Distribution: General

Final report

S-Risk version for the Walloon region: Technical guidance document

C. Cornelis, A. Standaert, H. Willems

Adapted for the Walloon Region by S. Crévecoeur (ISSeP)

Adaptations for Walloon Region accomplished under the authority of DGO3

2016/MRG/R/0771

February 2017

VITO NV
Boeretang 200 - 2400 MOL - BELGIE
Tel. + 32 14 33 55 11 - Fax + 32 14 33 55 99
vito@vito.be - www.vito.be

BTW BE-0244.195.916 RPR (Turnhout)
Bank 375-1117354-90 ING
BE34 3751 1173 5490 - BBRUBEBB

SUMMARY

S-Risk is a model for human exposure and health risk assessment at contaminated sites. It replaces the Vlier-Humaan model that has been in use since 1995 within the framework of the Flemish regulation on contaminated sites. S-Risk provides a full revision of Vlier-Humaan, updating model concepts, model equations and parameter values. It also provides increased flexibility for the user.

The technical guidance document provides the full set of model equations of S-Risk with links to information sources. Default values to be used in the calculation of soil remediation values are provided as well as guidance for site-specific parameter values were applicable. S-Risk was parameterized for use within the Flemish regulatory framework for contaminated sites assessment. Following a decision by the Walloon administration, S-Risk will also be applied in Wallonia after the implementation of a series of modifications. These modifications apply to the parameterization of the model. Equations were not modified. The technical guidance document presented here provides the background information in line with the S-Risk version developed for the Walloon region.

The development of the initial S-Risk model was followed by a steering committee being chaired by OVAM and consisting of the developers (VITO), representatives of OVAM and of the Accredited Soil Remediation Experts Association (VEB). A separate version has been developed in 2016 for the Walloon region on behalf of the Walloon administration (DGO3) and ISSEP and in collaboration with SPAQuE, ULg Gembloux Agro BioTech and AWAC.

REVISION HISTORY

Date	*revision*

TABLE OF CONTENTS

LIST OF FIGURES

LIST OF TABLES

LIST OF SYMBOLS

A

a	1/d	Total chemical elimination constant for removal out of the plant
A	m²	Surface of aboveground plant parts
a_1	-	Correction factor for the difference in density between water and n-octanol ($1/\rho_{octanol}$)
ABS_{dermal}	-	Dermal absorption factor for soil and dust
AD_{dermal}^{daily}	mg/kg.d	Daily uptake via dermal contact
$AD_{dermal\_bathing}^{daily}$	mg/kg.d	Daily uptake via dermal contact with water during bathing
$AD_{dermal\_dust}^{daily}$	mg/kg.d	Daily uptake via dermal contact with settled dust particles
$AD_{dermal\_showering}^{daily}$	mg/kg.d	daily uptake via dermal contact with water during showering
$AD_{dermal\_soil}^{daily}$	mg/kg.d	daily uptake via dermal contact with soil (outdoor)
$AD_{dermal\_soil/dust}^{daily}$	mg/kg.d	Total daily uptake via dermal contact with soil and settled dust
$ADE_{dermal\_bathing}$	mg/m².event	Absorbed dose via skin contact through bathing
$ADE_{dermal\_showeirng}$	mg/m².event	Absorbed dose via skin contact through showering
AD_{dermal}^{yearly}	mg/kg.d	Yearly average uptake via dermal contact
$AD_{dermal\_bathing}^{yearly}$	mg/kg.d	Yearly average uptake via dermal contact with water during bathing
$AD_{dermal\_dust}^{yearly}$	mg/kg.d	Yearly average uptake via dermal contact with settled dust
$AD_{dermal\_dust/soil}^{yearly}$	mg/kg.d	Yearly average uptake via dermal contact with settled dust and soil
$AD_{dermal\_showering}^{yearly}$	mg/kg.d	yearly average uptake via dermal contact with water during showering
$AD_{dermal\_soil}^{yearly}$	mg/kg.d	Yearly average uptake via dermal contact with soil
$AD_{dermal\_water}^{yearly}$	mg/kg.d	yearly average uptake via dermal contact with water
A_f	m²	surface area of the floor
$A_{f,b}$	m²	surface area of the floor of the basement
$A_{f,c}$	m²	surface area of the floor of the crawl space
AF_{dust_skin}	mg/m²	average dust adherence on skin
AF_{soil_skin}	mg/m²	average soil adherence on skin
a_{growth}	1/d	Chemical elimination via growth
$a_{metabolism}$	1/d	loss due to metabolization in the plant
$a_{photodegradation}$	1/d	Chemical elimination via photo-degradation
$a_{volatilization}$	1/d	Chemical elimination via volatilization
A_w	m²	surface area of the basement walls
$A_{w,d}$	m²	surface area of the basement walls for direct flux
$A_{w,i}$	m²	surface area of the basement walls for indirect flux

B

b	-	correlation coefficient
B	-	ratio of permeability through stratum corneum versus viable epidermis
b_1	-	Briggs factor for root plants
BCF_{inorg}	(mg/kg plant dm)/(mg/kg soil	Bioconcentration factor for inorganic contaminants

	dm)	
BCF_{org}	(mg/kg plant dm)/(mg/m³)	bioconcentration factor for organic contaminants
b_s	mg/m³.d	Source term which describes transfer from soil and gas deposition
$BTF_{feed,egg}$	(mg/kg fw)/(mg/d)	biotransfer factor from feed to egg
BTF_{kidney}	(mg/kg fw)/(mg/d)	biotransfer factor to kidney
BTF_{liver}	(mg/kg fw)/(mg/d)	biotransfer factor to liver
BTF_{meat}	(mg/kg fw)/(mg/d)	biotransfer factor to meat
$BTF_{meat,org}$	(mg/kg fw)/(mg/d)	biotransfer factor to meat for organic contaminants
BTF_{milk}	(mg/kg fw)/(mg/d)	biotransfer factor to milk
$BTF_{milk,org}$	(mg/kg fw)/(mg/d)	biotransfer factor to milk for organic contaminants
$BTF_{soil,egg}$	(mg/kg fw)/(mg/d)	biotransfer factor from soil to egg
BW	kg	body weight

