = 1	
	L: organic, metal: Fdiss_sed = Fwater_sed/K_sedwater L: gas: Fdiss_sed = 1	SB2 (32)
	S: organic, metal: Fdiss_seased = Fwater_sed/K_seasedseawater S: gas: Fdiss_seased = 1	
	L: organic, metal: Fdiss_soil = Fwater_soil/K_soilwater L: gas: Fdiss_soil = 1	
	L: organic, metal: Fdiss_agr = Fwater_agr/K_agrwater L: gas: Fdiss_agr = 1	
	L: organic, metal: Fdiss_nonagr = Fwater_nonagr/K_nonagrwater L: gas: Fdiss_nonagr = 1	
	L: organic, metal: Fdiss_deepsoil = Fwater_deepsoil/K_deepsoilwater L: gas: Fdiss_deepsoil = 1	

*Legend: U1 = USES 1.0 (+ page number); U2 = USES 2.0 (+ page number); EU1 = EUSES 1.00 (+ page number); EU II = EUSES 2.0 (+ page number); SB2 = SimpleBox 2.0 (+ page number); input = to be provided by the user; references: sea reference list below.

Table 4: Overview of chemical-independent equations

Number	Equation	Reference*
CLIMATIC PARAMETERS		
	L: AREA_lake>0: RAINDIRECT_lake = RAINRATE*AREA_lake	
	L: RAINDIRECT_saltlake = RAINRATE*AREA_saltlake	
	L: AREA_lake>0: EVAP_lake = EVAPrate_lake*AREA_lake	
	Ftime_rain = 0.1*RAINDAYS/365	
	Ftime_frost = FROSTMONTHS/12	
FLOW PARAMETERS		
	L: AREA_lake > 0: FLOW_river_lake = (AREA_lake*TOTALDEPTH_lake/RESTIME_lake)-RAINDIRECT_lake L: AREA_lake = 0: FLOW_river_lake = 0	
	L: AREA_lake > 0: FLOW_lake_river = (AREA_lake*TOTALDEPTH_lake/RESTIME_lake)-EVAP_lake L: AREA_lake = 0: FLOW_lake_river = 0	
	L: FLOW_river_saltlake = EVAP_saltlake-RAINDIRECT_saltlake	
DIMENSIONAL PARAMETERS		
	L: AREA_saltlakesed = AREA_saltlake	
	L: AREA_nat = SYSTEMAREA*Farea_nat	U1 (76)
	L: AREA_agr = SYSTEMAREA*Farea_agr	U1 (76)
	L: AREA_urb = SYSTEMAREA*Farea_urb	U1 (76)
	V_air = SYSTEMAREA*HEIGHT_air	SB2 (37)
	L: V_lake = AREA_lake*MIXDEPTH_lake	
	L: V_saltlake = AREA_saltlake*TOTALDEPTH_saltlake	
	S: V_seawater = SYSTEMAREA*MIXDEPTH_seawater	
	L: V_lakesed = AREA_lakesed*DEPTH_sed	SB2 (56)
	L: V_saltlakesed = AREA_saltlakesed*DEPTH_sed	
	S: V_seased = AREA_seased*DEPTH_sed	
	L: V_nat = AREA_nat*DEPTH_nonagr	SB2 (57)

Number	Equation	Reference*
	L: V_agr = AREA_agr*DEPTH_agr	SB2 (57)
	L: V_urb = AREA_urb*DEPTH_nonagr	SB2 (57)
	L: TOTALDEPTH_lake ≤ DEPTH_groundwater: V_groundwater = ((SYSTEMAREA*DEPTH_groundwater)-V_lake)*Fwater_deepsoil TOTALDEPTH_lake > DEPTH_groundwater: V_groundwater = ((SYSTEMAREA-AREA_lake)*DEPTH_groundwater)*Fwater_deepsoil	
IMPORT PARAMETERS		
5.1		
DEGRADATION		
	BACTporew_sed = BACT_sed/Fwater_sed	SB2 (73)
	organic: PASSreadytest = 'yes': kdeg_test = ln(2)/(5*24*3600) organic: PASSreadytest = 'no': kdeg_test = ln(2)/(1000*24*3600)	SB2 (72)
	DT50bio_freshwater_TEMPtest unknown: organic: inherently_biodegradable = yes: readily_biodegradable = yes: fulfilling_10d_window = yes: DT50bio_freshwater_TEMPtest = 15*24*3600 DT50bio_freshwater_TEMPtest unknown: organic: inherently_biodegradable = yes: readily_biodegradable = yes: fulfilling_10d_window = no: DT50bio_freshwater_TEMPtest = 50*24*3600 DT50bio_freshwater_TEMPtest unknown: organic: inherently_biodegradable = yes: readily_biodegradable = no: fulfilling_10d_window = no: DT50bio_freshwater_TEMPtest = 150*24*3600 DT50bio_freshwater_TEMPtest unknown: organic: inherently_biodegradable = no: readily_biodegradable = no: fulfilling_10d_window = no: DT50bio_freshwater_TEMPtest = infinite	SB2 (72)
	metal, gas: L: DT50bio_freshwater = DT50bio_freshwater_TEMPtest organic: L: $DT50bio\_freshwater = DT50bio\_freshwater\_TEMPtest \times e^{(0.08 \times (TEMPtest - TEMP))}$ [DT50bio_freshwater, DT50bio_freshwater_TEMPtest, TEMPtest, TEMP]	SB2 (72); EU2 (III-88)
	L: DT50bio_saltlake = DT50bio_freshwater/SALINITYcorr	
	DT50bio_seawater_TEMPtest unknown: DT50bio_seawater_TEMPtest = DT50bio_freshwater_TEMPtest/SALINITYcorr	
	metal, gas: S: DT50bio_seawater = DT50bio_seawater_TEMPtest organic: S: $DT50bio\_seawater = DT50bio\_seawater\_TEMPtest \times e^{(0.08 \times (TEMPtest - TEMP))}$ [DT50bio_seawater, DT50bio_seawater_TEMPtest, TEMPtest, TEMP]	EU2 (III-88)

Number	Equation	Reference*
	organic: L: inherently_biodegradable = yes: readily_biodegradable = yes: fulfilling_10d_window = yes: DT50aerbio_sed_TEMPtest = 30*24*3600*10*Kp_sed organic: L: inherently_biodegradable= yes: readily_biodegradable = yes: fulfilling_10d_window = no: DT50aerbio_sed_TEMPtest = 90*24*3600*10*Kp_sed organic: L: inherently_biodegradable= yes: readily_biodegradable = no: fulfilling_10d_window = no: DT50aerbio_sed_TEMPtest = 300*24*3600*10*Kp_sed organic: L: inherently_biodegradable= no: readily_biodegradable = no: fulfilling_10d_window = no: DT50aerbio_sed_TEMPtest = infinite	SB2 (73)
	metal, gas: L: DT50aerbio_sed = DT50aerbio_sed_TEMPtest organic: L: $DT50aerbio\_sed = DT50aerbio\_sed\_TEMPtest \times e^{(0.08 \times (TEMPtest - TEMP))}$ [DT50aerbio_sed, DT50aerbio_sed_TEMPtest, TEMPtest, TEMP]	
	L: DT50aerbio_saltlakesed unknown: DT50aerbio_saltlakesed = DT50aerbio_sed/SALINITYcorr	
	L: DT50anaerbio_saltlakesed unknown: DT50anaerbio_saltlakesed = DT50anaerbio_sed/SALINITYcorr	
	metal, gas: S: DT50aerbio_seased = DT50aerbio_seased_TEMPtest organic: S: DT50aerbio_seased_TEMPtest unknown: inherently_biodegradable= yes: readily_biodegradable = yes: fulfilling_10d_window = yes: DT50aerbio_seased_TEMPtest = 30*24*3600*10*Kp_seased/ SALINITYcorr inherently_biodegradable= yes: readily_biodegradable = yes: fulfilling_10d_window = no: DT50aerbio_seased_TEMPtest = 90*24*3600*10*Kp_seased/SALINITYcorr inherently_biodegradable= yes: readily_biodegradable = no: fulfilling_10d_window = no: DT50aerbio_seased_TEMPtest = 300*24*3600*10*Kp_seased/SALINITYcorr inherently_biodegradable= no: readily_biodegradable = no: fulfilling_10d_window = no: DT50aerbio_seased_TEMPtest = infinite [DT50aerbio_seased, DT50aerbio_sed_TEMPtest, TEMPtest, TEMP, SALINITYcorr]	
	metal, gas: L: DT50aerbio_seased = DT50aerbio_seased_TEMPtest organic: L: $DT50aerbio\_seased = DT50aerbio\_seased\_TEMPtest \times e^{(0.08 \times (TEMPtest - TEMP))}$ [DT50aerbio_seased, DT50aerbio_seased_TEMPtest, TEMPtest, TEMP]	
	S: DT50anaerbio_seased unknown: DT50anaerbio_seased = DT50anaerbio_sed/SALINITYcorr	
	organic: L: DT50bio_soil_TEMPtest unknown:	EU2 (III-89)

