CalTOX™ 1.5: Seven-Compartment Multimedia Exposure Model

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Inputs:

Chemical name	Styrene
Site name	site name

Toxicity Criteria

	Cancer potencies 1/(mg/kg-d)	Non-cancer ADIs (mg/kg-d)
Inhalation	0.0 E+00	0.3
Ingestion	0.0 E+00	0.2
Dermal	0.0 E+00	0.2
Total dose		0

	Risk	Hazard quotient
Target Risk/Hazard =	1.0 E-06	1.00

Time after measured concentrations when exposure begins	3.65E+02 days

Measured Concentrations (at time = 0)

Root-zone soil	1	ppm (mg/kg)
Vadose-zone soil	0.1	ppm (mg/kg)
Ground water	n/a	ppm (mg/L)

Continuous inputs

Source term to air (mol/d)	0.0 E+00	Sa
Source term to ground-surface soil (mol/d)	0.0 E+00	Sg
Source term to surface water(mol/d)	0.0 E+00	Sw

Constants

Gas Constant (Pa-m^3/mol-K)	8.31E+00	Rgas

Outputs:

Target Soil Concentrations (in ppm)

Based on cancer risk:

	w/o b-milk	w b-milk
Root soil	n/a	n/a
Vadose soil	n/a	n/a

Based on hazard

	Adult	Infant
Root soil	>conc limit	>conc limit
Vadose soil	5.1 E+2	>conc limit

root soil	n/a
vadose soil	5.1 E+2

Un-mitigated risk and/or hazard ratio

Risk	0.0 E+0	0.0 E+0
Hazard ratio	2.0 E-3	6.6 E-6

Concentration limits (ppm-solid) without NAPL

Root soil	2651.04
Vadose soil	2079.53
Sediments	4449.57

Concentrations in environmental media

Air	8.5 E-19	mg/m3
Plants	8.3 E-16	mg/kg(FM)
Grnd-surface soil	1.4 E-17	mg/kg(total)
Root-zone soil	1.8 E-15	mg/kg(total)
Vadose-zone soil	3.3 E-06	mg/kg(total)
Ground water	4.2 E-07	mg/L(water)
Surface water	8.8 E-20	mg/L
Sediment	6.9 E-19	mg/kg

Chemical properties

Compound name	Styrene		0.00297	0.003	5.1 E+2	1	5.1 E+04
			Value used	Mean value	Coeff. Var.	Adjustment	Notes
Molecular weight (g/mol)		MW	1.04 E+02	1.04 E+02	0.0090271	1	
Octanol-water partition coefficient		Kow	8.92 E+02	8.92 E+02	0.338565	1	
Melting point (K)		Tm	2.43 E+02	2.43 E+02	0.028	1	
Vapor Pressure in (Pa)		VP	8.32 E+02	8.32 E+02	0.0380024	1	
Solubility in mol/m3		S	2.55 E+00	2.55 E+00	0.2451128	1	
Henry's law constant (Pa-m^3/mol)		**H -**	3.26 E+02	-99	0.46	1	
Diffusion coefficient in pure air (m2/d)		Dair	6.13 E-01	6.13 E-01	0.08	1	7.10 E-06
Diffusion coefficient; pure water (m2/d)		Dwater	7.92 E-05	7.92 E-05	0.25	1	9.16 E-10
Organic carbon partition coefficient Koc		**Koc -**	9.12 E+02	912	0.85	1	m^2/s
Partition coefficient in ground/root soil layer		**Kd_s -**	1.09 E+01	-99	0.1	A parameter with a "-" symbol after it, indicates a parameter that can be calculated by a default algoritm when **the value of mean for this parameter is <0**. Otherwise the liste value is	
Partition coefficient in vadose-zone soil layer		**Kd_v -**	9.12 E+00	-99	0.1		
Partition coefficient in aquifer layer		**Kd_q -**	n/a	-99	0.1		
Partition coeffic. in surface wtr sediments		**Kd_d -**	1.82 E+01	-99	0.1		
Prtn cff. plnt(abv-grd)/sl (kg[s]/kg[pFM])		**Kps -**	1.52 E-01	-99	4		
Biotrnsfr fctr, plant/air (m3[a]/kg[pFM])		**Kpa -**	6.78 E-02	-99	14		
Biotransfer factor; cattle-diet/milk (d/L)		**Bk -**	7.09 E-06	-99	11		
Biotransfer factor; cattle-diet/meat (d/L)		**Bt -**	2.24 E-05	-99	13		
Biotransfer factor; hen-diet/eggs (d/L)		**Be -**	1.41 E-04	-99	14		
Biotrnsfr fctr; brst mlk/mthr intake (d/kg)		**Bbmk -**	1.78 E-04	-99	10		
Bioconcentration factor; fish/water		**BCF -**	4.28 E+01	-99	0.6		
Skin permeability coefficient; cm/h		**Kp_w -**	1.69 E-01	-99	2.4		
Skin-water partition coefficient		**Km -**	5.80 E+01	-99	1.3		
Reaction half-life in air (d)		Thalf_a	1.71 E-01	1.7 E-01	1		
Reaction half-life in surface soil (d)		Thalf_g	4.50 E+01	4.5 E+01	1.1	1	
Reaction half-life in root-zone soil (d)		Thalf_s	4.50 E+01	4.5 E+01	1.2	1	
Reaction half-life in vadose-zone soil (d)		Thalf_v	1.19 E+02	1.2 E+02	1	1	
Reaction half-life in ground water (d)		Thalf_q	n/a	1.2 E+02	1.3	1	
Reaction half-life in surface water (d)		Thalf_w	2.10 E+01	2.1 E+01	1.2	1	
Reaction half-life in sediments (d)		Thalf_d	6.30 E+01	6.3 E+01	1.4	1	