C

C	mg/kg dm	total soil concentration
c	-	correlation coefficient
$C'_{background, grass,silage}$	mg/kg dm	background concentration in silage grass
$C'_{background, maize}$	mg/kg dm	background concentration in maize
$C'_{background,pasture}$	mg/kg dm	background concentration in pasture grass
C'_{grass}	mg/kg dm	concentration in grass dry weight basis
C'_{maize}	mg/kg dm	concentration in maize dry weight basis
$C'_{mixture}$	mg/kg dm	concentration in feed mixture for chicken
$C_{site,inhalation}^{adult}$	mg/m³	average yearly air exposure concentration from the location for an adult
$C_{total,inhalation}^{adult}$	mg/m³	average yearly total air exposure concentration for an adult
$C_{site,inhalation}^{age\ group}$	mg/m³	yearly average exposure air concentration from the location for the specified exposure duration / averaging time
$C_{ai,v}$	mg/m³	final concentration in the gas phase of indoor air
C_{ao}	mg/m³	total concentration in ambient air
$C_{ao,v}$	mg/m³	concentration in outdoor air due to volatilization
$C_{ao,vf}$	mg/m³	Concentration in the gas phase in the ambient air
$C_{ao,pl,vf}$	mg/m³	final concentration in ambient air at plant height due to volatilization
$C_{ao,y}$	mg/m³	concentration in ambient air
$C_{ao,Y,v}$	mg/m³	concentration in ambient air at height Y due to volatilization
$C_{ao,Y,v}$ (finite)	mg/m³	average finite source ambient air concentration at height Y due to volatilization
$C_{ao,Y,vf}$	mg/m³	final concentration in ambient air at height Y due to volatilization
$C_{ao,Y,v,i}$	mg/m³	concentration in ambient air at height Y due to volatilization from layer i
$C^{background}$	mg/kg fw (vegetable) mg/m³ (drinking-water)	average background concentration in vegetable category or drinking-water
$C_{inhalation}^{background}$	mg/m³	yearly average inhalation rate weighted background air concentration
$C_{ao}^{background}$		background concentration in outdoor air
$C_{air}^{background}$	mg/m³	background concentration in indoor air
$C_{inhalation}^{background,i}$	mg/m³	average yearly background air exposure concentration for age category i
C_{beef}	mg/kg fw	Concentration in beef

$C_{br,a}$	mg/m^3	Concentration in bathroom air
$C_{br,a,0}$	mg/m^3	Concentration in bathroom air at start
C_{butter}	mg/kg fw	concentration in butter
$C_{c,water}$	mg/m^3	concentration in water for cattle
C_{ca}	mg/m^3	concentration in crawl space
$C_{ch,water}$	mg/m^3	concentration in water for chicken
$C'_{concentrate}$	mg/kg dm	concentration in concentrate
$C^{child}_{site,inhalation}$	mg/m^3	average yearly air exposure concentration from the location for a child
$C^{child}_{total,inhalation}$	mg/m^3	average yearly total air exposure concentration for a child
$C^{daily}_{inhalation}$	mg/m^3	total daily inhalation rate weighted air concentration
$C^{daily}_{inhalation\_in}$	mg/m^3	daily inhalation rate weighted air concentration in indoor environment
$C^{daily}_{inhalation\_out}$	mg/m^3	daily inhalation rate weighted air concentration in outdoor environment
$C^{daily}_{inhalation\_shower}$	mg/m^3	daily inhalation rate weighted air concentration during showering
C_{dw}	mg/m^3	concentration in drinking-water
C_{dw}	mg/m^3	Drinking-water concentration
CEC	meq/100 g	cation exchange capacity
C_{eggs}	mg/kg fw	concentration in eggs
CF_{PM10}	kg/µg	Conversion factor from µg/m^3 to kg/m^3
CF	kg/mg	Conversion factor from mg/d to kg/d
CF_2	m/cm	unit conversion factor
Cf_a	-	Correction factor for organic acids
Cf_b	-	Correction factor for organic bases
C_{grass}	mg/kg fw	concentration in grass fresh weight basis
C_{gw}	mg/m^3	Concentration in groundwater
CI	-	concentration index
C_i	mg/kg or mg/m^3	concentration in compartment i
C_{ia}	mg/m^3	concentration in indoor air
$C_{ia,t}$	mg/m^3	total concentration in indoor air
$C_{ia,v}$	mg/m^3	gas-phase concentration in indoor air
C_{kidney}	mg/kg fw	concentration in kidney
CL	%	clay content
C_{liver}	mg/kg fw	concentration in liver
C_{maize}	mg/kg fw	concentration in maize fresh weight basis
C_{meat}	mg/kg fw	concentration in meat (beef or sheep)
C_{milk}	mg/kg fw	concentration in milk
C_o	-	Correction factor for terrain roughness length
C_p	mg/kg fw	Concentration in the potato
$C_{PM10.i}$	mg/m^3	Concentration in indoor air (on PM10) as a result of soil quality
$C_{PM10.o}$	mg/m^3	Concentration in outdoor air (on PM10) as a result of soil quality
C_s	mg/kg dm	concentration in the soil solid phase
C_{s+w}	mg/kg dm	Concentration in the soil solid + water phase
C_{sa}	mg/m^3	concentration in soil air
$C_{sa,g}$	mg/m^3	concentration in soil air due to volatilization from groundwater
$C_{sa,t}$	mg/m^3	concentration in topsoil air