Number	Equation	Reference*
	inherently_biodegradable= yes: readily_biodegradable = yes: fulfilling_10d_window = yes: DT50bio_soil_TEMPtest = 30*24*3600*10*Kp_soil inherently_biodegradable= yes: readily_biodegradable = yes: fulfilling_10d_window = no: DT50bio_soil_TEMPtest = 90*24*3600*10*Kp_soil inherently_biodegradable= yes: readily_biodegradable = no: fulfilling_10d_window = no: DT50bio_soil_TEMPtest = 300*24*3600*10*Kp_soil inherently_biodegradable= no: readily_biodegradable = no: fulfilling_10d_window = no: DT50bio_soil_TEMPtest = infinite	
	metal, gas: L: DT50bio_soil = DT50bio_soil_TEMPtest organic: L: $DT50bio\_soil = DT50bio\_soil\_TEMPtest \times e^{(0.08 \times (TEMPtest - TEMP))}$ [DT50bio_soil, DT50bio_soil_TEMPtest, TEMPtest, TEMP]	
	L: DT50bio_agr unknown: DT50bio_agr = DT50bio_soil*Fdiss_soil/Fdiss_agr	
	L: DT50bio_nonagr unknown: DT50bio_nonagr = DT50bio_soil*Fdiss_soil/Fdiss_nonagr	
	metal, gas: DT50hydro_water = DT50hydro_water_TEMPtest organic: DT50hydro_water_TEMPtest known: $DT50hydro\_water = DT50hydro\_water\_TEMPtest \times e^{(0.08 \times (TEMPtest - TEMP))}$ [DT50hydro_water, DT50hydro_water_TEMPtest, TEMPtest, TEMP]	
	L: DT50abio_saltlakesed unknown: DT50abio_saltlakesed = DT50abio_sed	
	S: DT50abio_seased unknown: DT50abio_seased = DT50abio_sed	
	organic, gas: krad_OH unknown: krad_OH = ln(2)/DT50photo_air	
	kdeg_air unknown: kdeg_air = (1-Fass_aer)* krad_OH*OHCONC_air/OHCONCref_air	EU2 (III-86)
	L: kbio_freshwater = ln(2)/DT50bio_freshwater	
	L: kbio_saltlake = ln(2)/DT50bio_saltlake	
	DT50hydro_water known: khydro_inlandwater = ln(2)/DT50hydro_water DT50hydro_water unknown: khydro_inlandwater = 0	
	DT50hydro_water known: khydro_seawater = ln(2)/DT50hydro_water DT50hydro_water unknown: khydro_seawater = 0	
	DT50photo_water known: kphoto_water = ln(2)/DT50photo_water DT50photo_water unknown: kphoto_water = 0	
	L: kdeg_freshwater = kbio_freshwater + khydro_inlandwater + kphoto_water	EU2 III-88

Number	Equation	Reference*
	L: kdeg_saltlake = kbio_saltlake + khydro_inlandwater + kphoto_water	EU2 III-88
	S: kbio_seawater = ln(2)/DT50bio_seawater	
	S: kdeg_seawater = kbio_seawater + khydro_seawater+ kphoto_water	
	L: kaerbio_sed = ln(2)/DT50aerbio_sed	EU2 (III-90)
	L: kanaerbio_sed = ln(2)/DT50anaerbio_sed	EU2 (III-90)
	kabio_sed = ln(2)/DT50abio_sed	
	kdeg_sed = Faer_sed*kaerbio_sed+(1-Faer_sed)*kanaerbio_sed+kabio_sed	EU2 (III-90)
	L: kaerbio_saltlakesed = ln(2)/DT50aerbio_saltlakesed	
	L: kanaerbio_saltlakesed = ln(2)/DT50anaerbio_saltlakesed	
	L: kabio_saltlakesed = ln(2)/DT50abio_saltlakesed	
	L: kdeg_saltlakesed = Faer_sed*kaerbio_saltlakesed+(1-Faer_sed)*kanaerbio_saltlakesed+kabio_saltlakesed	
	S: kaerbio_seased = ln(2)/DT50aerbio_seased	
	S: kanaerbio_seased = ln(2)/DT50anaerbio_seased	
	S: kabio_seased = ln(2)/DT50abio_seased	
	S: kdeg_seased = Faer_seased*kaerbio_seased+(1-Faer_seased)*kanaerbio_seased+kabio_seased	
	L: kbio_agr = ln(2)/DT50bio_agr	EU2 (III-90)
	L: kbio_nonagr = ln(2)/DT50bio_nonagr	EU2 (III-90)
	kabio_soil = ln(2)/DT50abio_soil	EU2 (III-90)
	L: kdeg_agr = kbio_agr+kabio_soil	EU2 (III-90)
	L: kdeg_nonagr = kbio_nonagr+kabio_soil	EU2 (III-90)
EXPOSURE PARAMETERS		
	L: CONVagr = RHO_agr/(RHO_solid*Fsolid_agr)	EU2 (III-77)
	BORDERLENGTH(i,j)>0: BORDERHEIGHT_air(i,j) = min(HEIGHT_air(i), HEIGHT_air(j))	
	BORDERLENGTH(i,j)>0: $\text{BORDERWINDSPEED(i,j)}=\frac{\text{WINDSPEED(i)}\times\sqrt{\text{SYSTEMAREA(i)}}}{\sqrt{\text{SYSTEMAREA(i)}}+\sqrt{\text{SYSTEMAREA(j)}}}+\frac{\text{WINDSPEED(j)}\times\sqrt{\text{SYSTEMAREA(j)}}}{\sqrt{\text{SYSTEMAREA(i)}}+\sqrt{\text{SYSTEMAREA(j)}}}$ [BORDERWINDSPEED, WINDSPEED, SYSTEMAREA]	

Number	Equation	Reference*
	L: PRODsusp_saltlake = PRODratesusp_inlandwater*AREA_saltlake	
SALTLAKE PARAMETERS		
	L: FLOW_river,saltlake = EVAP_saltlake	
SEAWATER PARAMETERS		
	S: PRODsusp_seawater = PRODratesusp_seawater*SYSTEMAREA	
SEASEDIMENT PARAMETERS		
SOIL PARAMETERS		
DISTRIBUTION PARAMETERS		
	$\text{kaw\_air}=0.01\times(0.3+0.2\times\text{WINDSPEED})\times\left(\frac{0.018}{\text{MOLW}}\right)^{0.67\times0.5}$ [kaw_air, WINDSPEED, MOLW]	EU2 (III-108)
	$\text{kaw\_water}=0.01\times(0.004+0.00004\times\text{WINDSPEED})\times\left(\frac{0.032}{\text{MOLW}}\right)^{0.5\times0.5}$ [kaw_water, WINDSPEED, MOLW]	EU2 (III-108)
	$\text{GASABS\_water}=(1\text{-Ftime\_frost})\times\frac{1\text{-Fass\_aer}}{\frac{\text{K\_airwater}}{\text{kaw\_water}}+\frac{1}{\text{kaw\_air}}}$ [GASABS_water, Ftime_frost, Fass_aer, K_airwater, kaw_water, kaw_air]	SB2 (75)
	L: $\text{VOLAT\_inlandwater}=(1\text{-Ftime\_frost})\times\frac{\text{GASABS\_water}}{1\text{-Fass\_aer}}\text{K\_airwater}\times\text{Fdiss\_inlandwater}$ [VOLAT_inlandwater, Ftime_frost, GASABS_water, Fass_aer, K_airwater, Fdiss_inlandwater]	SB2 (76)
	S: $\text{VOLAT\_seawater}=(1\text{-Farea\_seaice})\times\frac{\text{GASABS\_water}}{1\text{-Fass\_aer}}\times\text{K\_airwater}\times\text{Fdiss\_seawater}$ [VOLAT_seawater, Farea_seaice, GASABS_water, Fass_aer, K_airwater, Fdiss_seawater]	-