Landscape properties

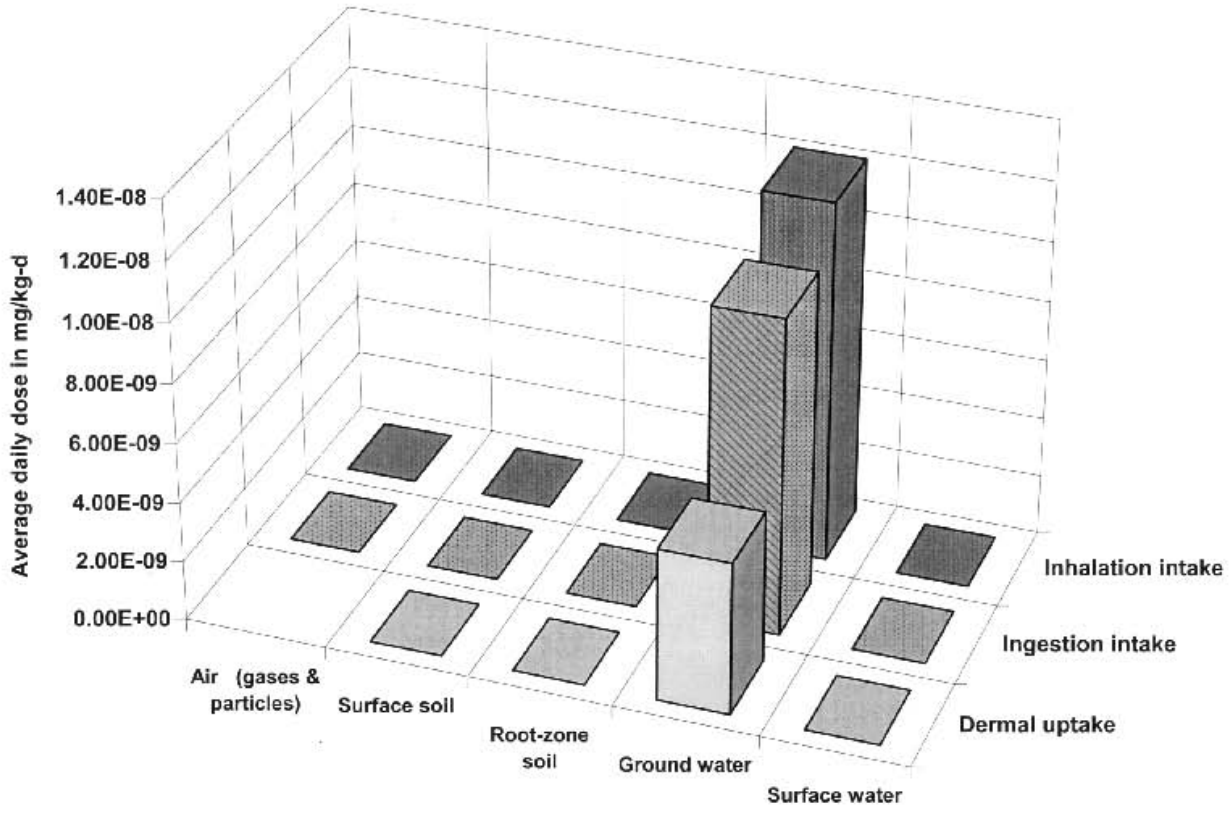
site name	site name	Value used	Mean value	Coeff. Var.	Adjustment	Notes
contaminated area in m2	Area	1.00 E+06	1.00 E+06	0.1	1	(m/y)
annual average precipitation (m/d)	rain	1.01 E-03	1.01 E-03	0.3	1	3.68 E-01
flux; surface water into landscape (m/d)	inflow	0.00 E+00	0.00 E+00	0.1	1	0.00 E+00
land surface runoff (m/d)	runoff	2.80 E-04	2.80 E-04	0.3	1	1.02 E-01
atmospheric dust load (kg/m3)	rhob_a	6.15 E-08	6.15 E-08	0.2	1	
deposition velocity of air particles (m/d)	v_d	5.00 E+02	5.00 E+02	0.3	1	
plant dry mass inventory (kg[DM]/m2)	bio_inv	7.00 E-01	7.00 E-01	0.2	1	
plant dry-mass fraction	bio_dm	2.00 E-01	2.00 E-01	0.2	1	
plant fresh-mass density kg/m^3	rho_p	1.00 E+03	1.00 E+03	0.2	1	
ground-water recharge (m/d)	recharge	2.00 E-04	2.00 E-04	1	1	7.30 E-02
evaporation of water from surface wtr (m/d)	evaporate	4.38 E-06	4.38 E-06	1	1	
thickness of the ground soil layer (m)	d_g	1.00 E-02	1.00 E-02	0.1	1	
soil particle density (kg/m3)	rhos_s	2.60 E+03	2.60 E+03	0.05	1	
water content in surface soil (vol fraction)	beta_g	1.00 E-01	1.00 E-01	0.2	1	
air content in the surface soil (vol frctn)	alpha_g	2.00 E-01	2.00 E-01	0.2	1	cm/y
erosion of surface soil (kg/m2-d)	erosion_g	3.00 E-04	3.00 E-04	0.2	1	0.00575
thickness of the root-zone soil (m)	d_s	2.00 E+00	2.00 E+00	0.1	1	
water content of root-zone soil (vol. frctn.)	beta_s	2.00 E-01	2.00 E-01	0.2	1	
air content of root-zone soil (vol. frctn.)	alpha_s	1.00 E-01	1.00 E-01	0.2	1	
thickness of the vadose-zone soil (m)	d_v	5.00 E+00	5.00 E+00	0.1	1	
water content; vadose-zone soil (vol. frctn.)	beta_v	3.00 E-01	3.00 E-01	0.2	1	
air content of vadose-zone soil (vol. frctn.)	alpha_v	1.00 E-01	1.00 E-01	0.2	1	
thickness of the aquifer layer (m)	d_q	n/a	3.00 E+00	0.1	1	
solid material density in aquifer (kg/m3)	rhos_q	n/a	2.60 E+03	0.05	1	
porosity of the aquifer zone	beta_q	n/a	2.00 E-01	0.2	1	
fraction of land area in surface water	f_arw	8.15 E-03	8.15 E-03	0.2	1	
average depth of surface waters (m)	d_w	5.00 E+00	5.00 E+00	1	1	
suspended sedmnt in surface wtr (kg/m3)	rhob_w	8.00 E-01	8.00 E-01	1	1	