$C_{settled\_dust}$	mg/kg dm	Concentration in settled dust indoors from soil
$C_{sh,a}$	mg/m³	Concentration in the shower stall air
$C_{site,inhalation}$	mg/m³	yearly average exposure air concentration from the location
$C_{site,inhalation}$	mg/m³	yearly average exposure air concentration from the location
$C_{total,inhalation}$	mg/m³	yearly average total exposure air concentration for the specified exposure duration / averaging time
C_v	mg/kg fw	Total plant concentration
$C_{v,i,j}$	mg/kg fw	concentration in vegetable i from vegetable category j
$C_{v,p}$	mg/kg fw	Plant concentration due to particle deposition
$C_{v,s}$	mg/kg fw	Plant concentration due to soil – plant transfer
$C_{v,sg}$	mg/kg fw	Plant concentration as a result of gas exchange and translocation from the root to the stem and leafs
$C_{v,sp}$	mg/kg fw	Plant concentration as a result of splashed soil particles
$C_{veg\_category}$	mg/kg fw	Concentration in vegetable category
$C_{veg\_category,j}$	mg/kg fw	Concentration in vegetable category j
C_w	mg/m^3	soil pore water concentration
C_w(max)	mg/m³	maximum soil water concentration for organic contaminants
$C_{w,i}$	mg/m^3	Concentration in soil pore water of layer i
$C_{water,other}$	mg/m³	concentration in other water
C_{wp}	mg/m³	Water concentration in a pipe as a result of permeation
$C^{yearly}_{inhalation}$	mg/m³	average yearly air exposure concentration from the location
$C^{yearly,i}_{inhalation}$	mg/m³	average yearly air exposure concentration from the location for age category i
$C^{yearly}_{inhalation\_in}$	mg/m³	yearly averaged inhalation rate weighted air concentration in indoor environment
$C^{yearly}_{inhalation\_out}$	mg/m³	yearly averaged inhalation rate weighted air concentration in outdoor environment
$C^{yearly}_{inhalation\_shower}$	mg/m³	yearly averaged inhalation rate weighted air concentration during showering

D

d	m	depth of the floor of the concrete slab or basement floor below soil surface
d_a	m	Thickness of the phreatic groundwater layer
D_a	m²/d	diffusion coefficient in air
$D^{adult}_{site,oral/dermal}$	mg/kg.d	average yearly intake/uptake from the location for an adult by the oral or dermal route
$D^{adult}_{total,oral/dermal}$	mg/kg.d	average total yearly intake/uptake for an adult by the oral or dermal route
$D^{age\ group}_{site,oral/dermal}$	mg/kg.d	yearly average intake/uptake from the location by the oral or dermal route for the specified exposure duration / averaging time
$D^{background,i}_{oral/dermal}$	mg/kg.d	average background intake by the oral or dermal route and age category i
$D^{background}_{oral/dermal}$	mg/kg.d	average background intake by the oral or dermal route
$D^{child}_{site,oral/dermal}$	mg/kg.d	average yearly intake/uptake from the location for a child by the oral or dermal route
d_c	m	depth of the crawl space beneath soil surface
$D^{cz}{}_{eff}$	m²/d	effective diffusion coefficient in the capillary zone
d_e	m	Thickness of the drinking-water pipe
$D^{fa}{}_{eff}$	m²/d	effective diffusion coefficient in the floor
DF_{gw}	-	Dilution factor from pore water to groundwater
$D^{gw}{}_{eff,o}$	m²/d	effective diffusion coefficient in soil air for transfer from groundwater to topsoil

dm	%	Dry matter content of the plant
D_p	m^2/d	Permeation coefficient
$D_{p,p}$	m^2/d	effective diffusion coefficient in the potato
D_{pe}	m^2/d	Permeation organic substance through PE drinking-water service pipe
D_{pvc}	m^2/d	Permeation organic substance through PVC drinking-water service pipe – if not filled in for organics, the value is set at D_{pe} / 1000
d_{sa}	m	depth of the top of the contamination
D^{sa}_{eff}	m^2/d	Effective diffusion coefficient in soil air
$D^{sa}_{eff,f}$	m^2/d	effective diffusion coefficient in soil for vapour intrusion through floor of building, basement or bottom of crawl space
$D^{sa}_{eff,i}$	m^2/d	effective diffusion coefficient of a soil layer
$D^{sa}_{eff,o}$	m^2/d	effective diffusion coefficient in soil for ambient air calculations
$D^{sa}_{eff,w}$	m^2/d	effective diffusion coefficient in soil for walls
$D^{sa,u}_{eff}$		effective diffusion coefficient in soil air for the soil layer below the floor of the building
D_{sc}	cm^2/hr	effective diffusion coefficient for chemical transfer through the stratum corneum
$D_{site,oral/dermal}$	mg/kg.d	average yearly lifelong intake/uptake from the location for by the oral or dermal route
$D_{site,oral/inhalation}$	mg/kg.d	yearly average lifelong intake/uptake from the location for by the oral or dermal route
dt	h/d	Standard stagnation time in pipe
$D_{total,oral/dermal}$	mg/kg.d	total yearly average intake/uptake for by the oral or dermal route for the specified exposure duration / averaging time
D_w	m^2/d	diffusion coefficient in water
D^{wa}_{eff}	m^2/d	effective diffusion coefficient in the basement wall
$D^{yearly,i}_{oral/dermal}$	mg/kg.d	yearly average intake/uptake from the location by the oral or dermal route and age category i
$D^{yearly,i}_{route}$	mg/kg.d	average yearly intake/uptake from the location by the oral or dermal route and age category i