Number	Equation	Reference*
	L: K_airnonagr>0: $\text{GASABS\_nat}=\dfrac{1\text{-Fass\_aer}}{\dfrac{1}{\text{kasl\_air}}+\dfrac{1}{\text{kasl\_soilair}+\dfrac{\text{kasl\_soilwater}}{\text{K\_airnonagr}}}}$ [GASABS_nat, Fass_aer, kasl_air, kasl_soilair, kasl_soilwater, K_airnonagr] L: K_airnonagr=0: GASABS_nat = 0	SB2 (76)
	L: K_airagr>0: $\text{GASABS\_agr}=\dfrac{1\text{-Fass\_aer}}{\dfrac{1}{\text{kasl\_air}}+\dfrac{1}{\text{kasl\_soilair}+\dfrac{\text{kasl\_soilwater}}{\text{K\_airagr}}}}$ [GASABS_agr, Fass_aer, kasl_air, kasl_soilair, kasl_soilwater, K_airagr] L: K_airagr=0: GASABS_agr = 0	SB2 (76)
	L: K_airnonagr>0: $\text{GASABS\_urb}=\dfrac{1\text{-Fass\_aer}}{\dfrac{1}{\text{kasl\_air}}+\dfrac{1}{\text{kasl\_soilair}+\dfrac{\text{kasl\_soilwater}}{\text{K\_airnonagr}}}}$ [GASABS_urb, Fass_aer, kasl_air, kasl_soilair, kasl_soilwater, K_airnonagr] L: K_airnongagr=0: GASABS_urb = 0	SB2 (76)
	L: AREA_nat>0: $\text{VOLAT\_nat}=\dfrac{\left(1\text{-}\left(\text{AREA\_landice/AREA\_nat}\right)\right)\times\left(1\text{-Ftime\_frost}\right)\times\text{GASABS\_nat}}{\left(1\text{-Fass\_aer}\right)}\times\text{K\_airnonagr}$ [VOLAT_nat, AREA_landice, AREA_nat, Ftime_frost, GASABS_nat, Fass_aer, K_airnonagr]	SB2 (76)
	L: AREA_agr>0: $\text{VOLAT\_agr}=\dfrac{\left(1\text{-Ftime\_frost}\right)\times\text{GASABS\_agr}}{\left(1\text{-Fass\_aer}\right)}\times\text{K\_airagr}$ [VOLAT_agr, Ftime_frost, GASABS_agr, Fass_aer, K_airagr]	SB2 (76)
	L: AREA_urb>0: $\text{VOLAT\_urb}=\dfrac{\left(1\text{-Ftime\_frost}\right)\times\text{GASABS\_urb}}{\left(1\text{-Fass\_aer}\right)}\times\text{K\_airnonagr}$	SB2 (76)

Number	Equation	Reference*
	[VOLAT_urb, Ftime_frost, GASABS_urb, Fass_aer, K_airnonagr]	
	DRYDEP_aer = AEROSOLDEPRATE*Fass_aer	SB2 (75)
	WASHOUT = RAINRATE*SCAVratio	SB2 (75)
	L: AREA_nat>0: EROSION_nat= RAINRATE*Fsolid_runoff/Fsolid_nonagr	-
	L: AREA_agr>0: EROSION_agr= RAINRATE*Fsolid_runoff/Fsolid_agr	-
	L: AREA_urb>0: EROSION_urb= RAINRATE*Fsolid_runoff/Fsolid_nonagr	-
	L: AREA_nat>0: RUNOFF_nat = ((WATERrunoff/AREA_nat)/K_nonagrwater)+EROSION_nat	SB2 (79)
	L: AREA_agr>0: RUNOFF_agr = ((WATERrunoff/AREA_agr)/K_agrwater)+EROSION_agr	SB2 (79)
	L: AREA_urb>0: RUNOFF_urb = ((WATERrunoff/AREA_urb)/K_nonagrwater)+EROSION_urb	SB2 (79)
	L: RAINRATE > 0: Finf_soil = FLOW_soil_groundwater/(RAINRATE*(AREA_nat+AREA_agr+AREA_urb)) L: RAINRATE = 0: Finf_soil = 0	
	L: LEACH_agr = Finf_soil*RAINRATE/K_agrwater	SB2 (80)
	L: LEACH_nonagr = Finf_soil*RAINRATE/K_nonagrwater	SB2 (80)
	L: ADSORB_sed = Fdiss_inlandwater/(1/kws_water+1/kws_sed)	SB2 (78)
	L: DESORB_sed = ADSORB_sed/(K_sedwater*Fdiss_sed)	SB2 (78)
	S: ADSORB_seased = Fdiss_seawater/(1/kws_water+1/kws_sed)	
	S: DESORB_seased = ADSORB_seased/(K_seasedseawater*Fdiss_seased)	
	L: $\text{sin(i)}=\text{EROSION\_nat(i)}\times\text{AREA\_nat(i)}\times\text{Fsolid\_nonagr(i)}+\text{EROSION\_agr(i)}\times\text{AREA\_agr(i)}\times\text{Fsolid\_agr(i)}+\text{EROSION\_urb(i)}\times\text{AREA\_urb(i}$ $\text{riverinflow\_solid}(i)=\sum_{j\in L}\text{SUSPCONC\_inlandwater}(j)\times\text{FLOW\_river\_river}(j,i)+\text{sin(i)}\times\text{RHO\_solid(i)}$ [riverinflow_solid, SUSPCONC_inlandwater, FLOW_river_river, EROSION_nat, AREA_nat, Fsolid_nonagr, EROSION_agr, AREA_agr, Fsolid_agr, EROSION_urb, AREA_urb, RHO_solid]	
	L: $\text{riveroutflow\_solid}(i)=\sum_{j\in L}\text{SUSPCONC\_inlandwater}(i)\times\text{FLOW\_river\_river}(i,j)$ [riveroutflow_solid, SUSPCONC_inlandwater, FLOW_river_river]	
	L: AREA_saltlake>0:	

Number	Equation	Reference*
	$ein(i)=EROSION\_nat(i)\times AREA\_nat(i)\times Fsolid\_nonagr(i)+EROSION\_agr(i)\times AREA\_agr(i)\times Fsolid\_agr(i)+EROSION\_urb(i)\times AREA\_urb(i$ $win(i)=\sum_{j\in L}\left(SUSPCONC\_inlandwater(j)\times FLOWriver\_river(j,i)\right)$ $NETSEDRATE\_saltlake(i)=\frac{PRODSUSP\_saltlake(i)+win(i)+ein(i)\times RHO\_solid}{Fsolid\_sed(i)\times RHO\_solid\times AREA\_saltlake(i)}$ [NETSEDRATE_saltlake, PRODSUSP_saltlake, SUSPCONC_inlandwater, FLOW_river_river, EROSION_nat, AREA_nat, Fsolid_nonagr, EROSION_agr, AREA_agr, Fsolid_agr, EROSION_urb, AREA_urb]	
	S: $rin(i)=\sum_{j\in L} SUSPCONC\_inlandwater(j)\times FLOW\_river\_seawater(j,i)$ $sin(i)=\sum_{j\in S} SUSPCONC\_seawater(j)\times FLOW\_seawater\_seawater(j,i)$ $sout(i)=\sum_{j\in S} SUSPCONC\_seawater(i)\times FLOW\_seawater\_seawater(i,j)$ $NETSEDRATE\_seawater(i)=\frac{PRODSUSP\_seawater(i)+rin(i)+sin(i)-sout(i)}{Fsolid\_sed(i)\times RHO\_solid\times SYSTEMAREA(i)}$ [NETSEDRATE_seawater, PRODSUSP_seawater, SUSPCONC_inlandwater, FLOW_river_seawater, SUSPCONC_seawater, FLOW_seawater_seawater, Fsolid_sed, RHO_solid, SYSTEMAREA]	
	L: sedrate_inlandwater = SETTLvelocity_susp*SUSPCONC_inlandwater/(Fsolid_sed*RHO_solid)	SB2 (49)
	S: sedrate_seawater = SETTLvelocity_susp*SUSPCONC_seawater/(Fsolid_sed*RHO_solid)	
	L: sedrate_inlandwater>NETsedrate_saltlake: GROSSsedrate_saltlake = sedrate_inlandwater L: sedrate_inlandwater<NETsedrate_saltlake: GROSSsedrate_saltlake = NETsedrate_saltlake	SB2 (49)
	S: sedrate_seawater>NETsedrate_seawater: GROSSsedrate_seawater = sedrate_seawater S: sedrate_seawater<NETsedrate_seawater: GROSSsedrate_seawater = NETsedrate_seawater	
	L: sedrate_inlandwater>NETsedrate_saltlake: RESUSPrate_saltlake = GROSSsedrate_saltlake-NETsedrate_saltlake L: sedrate_inlandwater≤NETsedrate_saltlake: RESUSPrate_saltlake =0	
	S: sedrate_seawater>NETsedrate_seawater: RESUSPrate_seawater = GROSSsedrate_seawater-NETsedrate_seawater S: sedrate_seawater≤NETsedrate_seawater: RESUSPrate_seawater = 0	
INTERMEDIA TRANSFER PARAMETERS		
	L: DIFF_air_lake = GASABS_water*AREA_lake	SB2 (87)