Landscape properties (continued)

site name	site name	Value used	Mean value	Coeff. Var.	Adjustment	Notes
suspended sdmnt deposition (kg/m2/d)	deposit	1.05 E+01	1.05 E+01	0.3	1	(m/s)
thickness of the sediment layer (m)	d_d	5.00 E-02	5.00 E-02	1	1	
solid material density in sediment (kg/m3)	rhos_d	2.60 E+03	2.60 E+03	0.05	1	
porosity of the sediment zone	beta_d	2.00 E-01	2.00 E-01	0.2	1	m/y
sediment burial rate (m/d)	bury_d	4.00 E-06	4.00 E-06	5	1	1.46 E-03
ambient environmental temperature (K)	Temp	2.83 E+02	2.83 E+02	0.05	1	(m/s)
Surface water current in m/d	current_w	0.00 E+00	0.00 E+00	1	1	0.00 E+00
organic carbon fraction in upper soil zone	foc_s	1.20 E-02	1.20 E-02	1	1	
organic carbon fraction in vadose zone	foc_v	1.00 E-02	1.00 E-02	1	1	
organic carbon fraction in aquifer zone	foc_q	n/a	1.00 E-02	1	1	
organic carbon fraction in sediments	foc_d	2.00 E-02	2.00 E-02	1	1	
bndry lyr thickness in air above soil (m)	del_ag	5.00 E-03	5.00 E-03	0.2	1	(m/s)
yearly average wind speed (m/d)	v_w	1.50 E+05	1.50 E+05	0.2	1	1.74 E+00

Human Exposure Factors (Residential)		Value used	Mean value	Coeff. Var.	Adjustment	Notes
Body weight (kg)	BW	6.20 E+01	6.20 E+01	0.2	1	
Surface area (m2/kg)	SAb	2.60 E-02	2.60 E-02	0.07	1	
Active breathing rate (m3/kg-h)	BRa	1.90 E-02	1.90 E-02	0.3	1	
Resting breathing rate (m3/kg-h)	BRr	6.40 E-03	6.40 E-03	0.2	1	
Fluid Intake (L/kg-d)	Ifl	2.20 E-02	2.20 E-02	0.2	1	
Fruit and vegetable intake (kg/kg-d)	Ifv	4.90 E-03	4.90 E-03	0.2	1	
Grain intake (kg/kg-d)	Ig	3.70 E-03	3.70 E-03	0.2	1	
Milk intake (kg/kg-d)	Imk	6.50 E-03	6.50 E-03	0.2	1	
Meat intake (kg/kg-d)	Imt	3.00 E-03	3.00 E-03	0.2	1	
Egg intake (kg/kg-d)	Iegg	4.60 E-04	4.60 E-04	0.3	1	
Fish intake (kg/kg-d)	Ifsh	2.90 E-04	2.90 E-04	0.4	1	
Soil ingestion (kg/kg-d)	Isl	3.50 E-07	3.50 E-07	3	1	
Breast milk ingestion by infants (kg/kg-d)	Ibm	1.10 E-01	1.10 E-01	0.2	1	
Inhalation by cattle (m3/d)	Inc	1.22 E+02	1.22 E+02	0.3	1	
Inhalation by hens (m3/d)	Inh	2.20 E+00	2.20 E+00	0.3	1	
Ingestion of pasture, dairy cattle (kg[FM]/d)	Ivdc	8.50 E+01	8.50 E+01	0.2	1	
Ingestion of pasture, beef cattle (kg[FM]/d)	Ivbc	6.00 E+01	6.00 E+01	0.4	1	
Ingestion of pasture by hens (kg[FM]/d)	Ivh	1.20 E-01	1.20 E-01	0.04	1	
Ingestion of water by dairy cattle (L/d)	Iwdc	3.50 E+01	3.50 E+01	0.2	1	
Ingestion of water by beef cattle (L/d)	Iwbc	3.50 E+01	3.50 E+01	0.2	1	
Ingestion of water by hens (L/d)	Iwh	8.40 E-02	8.40 E-02	0.1	1	
Ingestion of soil by cattle (kg/d)	Isc	4.00 E-01	4.00 E-01	0.7	1	
Ingestion of soil by hens (kg/d)	Ish	1.30 E-05	1.30 E-05	1	1	
Fraction of water needs from ground water	fw_gw	8.00 E-01	8.00 E-01	0.1	1	
Fraction of water needs from surface water	fw_sw	2.00 E-01	2.00 E-01	0.1	1	
Frctn irrgtn wtr contamnnts trnsfrd to soil	f_ir	2.50 E-01	2.50 E-01	1	1	
Frctn frts & vgtbls that are exposed produce	fabv_grd_v	4.70 E-01	4.70 E-01	0.1	1	
Fraction of fruits and vegetables local	flocal_v	2.40 E-01	2.40 E-01	0.7	1	
Fraction of grains local	flocal_g	1.20 E-01	1.20 E-01	0.7	1	