E

$ED_{animal\ products}$	mg/kg.d	yearly average intake through consumption of locally produced animal products
$ED^{background}_{drinking\_water}$	mg/kg.d	yearly average intake from drinking-water
$ED^{background}_{food}$	mg/kg.d	yearly average background intake from food
$ED^{background}_{oral}$	mg/kg.d	yearly average oral background intake
ED^{yearly}_{beef}	mg/kg.d	yearly average intake through consumption of locally produced beef
ED^{yearly}_{butter}	mg/kg.d	yearly average intake through consumption of locally produced butter
$ED^{daily}_{drinking\_water}$	mg/kg.d	Daily average intake through drinking-water
ED^{daily}_{oral}	mg/kg d	Total daily oral dose
$ED^{daily}_{oral\_dust}$	mg/kg.d	Daily average intake via dust particles
$ED^{daily}_{oral\_soil}$	mg/kg.d	Daily average intake via soil particles
$ED^{daily}_{oral\_soil/dust}$	mg/kg.d	Daily average intake via soil and dust particles
EDE_{dermal_dust}	mg/kg.d	Intake via dermal contact with settled dust particles, per event
EDE_{dermal_soil}	mg/kg.d	Intake via dermal contact with soil particles, per event

ED_{eggs}^{yearly}	mg/kg.d	yearly average intake through consumption of locally produced eggs
ED_{milk}^{yearly}	mg/kg.d	yearly average intake through consumption of locally produced milk
$ED_{organ\_meat}^{yearly}$	mg/kg.d	yearly average intake through consumption of locally produced organ meat
$ED_{food}^{populatior}$	mg/kg.d	yearly average intake of the general population from food
$ED_{veg\_category}^{yearly}$	mg/kg.d	Yearly average intake through consumption of locally grown vegetables by vegetable category
$ED_{vegetables}^{yearly}$	mg/kg.d	yearly average intake through consumption of locally grown vegetables
$ED_{animal\_products}^{yearly}$	mg/kg d	Yearly average intake via animal products
$ED_{drinking\_water}^{yearly}$	mg/kg d	Yearly average intake via drinking-water
ED_{oral}^{yearly}	mg/kg d	Total yearly oral dose
$ED_{oral\_dust}^{yearly}$	mg/kg.d	Yearly average oral intake via dust particles
$ED_{oral\_soil}^{yearly}$	mg/kg.d	Yearly average intake via soil and dust particles
$ED_{oral\_soil/dust}^{yearly}$	mg/kg.d	Yearly average intake via soil and dust particles
EF	d/y	exposure frequency
$EF_{bathing}$	d/y	exposure frequency for bathing
$EF_{bathing/showering}$	d/y	Exposure frequency for bathing or showering
$EF_{showering}$	d/y	exposure frequency for showering
$EF_{soil/settled\_dust}$	-	Enrichment factor from soil to indoor settled dust
EF_{week}	d/w	Frequency on a weekly basis
$EF_{week;bathing/showering}$	d/w	Frequency of bathing/showering on a weekly basis
EF_{year}	w/y	Frequency on a yearly basis
$EV_{bathing}$	baths/d	number of baths per day
EV_{in}	events/d	number of “dust” events
EV_{out}	events/d	number of “soil” events
$EV_{showering}$	showers/d	number of showers per day
ExCR	-	overall excess lifelong cancer risk for systemic effects
$ExCR_{inhalation}$	-	excess lifelong cancer risk by inhalation
$ExCR_{oral/dermal}$	-	excess lifelong cancer risk by the oral or dermal route

F

FA	-	Fraction absorbed water
$f_{vegetable\_category}^{garden}$	-	fraction of locally grown vegetables by category
$f_{animal\_product}^{local}$	-	fraction of animal product from local production
$f_{veg\_category}^{garden}$	-	Fraction of locally grown vegetables by category
f_{beef}^{local}	-	Fraction beef from locally produced farm product
$f_{c,water,gw}$	-	fraction of groundwater for cattle (summer / winter)
$f_{c,water,other}$	-	fraction of other water for cattle (summer / winter)
$f_{c,water,wp}$	-	fraction of drinking-water for cattle (summer / winter)
f_{CH}	-	fraction of carbohydrates in potato
$f_{ch,water,other}$	-	fraction of other water for chicken
$f_{ch,water,gw}$	-	fraction of groundwater for chicken
$f_{ch,water,wp}$	-	fraction of drinking-water for chicken
F_{ci}	m^3/m^2.d	air flux from crawl space to indoor space

f_{eff}	-	Fraction of soil particles taken up by the plant
$f_{f,butter}$	-	fat content of butter
$f_{f,milk}$	-	fat content of milk
$f_{free\text{-}range}$	-	fraction of free-range
f_g	-	Fraction of groundwater used as drinking-water
F_{gap}	m^3/m^2.d	air flux through gaps in the floor (per area of holes)
f_{local}	-	fraction of pasture grass, silage grass or maize coming from contaminated area
f_{of}	m^2/m^2	fraction of openings in floor
F_{oral_soil}	-	fraction of soil in soil and dust ingestion
$F_{out/in}$	-	contribution of the concentration on ambient PM_{10} to the concentration on indoor PM_{10}
f_p	-	fraction paved
F_{sc}	m^3/m^2.d	air flux from soil to the crawl space
$F_{sc,w,d}$	m^3/m^2.d	direct air flux through crawl space walls
$F_{sc,w,i}$	m^3/m^2.d	indirect air flux through crawl space walls
F_{si}	m^3/m^2.d	air flux from soil to indoor air through floor
$F_{si,f}$	m^3/m^2.d	air flux from soil to indoor air through the basement floor
$F_{si,w}$	m^3/m^2.d	air flux from soil to indoor air through basement walls
$F_{si,w,d}$	m^3/m^2.d	direct air flux from soil to indoor air through basement walls
$F_{si,w,i}$	m^3/m^2.d	indirect air flux from soil to indoor air through basement walls
$F_{soil/settled\text{-}dust}$	-	Fraction soil in indoor settled dust
f_u	-	fraction unpaved

G

g	m/d	Conductance of the leaf

H

H	Pa.m^3/mol	Henry coefficient
h	m	Height for wind velocity V_h
H'	-	Dimensionless Henry coefficient
$H\ (T_B)$	Pa.m^3/mol	Henry coefficient at soil temperature
$H\ (T_H)$	Pa.m^3/mol	Henry coefficient at specified temperature
H_{sh}	Pa.m^3/mol	Henry coefficient at shower temperature