Number	Equation	Reference*
	L: DIFF_lake_air = VOLAT_inlandwater*AREA_lake	SB2 (88)
	L: ADV_air_lake = (DRYDEP_aer+WASHOUT)*AREA_lake	SB2 (86)
	L: DIFF_air_saltlake = GASABS_water*AREA_saltlake	SB2 (87)
	L: DIFF_saltlake, air = VOLAT_inlandwater*AREA_saltlake	SB2 (88)
	L: ADV_air_saltlake = (DRYDEP_aer+WASHOUT)*AREA_saltlake	SB2 (86)
	S: DIFF_air_seawater = GASABS_water*SYSTEMAREA	
	S: DIFF_seawater_air = VOLAT_seawater*SYSTEMAREA	
	S: ADV_air_seawater = (DRYDEP_aer+WASHOUT)*SYSTEMAREA	
	L: DIFF_air_nat = GASABS_nat*AREA_nat	SB2 (88)
	L: DIFF_air_agr = GASABS_agr*AREA_agr	SB2 (88)
	L: DIFF_air_urb = GASABS_urb*AREA_urb	SB2 (88)
	L: DIFF_nat_air = VOLAT_nat*AREA_nat	SB2 (88)
	L: DIFF_agr_air = VOLAT_agr*AREA_agr	SB2 (88)
	L: DIFF_urb_air = VOLAT_urb*AREA_urb	SB2 (88)
	L: ADV_air_nat = (DRYDEP_aer+WASHOUT)*AREA_nat	SB2 (86)
	L: ADV_air_agr = (DRYDEP_aer+WASHOUT)*AREA_agr	SB2 (86)
	L: ADV_air_urb = (DRYDEP_aer+WASHOUT)*AREA_urb	SB2 (86)
	L: ADV_nat_river = RUNOFF_nat*AREA_nat	SB2 (105)
	L: ADV_agr_river = RUNOFF_agr*AREA_agr	SB2 (105)
	L: ADV_urb_river = RUNOFF_urb*AREA_urb	SB2 (105)
	L: ADV_river_lake = FLOW_river_lake	
	L: ADV_river_saltlake = FLOW_river_saltlake	
	L: ADV_river_agr = FLOW_river_agr	
	L,S: ADV_river_seawater(i,j) = FLOW_river_seawater(i,j)	
	L: ADV_river_outside = (riverinflow_solid-riveroutflow_solid))/(Fsolid_sed*RHO_solid)	
	L: ADV_nat_groundwater = LEACH_nonagr*AREA_nat*Fdiss_deepsoil	
	L: ADV_agr_groundwater = LEACH_agr*AREA_agr *Fdiss_deepsoil	
	L: ADV_urb_groundwater = LEACH_nonagr*AREA_urb*Fdiss_deepsoil	
	L: ADV_lake_river= FLOW_lake_river	

Number	Equation	Reference*
	L: DIFF_lake_lakesed = ADSORB_sed*AREA_lakesed	SB2 (102)
	L: DIFF_lakesed_lake = DESORB_sed*AREA_lakesed	SB2 (102)
	L: ADV_lake_lakesed = sedrate_inlandwater*SUSPCONC_inlandwater*Kp_susp*AREA_lakesed	SB2 (100)
	L: ADV_lake_outside = sedrate_inlandwater*SUSPCONC_inlandwater*Kp_susp *(AREA_lake-AREA_lakesed)	
	L: ADV_lakesed_outside = sedrate_inlandwater*SUSPCONC_inlandwater*Kp_susp*AREA_lakesed	
	L: DIFF_saltlake_saltlakesed = ADSORB_sed*AREA_saltlakesed	SB2 (102)
	L: DIFF_saltlakesed_saltlake = DESORB_sed*AREA_saltlakesed	SB2 (102)
	L: ADV_saltlake_saltlakesed = GROSSsedrate_saltlake*AREA_saltlakesed	SB2 (100)
	L: ADV_saltlakesed_saltlake = RESUSPrate_saltlake* AREA_saltlakesed	SB2 (100)
	L: ADV_saltlakesed_outside = NETsedrate_saltlake*AREA_saltlakesed	
	L: ADV_groundwater_agr = FLOW_groundwater_agr	
	L: ADV_groundwater_river = FLOW_groundwater_river	
	L,S: ADV_groundwater_seawater(i,j) = FLOW_groundwater_seawater(i,j)	
	S: DIFF_seawater_seased = ADSORB_seased*AREA_seased	
	S: DIFF_seased_seawater = DESORB_seased*AREA_seased	
	S: ADV_seawater_seased = GROSSsedrate_seawater*AREA_seased	
	S: ADV_seased_seawater = RESUSPrate_seawater* AREA_seased	
	S: ADV_seawater_outside = GROSSsedrate_seawater*(SYSTEMAREA-AREA_seased)	
	S: ADV_seased_outside = NETsedrate_seawater*AREA_seased	
INTRAMEDIUM TRANSPORT PARAMETERS		
	ADV_air_air(i,j) = BORDERWINDSPEED(i,j)*BORDERLENGTH(i,j)*BORDERHEIGHT_air(i,j)	
	L,L: ADV_river_river(i,j) = FLOW_river_river(i,j)	SB2 (38)
	L,L: ADV_groundwater_groundwater(i,j) = FLOW_groundwater_groundwater(i,j)	
	S,S: ADV_seawater_seawater(i,j) = FLOW_seawater_seawater(i,j)	SB2 (38)
BALANCE EQUATIONS		