Human Exposure Factors (continued)		Value used	Mean value	Coeff. Var.	Adjustment	Notes
Fraction of milk local	flocal_mk	4.00 E-01	4.00 E-01	0.7	1	
Fraction of meat local	flocal_mt	4.40 E-01	4.40 E-01	0.5	1	
Fraction of eggs local	flocal_egg	4.00 E-01	4.00 E-01	0.7	1	
Fraction of fish local	flocal_fsh	7.00 E-01	7.00 E-01	0.3	1	
Plant-air prttn fctr, particles, m3/kg[FM]	Kpa_part	3.30 E+03	3.30 E+03	1.8	1	
Rainsplash (mg/kg[plnt FM])/(mg/kg[soil])	rainsplash	3.40 E-03	3.40 E-03	1	1	
Water use in the shower (L/min)	Wshower	8.00 E+00	8.00 E+00	0.4	1	
Water use in the House (L/h)	Whouse	4.00 E+01	4.00 E+01	0.4	1	
Room ventilation rate, bathroom (m3/min)	VRbath	1.00 E+00	1.00 E+00	0.4	1	
Room ventilation rate, house (m3/h)	VRhouse	7.50 E+02	7.50 E+02	0.3	1	
Exposure time, in shower or bath (h/day)	ETsb	2.70 E-01	2.70 E-01	0.6	1	
Exposure time, active indoors (h/day)	ETai	8.00 E+00	8.00 E+00	0.14	1	
Exposure time, outdoors at home (h/day)	ETao	3.00 E-01	3.00 E-01	0.14	1	
Exposure time, indoors resting (h/day)	ETri	8.00 E+00	8.00 E+00	0.04	1	
Indoor dust load (kg/m^3)	dust_in	3.00 E-08	3.00 E-08	0.4	1	
Exposure frequency to soil on skin, (d/y)	EFsl	1.37 E+02	1.37 E+02	0.6	1	
Soil adherence to skin (mg/cm^2)	Slsk	5.00 E-01	5.00 E-01	0.4	1	
Ratio of indoor gas conc. to soil gas conc.	alpha_inair	1.00 E-04	1.00 E-04	2	1	
Exposure time swimming (h/d)	ETsw	5.00 E-01	5.00 E-01	0.5	1	
Exposure frequency, swimming (d/y)	EFsw	1.50 E+01	1.50 E+01	4	1	
Water ingestion while swimming (L/kg-h)	Isww	7.00 E-04	7.00 E-04	1	1	
Exposure duration (years)	ED	1.40 E+01	1.40 E+01	1.15	1	
Averaging time (days)	AT	2.56 E+04	2.56 E+04	0.1	1	


Average daily dose in mg/kg-d
1.40E-08
1.20E-08
1.00E-08
8.00E-09
6.00E-09
4.00E-09
2.00E-09
0.00E+00
Air (gases & particles)
Surface soil
Root-zone soil
Ground water
Surface water
Inhalation intake
Ingestion intake
Dermal uptake