I

i	m/m	Hydraulic gradient
IR_{dust_hourly}	mg/h	Hourly ingestion of settled dust
$IR_{soil/dust\_daily}$	mg/d	Daily ingestion of soil and settled dust
IR_{soil_hourly}	mg/h	Hourly ingestion of soil
I_V	-	Fraction of particles intercepted

J

J_{ci}	mg/m^2.d	contaminant flux from crawl space to indoor space
$J_{concentrate}$	mg/d	daily contaminant intake via concentrate
J_f	mg/d	daily contaminant intake in summer or winter
$J_{f,chicken}$	mg/d	daily contaminant intake via feed
$J_{f,year}$	mg/d	daily contaminant intake on yearly basis
$J_{grass,chicken}$	mg/d	daily contaminant intake via grass
$J_{grass,silage}$	mg/d	daily contaminant intake via silage grass
J_{maize}	mg/d	daily contaminant intake via maize

$J_{mixture,chicken}$	mg/d	daily contaminant intake via feed mixture
$J_{pasture}$	mg/d	daily contaminant intake via pasture
J_{sc}	mg/m^2.d	contaminant flux from soil to crawl space
J_{si}	mg/m^2.d	contaminant flux from soil to indoor air through floor
$J_{si,f}$	mg/m^2.d	contaminant flux from soil to indoor air through the basement floor
$J_{si,w}$	mg/m^2.d	contaminant flux from soil to indoor air through basement walls
$J_{si,w,d}$	mg/m^2.d	direct contaminant flux from soil to indoor air through basement walls
$J_{si,w,i}$	mg/m^2.d	indirect contaminant flux from soil to indoor air through basement walls
J_{soil}	mg/d	daily contaminant intake via soil
$J_{soil,chikcen}$	mg/d	daily contaminant intake via soil
J_{water}	mg/d	daily contaminant intake via water

K

k	m/yr	Hydraulic conductivity of the phreatic groundwater layer
k_1	1/d	Uptake rate in the potato
k_2	1/d	depuration rate from the potato
K_{bw}	m^2/Pa.d	air conductivity of an intact basement wall
K_{CH}	l/kg fw	partition coefficient between carbohydrates and water
K_d	l/kg	Soil-water distribution coefficient
K_f	m^2/Pa.d	air conductivity of the floor
K_g	m/h	Gas phase mass transfer coefficient of H_2O
k_G	m/h	gas phase mass transfer coefficient
k_{karman}	-	von Karman constant
k_L	m/h	Fluid mass transfer coefficient
K_l	m/h	Liquid phase mass transfer coefficient of CO_2
K_{oa}	-	Octanol-air partition coefficient – if not filled in, the value is calculated
K_{oc}	l/kg	Organic carbon-water partition coefficient – calculated if no value is filled in – choice of equations
K_{ow}	-	Octanol-water partition coefficient
K_p	cm/h	dermal permeability coefficient
K_{PA}	m^3/m^3	Gas-plant partition coefficient
k_{plant}	1/d	Loss due to growth of the plant - 1st order rate
K_{PW}	l/kg fw	partition coefficient between potato and water
K_{RW}	l/kg	Partition factor plant tissue – pore water
K_{sa}	m^2/Pa.d	air conductivity of the soil layer
$K_{sa,w}$	m^2/Pa.d	air conductivity of the soil profile for basement walls
k_v	m^2	soil air permeability
$k_{v,eff}$	m^2	effective air permeability of the soil for vapour intrusion
$k_{v,eff,w}$	m^2	effective air permeability of the soil profile for basement walls
$k_{v,f}$	m^2	air permeability of the floor, intact floor
$k_{v,w}$	m^2	air permeability of the basement wall
k_w	1/d	Plant weathering constant
k_{wa}	-	Degree of volatilization (weight fraction)

L

L	m	Length of the contaminated area in dominant wind direction
L_{bs}	m	thickness of buffer space
L_{bw}	m	thickness of the basement walls

L_{cz}	m	height of the capillary zone
L_f	m	thickness of the floor
L_i	m	thickness of the ith soil layer
LIM_i	mg/kg mg/m³	Concentration Limit in compartment i
L_{leach}	m	Length of the source area
L_p	m	Total length of the drinking-water pipe through the contaminated area
L_{plant}	kg/kg	Lipid content of the plant
L_s	m	length of the zone between top of the contamination and bottom of the building floor or crawl space floor
$L_{s,w}$	m	transfer distance for wall flux, indirect or direct
$L_{s,w,d}$	m	transfer distance for direct wall flux
$L_{s,w,i}$	m	transfer distance for indirect wall flux
l_{sc}	cm	apparent thickness of the stratum corneum
$L_{T,gw,o}$	m	thickness of soil layers between the top of the groundwater layer and the soil surface
$L_{T,s,o}$	m	Thickness of soil layers between the top of the contamination and the soil surface

M

M	g/mol	Molecular weight
m	-	Regression constant
M_Z	m	thickness of the mixing zone

N

n	-	Regression constant
n_f	1/m²	number of openings per floor area

O

OC	-	Fraction organic carbon
OM	%	organic matter content

P

P	Pa	Vapour pressure
pH	-	Soil pH (pH-H_2O)
pH-KCl	-	soil pH determined with KCl
pKa	-	Acid dissociation constant
PM_{10}^{soil}	µg/m³	Concentration of PM_{10} resulting from soil

Q

Q_{beef}	g/d	Consumption of beef
Q_{butter}	g/d	consumption of butter
$q_{concentrate}$	kg dm/d	daily intake of concentrate
$Q_{drinking\_water}$	l/d	Consumption of drinking-water
Q_{dw}	m³/d	Daily drinking-water use (water use per house)
Q_{eggs}	g/d	consumption of eggs
$q_{grass,chicken}$	kg dm/d	daily consumption of grass
$q_{grass,silage}$	kg dm/d	daily consumption of silage grass
q_{maize}	kg dm/d	daily consumption of silage maize
Q_{milk}	g/d	consumption of milk