Number	Equation	Reference*
	V((i-1)×nregion+1) = V_air(i) L: V((i-1)×nregion+2) = V_nat(i) L: V((i-1)×nregion+3) = V_agr(i) L: V((i-1)×nregion+4) = V_urb(i) L: V((i-1)×nregion+5) = V_river(i) L: V((i-1)×nregion+6) = V_lake(i) L: V((i-1)×nregion+7) = V_lakesed(i) L: V((i-1)×nregion+8) = V_saltlake(i) L: V((i-1)×nregion+9) = V_saltlakesed(i) L: V((i-1)×nregion+10) = V_groundwater(i) S: V((i-1)×nregion+11) = V_seawater(i) S: V((i-1)×nregion+12) = V_seased(i)	
	L: DIFF((i-1)×nregion+1, (i-1)×nregion+2) = DIFF_air_nat(i,i) L: DIFF((i-1)×nregion+1, (i-1)×nregion+3) = DIFF_air_agr(i,i) L: DIFF((i-1)×nregion+1, (i-1)×nregion+4) = DIFF_air_urb(i,i) L: DIFF((i-1)×nregion+1, (i-1)×nregion+6) = DIFF_air_lake(i,i) L: DIFF((i-1)×nregion+1, (i-1)×nregion+8) = DIFF_air_saltlake(i,i) S: DIFF((i-1)×nregion+1, (i-1)×nregion+11) = DIFF_air_seawater(i,i)	
	L: DIFF((i-1)×nregion+2, (i-1)×nregion+1) = DIFF_nat_air(i,i) L: DIFF((i-1)×nregion+3, (i-1)×nregion+1) = DIFF_agr_air(i,i) L: DIFF((i-1)×nregion+4, (i-1)×nregion+1) = DIFF_urb_air(i,i)	
	L: DIFF((i-1)×nregion+6, (i-1)×nregion+1) = DIFF_lake_air(i,i) L: DIFF((i-1)×nregion+6, (i-1)×nregion+7) = DIFF_lake_lakesed(i,i) L: DIFF((i-1)×nregion+7, (i-1)×nregion+6) = DIFF_lakesed_lake(i,i)	
	L: DIFF((i-1)×nregion+8, (i-1)×nregion+1) = DIFF_saltlake_air(i,i) L: DIFF((i-1)×nregion+8, (i-1)×nregion+9) = DIFF_saltlake_ saltlakesed(i,i) L: DIFF((i-1)×nregion+9, (i-1)×nregion+8) = DIFF_saltlakesed_saltlake(i,i)	

Number	Equation	Reference*
	S: DIFF((i-1)×nregion+11, (i-1)×nregion+1) = DIFF_seawater_air(i,i) S: DIFF((i-1)×nregion+11, (i-1)×nregion+12) = DIFF_seawater_seased(i,i) S: DIFF((i-1)×nregion+12, (i-1)×nregion+11) = DIFF_seased_seawater(i,i)	
	ADV((i-1)×nregion+1, (j-1)×nregion+1) = ADV_air_air(i,j) L: ADV((i-1)×nregion+1, (i-1)×nregion+2) = ADV_air_nat(i,i) L: ADV((i-1)×nregion+1, (i-1)×nregion+3) = ADV_air_agr(i,i) L: ADV((i-1)×nregion+1, (i-1)×nregion+4) = ADV_air_urb(i,i) L: ADV((i-1)×nregion+1, (i-1)×nregion+6) = ADV_air_lake(i,i) L: ADV((i-1)×nregion+1, (i-1)×nregion+8) = ADV_air_saltlake(i,i) S: ADV((i-1)×nregion+1, (j-1)×nregion+11) = ADV_air_seawater(i,i)	
	L: ADV((i-1)×nregion+2, (i-1)×nregion+5) = ADV_nat_river(i,i) L: ADV((i-1)×nregion+2, (i-1)×nregion+10) = ADV_nat_groundwater(i,i) L: ADV((i-1)×nregion+3, (i-1)×nregion+5) = ADV_agr_river(i,i) L: ADV((i-1)×nregion+3, (i-1)×nregion+10) = ADV_agr_groundwater(i,i) L: ADV((i-1)×nregion+4, (i-1)×nregion+5) = ADV_urb_river(i,i) L: ADV((i-1)×nregion+4, (i-1)×nregion+10) = ADV_urb_groundwater(i,i)	
	L: ADV((i-1)×nregion+5, (i-1)×nregion+3) = ADV_river_agr(i,i) L: ADV((i-1)×nregion+5, (i-1)×nregion+6) = ADV_river_lake(i,i) L,L: ADV((i-1)×nregion+5, (j-1)×nregion+5) = ADV_river_river(i,j) L: ADV((i-1)×nregion+5, (i-1)×nregion+8) = ADV_river_saltlake(i,i) L,S: ADV((i-1)×nregion+5, (j-1)×nregion+11) = ADV_river_seawater(i,j)	
	L: ADV((i-1)×nregion+6, (i-1)×nregion+5) = ADV_lake_river(i,i) L: ADV((i-1)×nregion+6, (i-1)×nregion+7) = ADV_lake_lakesed(i,i)	
	L: ADV((i-1)×nregion+8, (i-1)×nregion+9) = ADV_saltlake_saltlakesed(i,i) L: ADV((i-1)×nregion+9, (i-1)×nregion+8) = ADV_saltlakesed_saltlake(i,i)	

Number	Equation	Reference*
	L: ADV((i-1)×nregion+10, (i-1)×nregion+3) = ADV_groundwater_agr(i,i) L: ADV((i-1)×nregion+10, (i-1)×nregion+5) = ADV_groundwater_river(i,i) L,L: ADV((i-1)×nregion+10, (j-1)×nregion+10) = ADV_groundwater_groundwater(i,j) L,S: ADV((i-1)×nregion+10, (j-1)×nregion+11) = ADV_groundwater_seawater(i,j)	
	S,S: ADV((i-1)×nregion+11, (j-1)×nregion+11) = ADV_seawater_seawater(i,j) S: ADV((i-1)×nregion+11, (i-1)×nregion+12) = ADV_seawater_seased(i,i) S: ADV((i-1)×nregion+12, (i-1)×nregion+11) = ADV_seased_seawater(i,i)	
	kdeg((i-1)×nregion+1) = kdeg_air(i) L: kdeg((i-1)×nregion+2) = kdeg_nonagr(i) L: kdeg((i-1)×nregion+3) = kdeg_agr(i) L: kdeg((i-1)×nregion+4) = kdeg_nonagr(i) L: kdeg((i-1)×nregion+5) = kdeg_freshwater(i) L: kdeg((i-1)×nregion+6) = kdeg_freshwater(i) L: kdeg((i-1)×nregion+7) = kdeg_sed(i) L: kdeg((i-1)×nregion+8) = kdeg_saltlake(i) L: kdeg((i-1)×nregion+9) = kdeg_saltlakesed(i) L: kdeg((i-1)×nregion+10) = kdeg_freshwater(i) S: kdeg((i-1)×nregion+11) = kdeg_seawater(i) S: kdeg((i-1)×nregion+12) = kdeg_seased(i)	
	L: ADV_outside((i-1)×nregion+5) = ADV_river_outside(i) L: ADV_outside((i-1)×nregion+6) = ADV_lake_outside(i) L: ADV_outside((i-1)×nregion+7) = ADV_lakesed_outside(i) L: ADV_outside((i-1)×nregion+9) = ADV_saltlakesed_outside(i) L: ADV_outside((i-1)×nregion+11) = ADV_seawater_outside(i) L: ADV_outside((i-1)×nregion+12) = ADV_seased_outside(i)	

Number	Equation	Reference*
	EMIS((i-1)×nregion+1) =to_air(i) L: EMIS((i-1)×nregion+2) =to_nat(i) L: EMIS((i-1)×nregion+3) =to_agr(i) L: EMIS((i-1)×nregion+4) =to_urb(i) L: EMIS((i-1)×nregion+5) =to_river(i) L: EMIS((i-1)×nregion+6) =to_lake(i) L: EMIS((i-1)×nregion+8) =to_saltlake(i) S: EMIS((i-1)×nregion+11) =to_seawater(i)	
	$\text{Abig(i,j)}=\begin{cases}\sum_{k\neq j}\left(\text{-ADV(k,j)-DIFF(k,j)}\right)\text{-kdeg(j)}\times\text{V(j)-ADV\_outside(j)} & \text{i=j}\\ \text{ADV(i,j)+DIFF(i,j)} & \text{i} \neq \text{j}\end{cases}$ [Abig, ADV, DIFF, kdeg, V, ADV_outside]	
	$\text{CONC(i)}=-\sum_{j}\text{Abig}^{-1}\text{(i,j)}\times\text{EMIS(j)}$ [CONC, Abig, EMIS]	
	MASS(i)=CONC(i) ×V(i)	
ENVIRONMENTAL CONCENTRATIONS		