Exposure Pathway-Include-and-Exclude Toggles

All inhalation exposures indoors active	1	Contaminant transfer, air to plants surfaces	1
All inhalation exposures indoors resting	1	Cntmnnt. transfer, grnd. soil to plant surfaces	1
Inhalation exposure in shower/bath	1	Contamnnt. transfer, root soil to plant tissues	1
Inhalation exposures outdoors active	1	On-site grazing of animals	1
Inhalation of air particles indoors	1		
Transfer of soil dust to indoor air	1	Ingestion of home-grown exposed produce	1
Transfer of soil vapors to indoor air	1	Ingestion of home-grown unexposed produce	1
On-site inhalation by animals	1	Ingestion of home-grown meat	1
		Ingestion of home-grown milk	1
Use of ground water as tap water	1	Ingestion of home-grown eggs	1
Use of surface water as tap water	1	Ingestion of locally caught fish	1
Ingestion of tap water	1	Direct soil ingestion	1
Use of ground water for irrigation	1	Soil contact exposure at home or at work	1
Use of surface water for irrigation	1	Dermal exposure during shower/bath	1
		Dermal & ingstn exposures while swimming	1
Use of ground water for feeding animals	1		
Use of surface water for feeding animals	1	Breast-milk ingestion by infants	1

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MEDIA AND CORRESPONDING POTENTIAL DOSES IN mg/kg-d (at the mean exposure time)

PATHWAYS	Air (gases & particles)	Surface soil	Root-zone soil	Ground water	Surface water	Totals	%
INHALATION	1.77E-19	8.80E-26	4.98E-19	1.21E-08	6.23E-22	**1.21E-08**	43.59
INGESTION:							
Water				7.41E-09	3.77E-22	7.41E-09	26.66
Exposed produce	5.74E-23	4.89E-23	2.93E-19	1.43E-10	7.33E-24	1.43E-10	0.51
Unexposed produce			6.41E-18	3.05E-09	1.57E-22	3.05E-09	10.98
Meat	3.15E-24	2.58E-25	5.22E-22	6.02E-13	3.10E-26	6.02E-13	0.00
Milk	1.99E-24	1.83E-25	4.60E-22	4.41E-13	2.27E-26	4.41E-13	0.00
Eggs	4.86E-26	1.58E-28	9.17E-25	1.18E-15	6.08E-29	1.18E-15	0.00
Fish					7.53E-22	7.53E-22	0.00
Soil		2.53E-24	3.39E-22			3.41E-22	0.00
Total ingestion	6.26 E-23	5.19 E-23	6.71 E-18	1.06 E-08	1.29 E-21	**1.06 E-08**	38.15
DERMAL UPTAKE		1.06E-22	1.42E-20	5.07E-09	3.80E-22	**5.07E-09**	18.26
Dose SUM	**1.77E-19**	**1.58E-22**	**7.22E-18**	**2.78E-08**	**2.30E-21**	**2.78E-08**	100.0

Breast milk concentration	Air (gases & particles)	Surface soil	Root-zone soil	Ground water	Surface water	total
	2.06 E-21	1.84 E-24	8.42 E-20	3.24 E-10	2.68 E-23	
Infant dose	2.27 E-22	2.02 E-25	9.26 E-21	3.57 E-11	2.95 E-24	**dose_bm 3.57 E-11**

ENVIRONMENTAL Media	Air (gases) mg/m^3	Air (dust) mg/m^3	Ground soil mg/kg	Root soil mg/kg	Ground water mg/L	Surface water mg/L
CONCENTRATIONS	**8.46 E-19**	**7.21 E-26**	**1.44 E-17**	**1.94 E-15**	**4.21 E-07**	**8.66 E-20**

EXPOSURE MEDIA CONCENTRATIONS (at the mean exposure time)

EXPOSURE	Air (gases)	Air (dust)	Ground soil	Root soil	Ground water	Surface water
Indoor air (mg/m^3)	8.46 E-19	7.21 E-26	4.33 E-25	2.45 E-18	1.41 E-08	7.27 E-22
Bathroom air (mg/m^3)					1.82 E-06	9.34 E-20
Outdoor air (mg/m^3)	8.46 E-19	7.21 E-26				
Tap water (mg/L)					3.37 E-07	1.71 E-20
Exposed produce (mg/kg)	5.74 E-20	2.38 E-22	4.91 E-20	2.94 E-16	1.43 E-07	7.35 E-21
Unexposed produce (mg/kg)				1.03 E-14	4.89 E-06	2.52 E-19
Meat (mg/kg)	2.39 E-21	3.20 E-25	1.95 E-22	3.95 E-19	4.56 E-10	2.35 E-23
Milk (mg/kg)	7.66 E-22	1.43 E-25	7.05 E-23	1.77 E-19	1.70 E-10	8.73 E-24
Eggs (mg/kg)	2.64 E-22	4.06 E-27	8.59 E-25	4.99 E-21	6.43 E-12	3.30 E-25
Fish and seafood (mg/kg)						3.71 E-18
Household soil (mg/kg)			7.22 E-18	9.68 E-16		
Swimming water (mg/L)						8.66 E-20

PATHWAY CONTACT FACTORS (CR/BW*FI)

EXPOSURE Media	Units	Inhalation	Ingestion	Dermal
Indoor air (active)		1.52 E-01		
Indoor air (resting)		5.12 E-02		
Indoor air (shower/bath)		5.13 E-03		
Outdoor air (active)		5.70 E-03		
Tap water			2.20 E-02	1.51 E-02
Exposed produce			9.97 E-04	
Unexposed produce			6.23 E-04	
Meat			1.32 E-03	
Milk			2.60 E-03	
Eggs			1.84 E-04	
Fish and seafood			2.03 E-04	
Household soil			3.50 E-07	1.46 E-05
Swimming wtr			1.44 E-05	1.42 E-03