$q_{mixture,chicken}$	kg dm/d	daily consumption of feed mixture
Q_{organ_meat}	g/d	consumption of organ meat
q_p	m/yr	infiltration in the vadose zone, paved area
$q_{pasture}$	kg dm/d	daily consumption of grass
q_{soil}	kg dm/d	daily intake of soil particles
$q_{soil,chicken}$	kg dm/d	daily intake of soil by chicken
Q_{transp}	m^3/m^2.d	Transpiration rate
$q_{\mathbf{u}}$	m/yr	Infiltration in the vadose zone, unpaved area
$Q_{veg\_category}$	g fw/d	Amount of consumed vegetable category
$Q_{vegetable,i,j}$	g fw/d	amount of consumed vegetable i from category j
q_{water}	m^3/d	daily intake of water
$q_{water,chicken}$	m^3/d	daily intake of water

R

r	m	Internal radius of the drinking-water pipe
R	g/g fw	Ratio of the particles on the leaves (weight) to the total weight of the plant
$RBA_{c,soil}$	-	relative bioavailability of contaminants in soil versus food, cattle
$RBA_{drinking\_water}$	-	Relative bioavailability in drinking-water
RBA_{dust}	-	Relative bioavailability of contaminants in settled dust
RBA_{soil}	-	Relative bioavailability of contaminants in soil
r_d	m	Diameter of a drop
$RF_{drinking\_water}$	-	Reduction factor for drinking-water consumption
R_g	Pa.m^3/mol.K	Universal gas constant
RI	-	risk index for systemic effects for the specified exposure period
RI^{adult}	-	risk index for an adult for systemic effects
$RI^{adult}_{inhalation}$	-	risk index for an adult by inhalation
$RI^{adult}_{oral/dermal}$	-	risk index for an adult by the oral or dermal route
RI^{child}	-	risk index for a child for systemic effects
$RI^{child}_{inhalation}$	-	risk index for a child by inhalation
$RI^{child}_{oral/dermal}$	-	risk index for a child by the oral or dermal route
$RI_{inhalation}$	-	risk index by inhalation for the specified exposure period
$RI_{oral/dermal}$	-	risk index by the oral or dermal route for the specified exposure period
R_n	m/d	Annual rainfall
r_p	m	radius of the potato
R_w	-	Fraction retained after rainfall

S

S	mg/l	Water solubility at T_S
S’	mol/m^3	Water solubility at T_S
SA_{in}	m^2	surface area covered with dust during inside activities
SA_{out}	m^2	surface area covered with soil during outside activities
SA_{total}	m^2	total body surface area
SF_{dermal_local}	(mg/kg.d)$^{-1}$	dermal Slope Factor for local effects (absorbed dose)
SF_{dermal_syst}	(mg/kg.d)$^{-1}$	dermal Slope Factor for systemic effects (absorbed dose)
$SF_{oral/dermal}$	(mg/kg.d)$^{-1}$	slope factor for non-threshold effects by the oral or dermal route
SF_{oral_local}	(mg/kg.d)$^{-1}$	oral Slope Factor for local effects
SF_{oral_syst}	(mg/kg.d)$^{-1}$	oral Slope Factor for systemic effects

S_z	m	Pasquill dispersion coefficient

T

T	d	Averaging time
t	d	Growth period of the plant
t*	h	time to reach steady-state
T_B	K	Soil temperature
$t_{bathing}$	h	time in bath
t_{br}	h	time spent in the bathroom after showering
TCA^{adult}	mg/m³	Tolerable Concentration in air for an adult
TCA^{child}	mg/m³	Tolerable Concentration in air for a child
TCA_{inhal_local}	mg/m³	Tolerable Concentration in air for local effects
TCA_{inhal_syst}	mg/m³	Tolerable Concentration in air for systemic effects
TC_{air}	mg/m³	Tolerable Concentration in air
$TC_{animal\_product}$	mg/kg fw	Tolerable Concentration by animal product
TC_{dw}	mg/m³	Tolerable Concentration in drinking-water
$TC_{vegetable\_category}$	mg/kg fw	Tolerable Concentration by vegetable category
TDU_{dermal_local}	mg/kg.d	dermal Tolerable Daily Uptake for local effects
TDI_{oral_local}	mg/kg.d	oral Tolerable Daily Intake for local effects
TDI_{oral_syst}	mg/kg.d	oral Tolerable Daily Intake for systemic effects
$TDI/U^{adult}_{oral/dermal}$	mg/kg.d	Tolerable Daily Intake/Uptake for an adult by the oral or dermal route
$TDI/U^{age\ group}_{orla/dermal}$	mg/kg.d	Tolerable Daily Intake/Uptake by the oral or dermal route for the age group
$TDI/U^{child}_{oral/dermal}$	mg/kg.d	Tolerable Daily Intake/Uptake for a child by the oral or dermal route
TDU_{dermal_syst}	mg/kg.d	dermal Tolerable Daily Uptake for systemic effects
t_f	h	Time of fall for a drop
TF_{net}	-	Net transfer factor of particles to the plant
$t_{f,summer}$	-	time fraction for summer diet
$t_{f,winter}$	-	time fraction for winter diet
T_H	K	temperature for H
t_{in}	h/d	Time spent inside
t_{out}	h/d	Time spent outside
T_P	°C	Temperature for P
T_S	°C	Temperature for S
TSCF	-	Transpiration stream concentration factor
t_{sh}	h	duration of shower
T_{sh}	K	Shower temperature
t_{sleep}	h/d	time sleeping
t^{RES}_{in}	h	time spent indoor in scenario RES
t^{RES}_{out}	h	time spent outdoor in scenario RES
t^{RES}_{sleep}	h	time sleeping in scenario RES