Number	Equation	Reference*
	C_air(i) = CONC((i-1)×nregion+1) L: C_nat(i) = CONC((i-1)×nregion+2) L: C_agr(i) = CONC((i-1)×nregion+3) L: C_urb(i) = CONC((i-1)×nregion+4) L: C_river(i) = CONC((i-1)×nregion+5) L: C_lake(i) = CONC((i-1)×nregion+6) L: C_lakesed(i) = CONC((i-1)×nregion+7) L: C_saltlake(i) = CONC((i-1)×nregion+8) L: C_saltlakesed(i) = CONC((i-1)×nregion+9) L: C_groundwater(i) = CONC((i-1)×nregion+10) S: C_seawater(i) = CONC((i-1)×nregion+11) S: C_seased(i) = CONC((i-1)×nregion+12)	
HUMAN EXPOSURE PARAMETERS		
	L: V_river*(1-Friver_frozen)+V_lake = 0: C_freshwaterfish=0 L: C_freshwaterfish = BCF_fish*(C_river*V_river*(1-Friver_frozen)+C_lake*V_lake)/ (V_river*(1-Friver_frozen)+V_lake)	EU2 (III-132)
	$\text{C\_freshwaterfishimp}=\frac{\sum_{j\in L}\text{C\_freshwaterfish(j)}\times\text{EXPORT\_freshwaterfish(j)}}{\sum_{j\in L}\text{EXPORT\_freshwaterfish(j)}}$ [C_freshwaterfishimp, C_freshwaterfish, EXPORT_freshwaterfish]	GLOBOX
	S: organic, gas: C_seafish = BCF_fish*C_seawater S: metal: C_seafish = BCF_fish*C_seawater*ACTCOEFF*FREEIONseawater S: gas: C_seafish = 0	EU2 (III-132)

Number	Equation	Reference*
	$C\_seafishaverage=\frac{\sum_{j\in S} C\_seafish(j)\times CATCH\_seafish(j)}{\sum_{j\in S} CATCH\_seafish(j)}$ [C_seafishaverage, C_seafish, CATCH_seafish]	GLOBOX
	L: C_leafcrops = (BCFsoil_leafcrops*C_agr)+ (BCFair_leafcrops*C_air)	EU2 (III-132)
	$C\_leafcropsimp=\frac{\sum_{j\in L} C\_leafcrops(j)\times EXPORT\_leafcrops(j)}{\sum_{j\in L} EXPORT\_leafcrops(j)}$ [C_leafcropsimp, C_leafcrops, EXPORT_leafcrops]	GLOBOX
	L: C_rootcrops = BCF_rootcrops*C_agr	EU2 (III-130)
	$C\_rootcropsimp=\frac{\sum_{j\in L} C\_rootcrops(j)\times EXPORT\_rootcrops(j)}{\sum_{j\in L} EXPORT\_rootcrops(j)}$ [C_rootcropsimp, C_rootcrops, EXPORT_rootcrops]	GLOBOX
	L: C_grass = (BCFsoil_leafcrops*C_nat)+ (BCFair_leafcrops*C_air)	EU2 (III-127/132)
	L: C_meat = BCF_meat*C_grass*ICdwt_grass*CONVgrass+C_agr*ICdwt_soil*CONVagr+C_air*IC_air	EU2 (III-134)
	$C\_meatimp=\frac{\sum_{j\in L} C\_meat(j)\times EXPORT\_meat(j)}{\sum_{j\in L} EXPORT\_meat(j)}$ [C_meatimp, C_meat, EXPORT_meat]	GLOBOX
	L: C_dairy = BCF_milk*C_grass*ICdwt_grass*CONVgrass+C_agr*ICdwt_soil*CONVagr+C_air*IC_air	EU2 (III-134)

Number	Equation	Reference*
	$C\_dairyimp=\frac{\sum_{j\in L} C\_dairy(j)\times EXPORT\_dairy(j)}{\sum_{j\in L} EXPORT\_dairy(j)}$ [C_dairyimp, C_dairy, EXPORT_dairy]	GLOBOX
	organic: log(Kow)≤4: fac1a = 1 organic: 4< log(Kow) ≤5: fac1a = 1/4 organic: log(Kow)>5: fac1a = 1/16	EU2 (III-135)
	organic: log(Kow)≤4: fac2a = 1 organic: 4< log(Kow) ≤ 5: fac2a = 1/2 organic: if log(Kow)>5: fac2a = 1/4	EU2 (III-135)
	organic: HENRY≤100: fac1b = 1 organic: HENRY>100: fac1b = 1/2	EU2 (III-135)
	organic: HENRY≤100: fac2b = 1 organic: HENRY>100: fac2b = 1/2	EU2 (III-135)
	organic: fac1c = 1	EU2 (III-135)
	organic: DT50bio_freshwater>10*24*3600: fac2c = 1 organic: DT50bio_freshwater≤10*24*3600: fac2c = 1/4	EU2 (III-135)
	organic: PURFsys1 = fac1a*fac1b*fac1c	EU2 (III-135)
	organic: PURFsys2 = fac2a*fac2b*fac2c	EU2 (III-135)
	organic: PURFsys1>PURFsys2: PURFsurfacew = PURFsys1 organic: PURFsys1≤PURFsys2: PURFsurfacew = PURFsys2 gas, metal: PURFsurfacew=0	EU2 (III-136)
	organic, gas: PURFgroundw = 1 metal: PURFgroundw = 0	
	L: C_purfgroundw=PURFgroundw*Fdiss_inlandwater*C_groundw	EU2 (III-136)
	L: V_river*(1-Friver_frozen)+V_lake = 0: C_purfsurfacew=0 L: V_river+V_lake > 0: C_purfsurfacew=PURFsurfacew*Fdiss_inlandwater*(C_river*V_river*(1-Friver_frozen)+C_lake*V_lake)/(V_river*(1-Friver_frozen)+V_lake)	EU2 (III-136)

Number	Equation	Reference*
	L: V_river*(1-Friver_frozen)+V_lake = 0: C_drw = Fdrw_safe*C_purfgroundw+(1-Fdrw_safe) *Fdiss_inlandwater *C_groundwater L: V_river+V_lake > 0: $C\_drw=\left(Fdrw\_grw\times\left(Fdrw\_safe\times C\_purfgroundw+\left(1\text{-}Fdrw\_safe\right)\times Fdiss\_inlandwater\times C\_groundwater\right)\right)+$ $\left(\left(1\text{-}Fdrw\_grw\right)\times\left(Fdrw\_safe\times C\_purfsurfacew+\left(1\text{-}Fdrw\_safe\right)\times Fdiss\_inlandwater\times\frac{C\_river\times V\_river\times\left(1\text{-}Friver\_frozen\right)}{V\_river\times\left(1\text{-}Friver\_frozen\right)}\right.\right.$ [C_drw, Fdrw_grw, Fdrw_safe, C_purfgroundw, Fdiss_inlandwater, C_groundwater, C_purfsurfacew, C_river, V_river, Friver_frozen, C_lake, V_lake]	EU2 (III-136) (mod)
	L: DOSE_drw = C_drw*IH_drw/BW	
	L: EXP_x-PROD_x>0: REEXP_x = EXP_x-PROD_x L: EXP_x-PROD_x<0: REEXP_x = 0	
	L: $DOSE\_x=\frac{IH\_x}{BW}\left(C\_x\times\frac{PROD\_x\text{-}EXP\_x}{PROD\_x\text{-}EXP\_x+IMP\_x}+C\_ximp\times\frac{IMP\_x}{PROD\_x\text{-}EXP\_x+IMP\_x}\right)$ with x = freshwaterfish	EU2 (III-136)
	L: DOSE_seafish = C_seafishaverage*IH_seafish/BW	GLOBOX equation
	L: $DOSE\_x=\frac{IH\_x}{BW}\left(C\_x\times\frac{PROD\_x\text{-}EXP\_x}{PROD\_x\text{-}EXP\_x+IMP\_x}+C\_ximp\times\frac{IMP\_x}{PROD\_x\text{-}EXP\_x+IMP\_x}\right)$ with x = leafcrops [DOSE_leafcrops, C_leafcrops, PROD_leafcrops, EXP_leafcrops, IMP_leafcrops, C_leafcropsimp]	EU2 (III-136)
	L: $DOSE\_x=\frac{IH\_x}{BW}\left(C\_x\times\frac{PROD\_x\text{-}EXP\_x}{PROD\_x\text{-}EXP\_x+IMP\_x}+C\_ximp\times\frac{IMP\_x}{PROD\_x\text{-}EXP\_x+IMP\_x}\right)$ with x = rootcrops [DOSE_rootcrops, C_rootcrops, PROD_rootcrops, EXP_rootcrops, IMP_rootcrops, C_rootcropsimp]	EU2 (III-136)
	L: $DOSE\_x=\frac{IH\_x}{BW}\left(C\_x\times\frac{PROD\_x\text{-}EXP\_x}{PROD\_x\text{-}EXP\_x+IMP\_x}+C\_ximp\times\frac{IMP\_x}{PROD\_x\text{-}EXP\_x+IMP\_x}\right)$ with x = meat [DOSE_meat, C_meat, PROD_meat, EXP_meat, IMP_meat, C_meat]	EU2 (III-136)