Dose ratios	inh-dose/Ns	ing-dose/Ns	drml-dose/Ns	inh-dose/Nv	ing-dose/Nv	drml-dose/Nv
	9.9 E-09	9.9 E-08	7.2 E-12	4.2 E-08	3.6 E-08	1.7 E-08

Time (y)	Total inhalation dose	Total ingestion dose	Total dermal dose	Total dose	Total dose from root soil	Total dose from ground water
1	4.4 E-04	4.0 E-04	1.8 E-04	1.0 E-03	1.4 E-05	1.0 E-03
2.4	2.2 E-05	2.0 E-05	9.4 E-06	5.1 E-05	4.5 E-09	5.1 E-05
3.8	1.1 E-06	1.0 E-06	4.8 E-07	2.6 E-06	1.5 E-12	2.6 E-06
5.2	5.8 E-08	5.1 E-08	2.4 E-08	1.3 E-07	5.0 E-16	1.3 E-07
6.6	3.0 E-09	2.6 E-09	1.2 E-09	6.8 E-09	1.7 E-19	6.8 E-09
8	1.5 E-10	1.3 E-10	6.3 E-11	3.5 E-10	5.5 E-23	3.5 E-10
9.4	7.7 E-12	6.7 E-12	3.2 E-12	1.8 E-11	1.8 E-26	1.8 E-11
10.8	3.9 E-13	3.4 E-13	1.6 E-13	9.0 E-13	6.0 E-30	9.0 E-13
12.2	2.0 E-14	1.7 E-14	8.3 E-15	4.6 E-14	2.0 E-33	4.6 E-14
13.6	1.0 E-15	8.9 E-16	4.2 E-16	2.3 E-15	6.6 E-37	2.3 E-15
15	5.2 E-17	4.5 E-17	2.2 E-17	1.2 E-16	2.2 E-40	1.2 E-16
Cumulative doses				0.288444706		
over ED by route, mg/kg	1.2 E-01	1.1 E-01	5.2 E-02	2.9 E-01	3.5 E-03	2.8 E-01
fraction	0.4317	0.3879	0.1804	1.0000	0.012	0.988
Average doses						
over ED by route, mg/kg-d	2.4 E-05	2.2 E-05	1.0 E-05	5.6 E-05	6.9 E-07	5.6 E-05
Maximum doses				1.0 E-03		
over ED by route, mg/kg-d	4.4 E-04	4.0 E-04	1.8 E-04	1.0 E-03	1.4 E-05	1.0 E-03
fraction	0.4312	0.3886	0.1801	1.0000	0.013	0.987

Time zero breast-milk dose	1.3 E-06	mg/kg-d
Max breast-milk dose	1.3 E-06	mg/kg-d

The Chemical Fate Diagram is unavailable in the PC version of CalTOX™.
Please refer to the Gain-loss table, available in the CalTOX pull-down menu.

Calculated Properties

Time at which mean exposures are calculated	2.17E+03	Time		
fugacity capacity of pure air	4.25 E-04	Zair		
fugacity capacity of pure water	3.07 E-03	Zwater		
diffusion lag time in skin (h)	1.42 E-01	tlag		
height of the air compartment (m)	5.53 E+01	d_a		
evapotranspiration of water from soil (m/d)	5.20 E-04	evapotrans	1.90 E-01	m/y
Total surface water runoff (m/d)	2.84 E-04	outflow	1.04 E-01	m/y
bndry lyr thickness in air above wtr (m)	3.11 E-03	del_aw		
bndry lyr thickness in wtr below air (m)	3.30 E-04	del_wa		
diffusion length in surface soil (m)	1.57 E-02	del_g		
diffusion length in upper soil (m)	2.10 E-01	del_s		
Thickness of the root-zone soil layer	2.00 E+00	d_s		
wtr-side bndry lyr thickness with sed (m)	2.00 E-02	del_wd		
sed-side bndry lyr thickness with wtr (m)	9.66 E-03	del_dw		
Initial concentration in soil (mol/m3)	1.94E-02	Cs0		
Initial conc. in the vadose zone (mol/m3)	1.79E-02	Cv0		
Sediment resuspension rate (kg/m2-d)	1.05E+01	resuspend		
soil particle density; surface layer(kg/m3)	2600	rhos_g		
soil particle density; vadose layer(kg/m3)	2600	rhos_v		
Initial iventory in groundwater zone	0	Nq0		
Reaction rate constant in air (1/d)	4.056585366	Ra		
Reaction rate constant, ground soil (1/d)	0.015413375	Rg		
Reaction rate constant, root-zone soil (1/d)	0.015413375	Rs		
Reaction rate constant, vadose-zone soil (1/d)	0.005823529	Rv		
Reaction rate constant, ground water (1/d)	n/a	Rq		
Reaction rate constant, surface water (1/d)	0.033	Rw		
Reaction rate constant, sediment (1/d)	0.011	Rd		