U

UR	$(mg/m^3)^{-1}$	unit risk for inhalation
$UR^{age\ Group}$	$(mg/m^3)^{-1}$	unit risk for non-threshold effects for the selected age group
UR_{inhal_local}	$(mg/m^3)^{-1}$	inhalation Unit Risk for local effects
UR_{inhal_syst}	$(mg/m^3)^{-1}$	inhalation Unit Risk for systemic effects

V

V	m^3	Volume of the aboveground plant parts
V^*	m/d	Friction velocity
V_b	m^3	volume of the basement
V_{br}	m^3	volume of the bathroom
V_c	m^3	volume of the crawl space
V_d	m/d	Dry particle deposition rate
V_f	m/d	dilution rate at height Y
V_g	m/d	Average air velocity
V_h	m/d	Wind velocity at height h
V_i	m^3	volume of the indoor space
V_r	m^3	Root volume
V_{sh}	m^3	Volume of the shower stall
V_{sh}	m^3	Volume of the shower stall
vv_{br}	1/h	ventilation rate in the bathroom
vv_c	1/d	air exchange rate for crawl space
$vv_{c,b}$	1/d	basic air exchange rate for crawl space
vv_i	1/d	air exchange rate for indoor space
$vv_{i,b}$	1/d	basic air exchange rate for indoor space
V_w	m^3/h	water use during showering
V_y	*m/d*	wind velocity at height Y

W

W	kg/kg	Water content of the plant
W_c	-	Volumetric washout factor for particles
WF_{act}	-	activity-dependent inhalation rate based weighting factor
WF_{age}	-	age-dependent inhalation rate based weighting factor
WF_{inh}^{RES}	-	inhalation rate based weighting factor in scenario RES

X

X	m	Lambert X coordinate

Y

Y	m	breathing height
Yr_i	-	number of years in age category i
Y_V	kg fw/m^2	Plant yield

Z

Zo_r	m	terrain roughness length

Symbols

ΔP_{ci}	Pa	pressure difference between indoor space and crawl space
ΔP_{sc}	Pa	pressure difference between crawl space and soil
ΔP_{si}	Pa	pressure difference between indoor space and soil
$\varepsilon_{T,f}$	-	total porosity of a concrete floor, intact floor
$\varepsilon_{T,w}$	-	total porosity of the basement wall
$\varepsilon_{v,f}$	-	air-filled porosity of a concrete floor, intact floor
$\varepsilon_{v,w}$	-	air-filled porosity of the basement wall
η	Pa.d	dynamic viscosity of air

θ_a	m^3/m^3	air-filled porosity
$\theta_{a,cz}$	-	air-filled porosity in the capillary zone
θ_s	m^3/m^3	total soil porosity
θ_w	m^3/m^3	water-filled porosity
$\theta_{w,cz}$	-	water-filled porosity in the capillary zone
ρ	kg fw/m^3	Density of the plant
ρ_r	kg fw/m^3	Density of the root
ρ_s	kg/m^3	dry bulk density of the soil
ρ_w	kg/m^3	density of water
τ_{event}	hr/event	lag time per event

CHAPTER 1 INTRODUCTION

This document provides technical background information to the S-Risk model version February 2013. The software enables the calculation of generic or site-specific human health-based screening levels and the prediction of human health risks from a contaminated site. The document contains the overall lay-out of the model, the description of equations and of parameter values.

The S-Risk equations are based on a review of available approaches for fate and transfer modeling and for exposure assessment. The parameter values are based on available databases, the choices are such that sufficient protection of human receptors is anticipated. However, as the software is aimed to be used within an existing regulatory framework and will replace the current software, some choices for default values are made based on the condition that remediation values should not be significantly more conservative than actual remediation values. The influence of this condition is most pronounced in the vapour intrusion module.

The development of the S-Risk model has been a stepwise approach, starting with an initial revision document (Cornelis, Provoost, Seuntjens, and De Raeymaecker, 2008). Side-projects as well contributed to the development of the S-Risk prototype and provide documentation to parameterization of the model (Cornelis and Swartjes, 2007; Van Holderbeke, Cornelis, Bierkens, and Torfs, 2008). A first evaluation of the prototype with 3 substances resulted in the identification of some bottlenecks that required further attention (Cornelis, Bierkens, Standaert, and Willems, 2011). The model was modified based on an assessment of these bottlenecks (Cornelis and Bierkens, 2012). An extended evaluation of model outcome was done by recalculating all soil remediation value proposals with the S-Risk model. This resulted in additional bottlenecks for which final decisions were documented in separate issue documents (Cornelis, 2012a, 2012b, 2013). The current document provides the integration of the whole development process.

	**Adaptations of the initial S-Risk TGD have been made in order to be used with the Walloon version of the S-Risk model. Elements specific to the Walloon Region are highlighted using $\boxed{W}$.** **However, the Walloon experts must use the present document along with the guidance reference document for human health risk assessment (GRER part B v.03). The latter document is available on http://dps.environnement.wallonie.be/home/sols/sols-pollues/code-wallon-de-bonnes-pratiques--cwbp-.html.**

1.1. MODEL DESCRIPTION

The S-Risk model is a steady-state, mass conservation model for calculating exposure and risk of humans to soil and groundwater contaminants. It can deal with both organic and inorganic contaminants. The schematic representation of transfer and exposure pathways is given in Figure 1. The model addresses following transfer pathways:

- transfer from surface and subsurface soil to outdoor air through volatilization;

- transfer from subsurface soil to indoor air through volatilization (vapour intrusion);
- transfer from surface soil to outdoor air and indoor air through soil resuspension;
- transfer from outdoor soil to indoor settled dust;
- transfer from surface soil to vegetation through root uptake and translocation;
- transfer from surface soil to above-ground vegetation through soil splash;
- transfer from outdoor air to vegetation through vapour and particle deposition;
- transfer from soil to plastic drinking-water pipes through permeation;
- transfer from groundwater to outdoor air through volatilization;
- transfer from groundwater to indoor air through volatilization (vapour intrusion);
- transfer from soil to groundwater through leaching;
- transfer from drinking-water to bathroom air through volatilization;
- transfer from soil, water and feed to meat, milk and eggs through exposure of cattle and chicken.