Number	Equation	Reference*
	L: $DOSE\_x=\frac{IH\_x}{BW}\left(C\_x\times\frac{PROD\_x\text{-}EXP\_x}{PROD\_x\text{-}EXP\_x+IMP\_x}+C\_ximp\times\frac{IMP\_x}{PROD\_x\text{-}EXP\_x+IMP\_x}\right)$ with x = dairy [DOSE_dairy, C_dairy, PROD_dairy, EXP_dairy, IMP_dairy, C_dairy]	EU2 (III-136)
	L: DOSE_totaloral = DOSE_drw+DOSE_freshwaterfish+DOSE_seafish+DOSE_leafcrops+DOSE_rootcrops+DOSE_meat+DOSE_dairy	EU2 (III-136)
	L: DOSE_air = (F_resp*IH_air/BW)*(BIO_inh/BIO_oral)*C_air	EU2 (III-136)
	L: DOSE_total = DOSE_totaloral+DOSE_air	EU2 (III-136)
	$INTAKE\_drw=\sum_{j\in L} DOSE\_drw(j)\times BW(j)\times Npop(j)$ [INTAKE_drw, DOSE_drw, BW, Npop]	
	$INTAKE\_freshwaterfish=\sum_{j\in L} DOSE\_freshwaterfish(j)\times BW(j)\times Npop(j)$ [INTAKE_freshwaterfish, DOSE_freshwaterfish, BW, Npop]	
	$INTAKE\_seafish=\sum_{j\in L} DOSE\_seafish(j)\times BW(j)\times Npop(j)$ [INTAKE_seafish, DOSE_seafish, BW, Npop]	
	$INTAKE\_leafcrops=\sum_{j\in L} DOSE\_leafcrops(j)\times BW(j)\times Npop(j)$ [INTAKE_leafcrops, DOSE_leafcrops, BW, Npop]	
	$INTAKE\_rootcrops=\sum_{j\in L} DOSE\_rootcrops(j)\times BW(j)\times Npop(j)$ [INTAKE_rootcrops, DOSE_rootcrops, BW, Npop]	
	$INTAKE\_meat=\sum_{j\in L} DOSE\_meat(j)\times BW(j)\times Npop(j)$ [INTAKE_meat, DOSE_meat, BW, Npop]	
	$INTAKE\_dairy=\sum_{j\in L} DOSE\_dairy(j)\times BW(j)\times Npop(j)$ [INTAKE_dairy, DOSE_dairy, BW, Npop]	

Number	Equation	Reference*
	$INTAKE\_totaloral=\sum_{j\in L} DOSE\_totaloral(j)\times BW(j)\times Npop(j)$ [INTAKE_totaloral, DOSE_totaloral, BW, Npop]	
	$INTAKE\_air=\sum_{j\in L} DOSE\_air(j)\times BW(j)\times Npop(j)$ [INTAKE_air, DOSE_air, BW, Npop]	
	$INTAKE\_total=\sum_{j\in L} DOSE\_total(j)\times BW(j)\times Npop(j)$ [INTAKE_total, DOSE_total, BW, Npop]	
	L: iF = DOSE_total*BW*Npop/EMIS	
	iFtot = INTAKE_total/EMIS	
INTEGRATED RISK PARAMETERS		
	L: RCRtox_river = C_river*EFFECT_aquatox	
	L: RCRtox_lake = C_lake*EFFECT_aquatox	EU2 (III-186)
	L: RCRtox_saltlake = C_saltlake*EFFECT_aquatox	
	L: RCRtox_soil = ((C_nat*V_nat+C_agr*V_agr+C_urb*V_urb)/(V_nat+V_agr+V_urb))*EFFECT_terrtox	EU2 (III-187)
	L: RCRtox_lakesed = C_lakesed*EFFECT_sedtox	
	L: RCRtox_saltlakesed = C_saltlakesed*EFFECT_sedtox	
	S: organic, gas: RCRtox_seawater = C_seawater*EFFECT_marinetox S: metal: RCRtox_seawater = C_seawater*ACTCOEFF*FREEIONseawater*EFFECT_marinetox	
	S: organic, gas: RCRatox_seased = C_seased*EFFECT_seasedtox S: metal: RCRtox_seased = C_seased*ACTCOEFF*FREEIONseawater *EFFECT_seasedtox	
	L: RCRtox_humnoncarc = DOSE_total*EFFECThum_noncarc	
	L: RCRtox_humcarc = DOSE_total*EFFECThum_carc	EU1 (III-110)
LCA CHARACTERISATION FACTORS FOR COMBINED POTENTIAL IMPACTS		

Number	Equation	Reference*
	$\text{IPICRtox\_river}=\frac{\sum_{\text{jÎL}}\text{RCRtox\_river(j)}\times\text{V\_river(j)}\times\left(\text{1-Friver\_frozen(j)}\right)}{\sum_{\text{jÎL}}\text{V\_river(j)}\times\left(\text{1-Friver\_frozen(j)}\right)}$ [IPICRtox_river, RCRtox_river, V_river, Friver_frozen]	
	$\text{IPICRtox\_lake}=\frac{\sum_{j\in L}\text{RCRtox\_lake(j)}\times\text{V\_lake(j)}}{\sum_{j\in L}\text{V\_lake(j)}}$ [IPICRtox_lake, RCRtox_lake, V_lake]	
	$\text{IPICRtox\_saltlake}=\frac{\sum_{j\in L}\text{RCRtox\_saltlake(j)}\times\text{V\_saltlake(j)}}{\sum_{j\in L}\text{V\_saltlake(j)}}$ [IPICRtox_saltlake, RCRtox_saltlake, V_saltlake]	
	$\text{IPICRtox\_seawater}=\frac{\sum_{j\in S}\text{RCRtox\_seawater(j)}\times\text{V\_sea(j)}}{\sum_{j\in S}\text{V\_sea(j)}}$ [IPICRtox_seawater, RCRtox_seawater, V_sea]	
	$\text{IPICRtox\_soil}=\frac{\sum_{j\in L}\text{RCRtox\_soil(j)}\times\left(\text{V\_nat(j)+V\_agr(j)+V\_urb(j)}\right)}{\sum_{j\in L}\left(\text{V\_nat(j)+V\_agr(j)+V\_urb(j)}\right)}$ [IPICRtox_soil, RCRtox_soil, V_nat, V_agr, V_urb]	

Number	Equation	Reference*
	$IPICRtox\_lakesed=\frac{\sum_{j\in L} RCRtox\_lakesed(j)\times V\_lakesed(j)}{\sum_{j\in L} V\_lakesed(j)}$ [IPICRtox_lakesed, RCRtox_lakesed, V_lakesed]	
	$IPICRtox\_saltlakesed=\frac{\sum_{j\in L} RCRtox\_saltlakesed(j)\times V\_saltlakesed(j)}{\sum_{j\in L} V\_saltlakesed(j)}$ [IPICRtox_saltlakesed, RCRtox_saltlakesed, V_saltlakesed]	
	$IPICRtox\_seased=\frac{\sum_{j\in S} RCRtox\_seased(j)\times V\_seased(j)}{\sum_{j\in S} V\_seased(j)}$ [IPICRtox_seased, RCRtox_seased, V_seased]	
	$IPICRtox\_humnoncarc=\frac{\sum_{j\in L} RCRtox\_humnoncarc(j)\times Npop(j)}{\sum_{j\in L} Npop(j)}$ [IPICRtox_humnoncarc, RCRtox_humnoncarc, N_pop]	
	$IPICRtox\_humcarc=\frac{\sum_{j\in L} RCRtox\_humcarc(j)\times Npop(j)}{\sum_{j\in L} Npop(j)}$ [IPICRtox_humcarc, RCRtox_humcarc, N_pop]	
	CFtoxpot_river = IPICRtox_river/IPICRtox_river(ref) with ref = {reference susbtance, emission region, and emission compartment}	
	CFtoxpot_lake = IPICRtox_lake/IPICRtox_lake(ref) with ref = {reference susbtance, emission region, and emission compartment}	