Warnings

0 Ground soil depth greater than 2 cm
0 Root-zone soil too shallow for accuracy of diffusion model (must be at least 0.4*del_s)
0 Starting time cannot be 0 and should be greater than 365 day
0 Recharge velocity is negative
0 Recharge velocity is too large accuracy of model
0 Concentration in root-zone soil-water exceeds solubility or < 0
0 Concentration in vadose-zone soil-water exceeds solubility or < 0
0 Concentration in groundwater exceeds solubility or < 0
0 Concentration in surface water exceeds solubility
0 Concentration in sediment-zone water exceeds solubility
0 Exposure time indoors and outdoors at home or at work exceeds 24 h
0 Exposure time in shower or bath << than lag time
0 Exposure time swimming << than lag time
0 Fraction of water from groundwater plus fraction from surface >1
0 total

Fugacity (Pa)

Air	fa	1.91E-20
Plants	fp	2.77E-16
Ground	fg	4.12E-18
Root	fs	5.53E-16
Vadose	fv	1.32E-06
Water	fw	2.71E-19
Sediment	fd	1.29E-19
Groundwater	fq	n/a

Compartment Volumes (m^3)

Va	5.5 E+07	Air compartment
Vpp	3.5 E+03	Plants compartment
Vg	9.9 E+03	Ground-soil compartment
Vs	2.0 E+06	Root-zone compartment
Vv	5.0 E+06	Vadose compartment volume
Vw	4.1 E+04	Water compartment
Vd	4.1 E+02	Sediment compartment
Vq	n/a	aquifer compartment

Fugacity Capacities (mol/m^3 per Pa)

Zap	1.53E+00	fugacity capacity of air particles in mol/m3[s]-Pa
Zgp	8.74E-02	fugacity capacity of ground soil compartment particles in mol/m3[s]-Pa
Zsp	8.74E-02	fugacity capacity of root zone compartment particles in mol/m3[s]-Pa
Zvp	7.28E-02	fugacity capacity of vadose zone compartment particles in mol/m3[s]-Pa
Zwp	1.46E-01	fugacity capacity of suspended sediment in surface water in mol/m3[s]-Pa
Zdp	1.46E-01	fugacity capacity of bottom sediment particles in mol/m3[s]-Pa
Zqp	n/a	fugacity capacity of aquifer solids in mol/m3-Pa
Za	4.25E-04	fugacity capacity of air compartment in mol/m3-Pa
Zp	2.88E-02	fugacity capacity of plant biomass
Zg	6.15E-02	fugacity capacity of ground soil compartment in mol/m3-Pa
Zs	6.18E-02	fugacity capacity of upper soil compartment in mol/m3-Pa
Zv	4.46E-02	fugacity capacity of vadose compartment in mol/m3-Pa
Zw	3.11E-03	fugacity capacity of water compartment in mol/m3-Pa
Zd	1.17E-01	fugacity capacity of sediment compartment in mol/m3-Pa
Zq	n/a	fugacity capacity of aquifer compartment in mol/m3-Pa

Diffusion coefficients in m2/d				Boundary-layer thickness (del)	Fugacity mass-transfer coefficients mol/Pa-m2 Y		Overall intercompartment mass transfer rate constants (1/day) T			
Compartment Phase		Compartment			one-sided	both-sides	Diffusion	Advection	Total	Compartment Interface
Dair	6.13E-01	Da	6.13E-01	3.11E-03	8.37E-02	7.30E-04	2.53E-04	1.08E-06	2.55 E-04	air-water, T_aw
Dwater	7.92E-05	Dw	7.81E-05	3.30E-04	7.37E-04		4.69 E-02		4.69 E-02	water-air, T_wa
Dair_g	3.19E-02	Dg	2.20E-04	5.00E-03	5.21E-02	8.49E-04	3.59E-02	1.31E-04	3.60 E-02	air-ground, T_ag
Dwater_	4.08E-07			1.57E-02	8.63E-04		1.38E+00	1.68E-06	1.38 E+00	ground-air, T_ga
Dair_s	3.16E-03	Ds	2.20E-05	1.57E-02	8.63E-04	6.43E-06	1.04E-02	9.98E-04	1.14 E-02	ground-soil, T_gs
Dwater_	4.12E-06			2.10E-01	6.48E-06		5.20E-05		5.20 E-05	soil-ground, T_sg
Dwater_	9.26E-06	Dd	2.43E-07	2.00E-02	1.23E-05	2.38E-06	1.53E-04	3.78E-02	3.79 E-02	water-sediment, T_wd
				9.66E-03	2.94E-06		4.06E-04	1.01E-01	1.01 E-01	sediment-water, T_dw
								9.95E-05	1.01 E-01	sediment-out, T_do
								3.45E+01	3.45 E+01	air-out, T_ao
							1.09E-03		1.09 E-03	air-plants, T_ap
							5.00E-01		5.00 E-01	plants-air, T_pa
								0.00E+00	0.00 E+00	plants-ground, T_pg
								1.00E-02	1.00 E-02	plants-soil, T_ps
								0.00E+00	0.00 E+00	ground-plants, T_gp
								1.41E-03	1.41 E-03	ground-water, T_gw
								2.08E-04	2.08 E-04	soil-plants, T_sp
								4.97E-06	4.97 E-06	soil-vadose, T_sv
								2.75E-06	2.75 E-06	vadose-aquifer, T_vq
								6.97E-03	6.97 E-03	water-out, T_wo

aaa1	2.38E-03	bbb1	0.00E+00
aaa2	1.32E-02	bbb2	0.00E+00
aaa3	3.58E-02	bbb3	0.00E+00
aaa4	5.29E-06	bbb4	0.00E+00
aaa5	3.71E-05	bbb5	0.00E+00
aaa6	3.85E+04		
aaa7	8.86E+04	Lam1	1.57E-02
aaa8	-1.94E+01		