Number	Equation	Reference*
	CFtoxpot_saltlake = IPICRsaltlake_river/IPICRtox_saltlake(ref) with ref = {reference susbtance, emission region, and emission compartment}	
	CFtoxpot_seawater = IPICRtox_seawater/IPICRtox_seawater(ref) with ref = {reference susbtance, emission region, and emission compartment}	
	CFtoxpot_soil = IPICRtox_soil/IPICRtox_soil(ref) with ref = {reference susbtance, emission region, and emission compartment}	
	CFtoxpot_lakesed = IPICRtox_lakesed/IPICRtox_lakesed(ref) with ref = {reference susbtance, emission region, and emission compartment}	
	CFtoxpot_saltlakesed = IPICRtox_saltlakesed/IPICRtox_saltlakesed(ref) with ref = {reference susbtance, emission region, and emission compartment}	
	CFtoxpot_seased = IPICRtox_seased/IPICRtox_seased(ref) with ref = {reference susbtance, emission region, and emission compartment}	
	CFtoxpot_humnoncarc = IPICRtox_humnoncarc/IPICRtox_humnoncarc(ref) with ref = {reference susbtance, emission region, and emission compartment	
	CFtoxpot_humcarc = IPICRtox_humcarc/IPICRtox_humcarc(ref) with ref = {reference susbtance, emission region, and emission compartment	
LCA CHARACTERISATION FACTORS FOR ACTUAL IMPACTS		
	$IAICRtox\_river=\frac{\sum_{j\hat{I}L} RCRtox\_river(j)\times SFtox\_river(j)\times TFtox\_river(j)\times V\_river(j)}{\sum_{j\hat{I}L} V\_river(j)}$ [IAICRtox_river, RCRtox_river, SFtox_river, TFtox_river, V_river]	
	$IAICRtox\_lake=\frac{\sum_{j\in L} RCRtox\_lake(j)\times SFtox\_lake(j)\times TFtox\_lake(j)\times V\_lake(j)}{\sum_{j\in L} V\_lake(j)}$ [IAICRtox_lake, RCRtox_lake, SFtox_lake, TFtox_lake, V_lake]	

Number	Equation	Reference*
	$$\text{IAICRtox\_saltlake}=\frac{\sum_{j\in L}\text{RCRtox\_saltlake(j)}\times\text{SFtox\_saltlake(j)}\times\text{TFtox\_saltlake(j)}\times\text{V\_saltlake(j)}}{\sum_{j\in L}\text{V\_saltlake(j)}}$$ [IAICRtox_saltlake, RCRtox_saltlake, SFtox_saltlake, TFtox_saltlake, V_saltlake]	
	$$\text{IAICRtox\_seawater}=\frac{\sum_{j\in S}\text{RCRtox\_seawater(j)}\times\text{SFtox\_seawater(j)}\times\text{TFtox\_seawater(j)}\times\text{V\_sea(j)}}{\sum_{j\in S}\text{V\_sea(j)}}$$ [IAICRtox_seawater, RCRtox_seawater, SFtox_seawater, TFtox_seawater, V_sea]	
	$$\text{IAICRtox\_soil}=\frac{\sum_{j\in L}\text{RCRtox\_soil(j)}\times\text{SFtox\_soil(j)}\times\left(\text{TFtox\_nat(j)}\times\text{V\_nat(j)}+\text{TFtox\_agr(j)}\times\text{V\_agr(j)}+\text{TFtox\_urb(j)}\times\text{V\_urb(j)}\right)}{\sum_{j\in L}\left(\text{V\_nat(j)}+\text{V\_agr(j)}+\text{V\_urb(j)}\right)}$$ [IAICRtox_soil, RCRtox_soil, SFtox_soil, TFtox_nat, TFtox_agr, TFtox_urb, V_nat, V_agr, V_urb]	
	$$\text{IAICRtox\_lakesed}=\frac{\sum_{j\in L}\text{RCRtox\_lakesed(j)}\times\text{SFtox\_lakesed(j)}\times\text{TFtox\_lakesed(j)}\times\text{V\_lakesed(j)}}{\sum_{j\in L}\text{V\_lakesed(j)}}$$ [IAICRtox_lakesed, RCRtox_lakesed, SFtox_lakesed, TFtox_lakesed, V_lakesed]	
	$$\text{IAICRtox\_saltlakesed}=\frac{\sum_{j\in L}\text{RCRtox\_saltlakesed(j)}\times\text{SFtox\_saltlakesed(j)}\times\text{TFtox\_saltlakesed(j)}\times\text{V\_saltlakesed(j)}}{\sum_{j\in L}\text{V\_saltlakesed(j)}}$$ [IAICRtox_saltlakesed, RCRtox_saltlakesed, SFtox_saltlakesed, TFtox_saltlakesed, V_saltlakesed]	
	$$\text{IAICRtox\_seased}=\frac{\sum_{j\in S}\text{RCRtox\_seased(j)}\times\text{SFtox\_seased(j)}\times\text{TFtox\_seased(j)}\times\text{V\_seased(j)}}{\sum_{j\in S}\text{V\_seased(j)}}$$ [IAICRtox_seased, RCRtox_seased, SFtox_seased, TFtox_seased, V_seased]	

Number	Equation	Reference*
	$IAICRtox\_humnoncarc=\frac{\sum_{j\in L} RCRtox\_humnoncarc(j)\times TFtox\_humnoncarc(j)\times Npop(j)}{\sum_{j\in L} Npop(j)}$ [IAICRtox_humnoncarc, RCRtox_humnoncarc, TFtox_humnoncarc, N_pop]	
	$IAICRtox\_humcarc=\frac{\sum_{j\in L} RCRtox\_humcarc(j)\times Npop(j)}{\sum_{j\in L} Npop(j)}$ [IAICRtox_humcarc, RCRtox_humcarc, N_pop]	
	CFtoxact_river = IEACRtox_river/IPICRtox_river(ref) with ref = {reference susbtance, emission region, and emission compartment}	
	CFtoxact_lake = IEACRlake_river/IPICRtox_lake(ref) with ref = {reference susbtance, emission region, and emission compartment}	
	CFtoxact_saltlake = IEACRsaltlake_river/IPICRtox_saltlake(ref) with ref = {reference susbtance, emission region, and emission compartment}	
	CFtoxact_seawater = IEACRtox_seawater/IPICRtox_seawater(ref) with ref = {reference susbtance, emission region, and emission compartment}	
	CFtoxact_soil = IEACRtox_soil/IPICRtox_soil(ref) with ref = {reference susbtance, emission region, and emission compartment}	
	CFtoxact_lakesed = IAICRtox_lakesed/IPICRtox_lakesed(ref) with ref = {reference susbtance, emission region, and emission compartment}	
	CFtoxact_saltlakesed = IAICRtox_saltlakesed/IPICRtox_saltlakesed(ref) with ref = {reference susbtance, emission region, and emission compartment}	
	CFtoxact_seased = IAICRtox_seased/IPICRtox_seased(ref) with ref = {reference susbtance, emission region, and emission compartment}	
	CFtoxact_humnoncarc = IAICRtox_humnoncarc/IPICRtox_humnoncarc(ref) with ref = {reference susbtance, emission region, and emission compartment}	
	CFtoxact_humcarc = IAICRtox_humcarc/IPICRtox_humcarc(ref) with ref = {reference susbtance, emission region, and emission compartment}	

*Legend: U1 = USES 1.0 (+ page number); U2 = USES 2.0 (+ page number); EU1 = EUSES 1.00 (+ page number); EU II = EUSES 2.0 (+ page number); SB2 = SimpleBox 2.0 (+ page number); input = to be provided by the user; references: sea reference list below.

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