Source term (g/d)

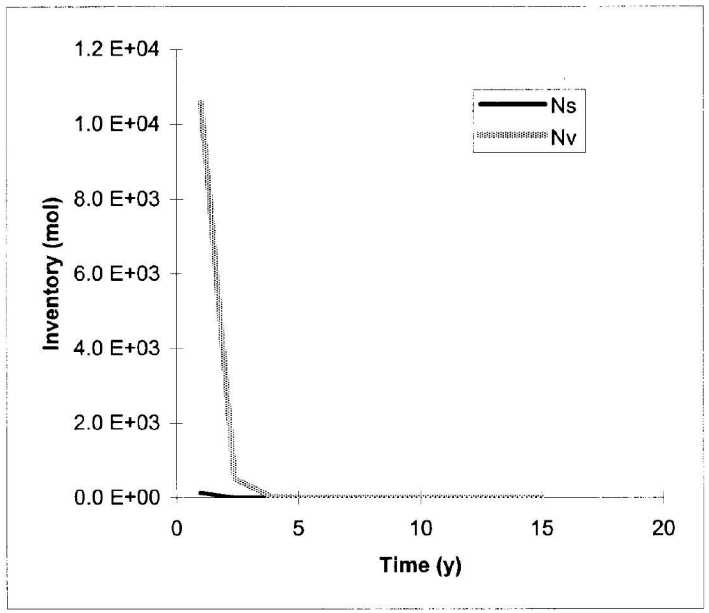
air	0.0 E+00	
ground	0.0 E+00	
water	0.0 E+00	

Compartment Name		Loss-rate constant (1/day) L	Total Inventory (moles) N	Concen-tration (mol/m3) C	Mass distri-bution %	Gains g/d	Losses g/d	Residence Time (days)
air	a	3.86 E+01	4.5 E-16	8.1 E-24	0.00%	1.80 E-12	1.80E-12	2.59 E-02
plants	p	5.10 E-01	2.8 E-14	8.0 E-18	0.00%	1.47 E-12	1.47E-12	1.96 E+00
ground-soil	g	1.41 E+00	2.5 E-15	2.5 E-19	0.00%	3.69 E-13	3.69E-13	7.10 E-01
root-soil	s	1.57 E-02	6.8 E-11	3.4 E-17	0.00%	3.18 E-14	1.11E-10	6.38 E+01
vadose-zone	v	5.83 E-03	2.9 E-01	5.9 E-08	100.00%	3.51 E-14	1.77E-01	1.72 E+02
surface water	w	1.25 E-01	3.4 E-17	8.4 E-22	0.00%	4.47 E-16	4.47E-16	8.01 E+00
sediment	d	2.13 E-01	6.1 E-18	1.5 E-20	0.00%	1.36 E-16	1.36E-16	8.95 E+00
aquifer	q	n/a	n/a	n/a	n/a	8.35 E-05		

Mass Flows (g/d)

air-ground	1.68 E-15	Tag*Na*MW
air-water	1.19 E-17	
air-out	1.61 E-12	
air-plants	5.08 E-17	
air-transform	1.90 E-13	
plants-air	1.44 E-12	
plants-ground	0.00 E+00	
plants-soil	2.88 E-14	
plants-trnsfrm	0.00 E+00	
ground-air	3.62 E-13	
ground-plants	0.00 E+00	
ground-soil	3.00 E-15	
ground-water	3.71 E-16	

ground-trnsfrm	4.04 E-15	
soil-ground	3.67 E-13	
soil-plants	1.47 E-12	
soil-vadose	3.51 E-14	
soil-trnsfrm	1.09 E-10	
vadose-aquifer	8.35 E-05	
vadose-trnsfrm	1.77 E-01	
water-air	1.68 E-16	
water-sediment	1.36 E-16	
water-out	2.49 E-17	
water-trnsfrm	1.18 E-16	
sediment-water	6.44 E-17	
sedmnt-trnsfrm	7.03 E-18	
sediment-out	6.44 e-17	

Time-dependent Compartment Inventories

Time (y)	Time (d)	Ns	Nv	
1	365	1.3 E+02	1.1 E+04	n/a
2.4	876	4.2 E-02	5.4 E+02	n/a
3.8	1387	1.4 E-05	2.7 E+01	n/a
5.2	1898	4.6 E-09	1.4 E+00	n/a
6.6	2409	1.5 E-12	7.1 E-02	n/a
8	2920	5.0 E-16	3.6 E-03	n/a
9.4	3431	1.7 E-19	1.8 E-04	n/a
10.8	3942	5.6 E-23	9.4 E-06	n/a
12.2	4453	1.8 E-26	4.8 E-07	n/a
13.6	4964	6.1 E-30	2.4 E-08	n/a
15	5475	2.0 E-33	1.2 E-09	n/a