The model does not cover the presence of a separate contaminant layer (pure product, floating or sinking layer in groundwater). If a calculated concentration in soil pore water exceeds solubility, the further fate and transfer calculations are based on the solubility. If a groundwater concentration exceeding the solubility is filled in, the model uses this user-defined concentration for further fate and transfer modeling. This is a conservative approach towards the concentration in pore water (which will be used for leaching and volatilization, where applicable) The concentration in pore water in equilibrium with pure product can be estimated by applying Raoult's law. The F-Leach model (available from http://www.ovam.be), developed for calculating leaching under the Flemish soil remediation policy, can be used to estimate pore water concentrations when total petroleum analysis results are available according to the TPH methodology. Evenly if time-dependency should be taken into account, complex models can be used and the output of these models can be used as input to the S-Risk model and thus overwrite intermediate results.

Exposure of humans can be calculated from following exposure pathways:

- ORAL EXPOSURE:
    - intake of soil and indoor settled dust particles;
    - intake of vegetables;
    - intake of animal products (meat, milk, eggs);
    - intake of water (drinking-water, ground water);
- INHALATION EXPOSURE:
    - inhalation of outdoor and indoor vapour phase contaminants;
    - inhalation of outdoor and indoor particle phase contaminants;
    - inhalation of vapour during showering;
- DERMAL EXPOSURE:
    - absorption from soil and settled dust particles;
    - absorption from water during bathing and showering.

Default scenarios are given, defining exposure routes and exposure parameters. The user can define own scenarios and modify exposure parameters.

Human health risk is calculated by comparing exposure dose (oral and dermal) and exposure concentration (inhalation) to toxicological reference values. The way exposure from the three exposure routes (oral, inhalation and dermal) is combined, depends on the toxicological characteristics of the compound and can be specified by the user. In a parallel step, concentrations in the environmental compartments are compared to legal or toxicological limits as to complete the risk assessment.

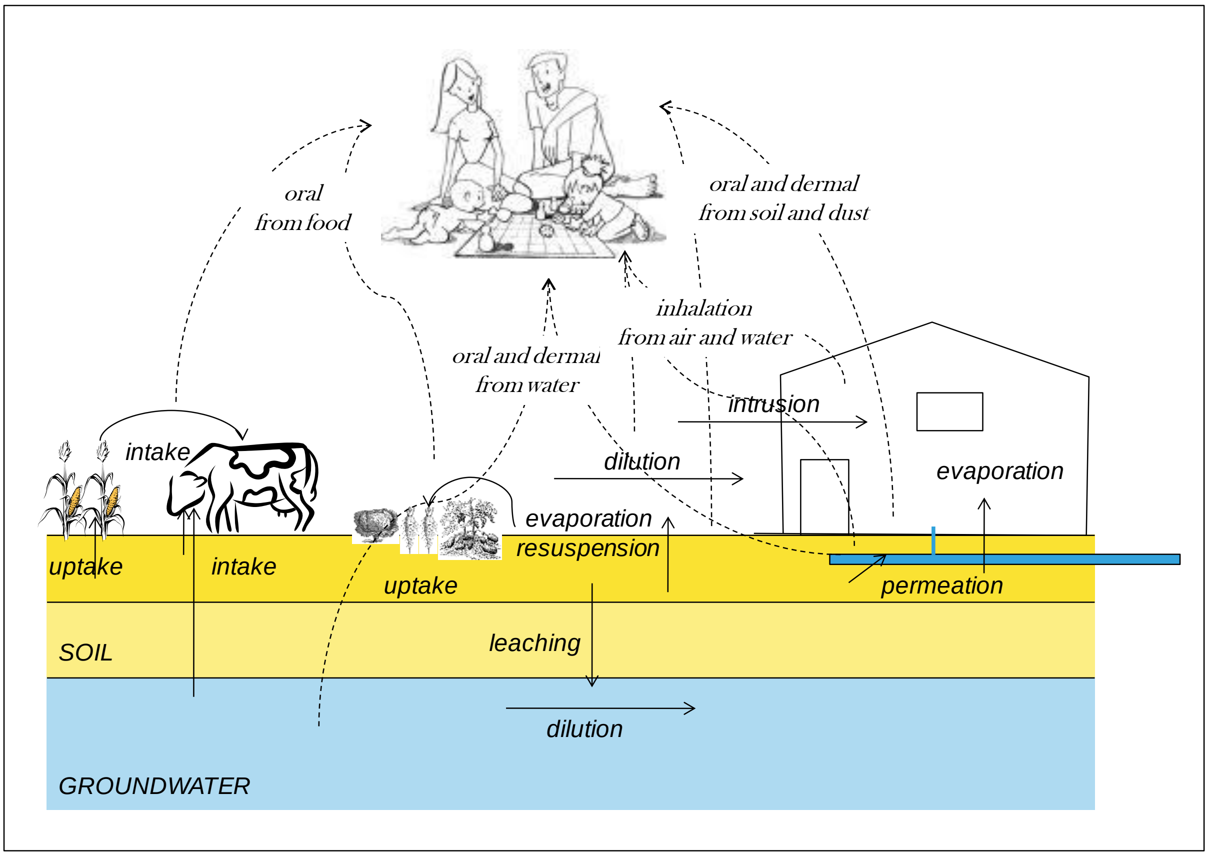

Figure 1: Scheme of transfer and intake pathways of the S-Risk model

1.2. MODEL APPLICATIONS

The S-Risk model is intended to be used for three fields of application:

- calculation of generic human health based soil remediation values as required within the legal framework in Wallonia, or as a first screening tool for local site risk assessment;
- calculation of site-specific human health risks within a detailed site assessment;
- calculation of site-specific remediation objectives.

The next paragraphs give a short overview of the characteristics of the three options.

1.2.1. APPLICATION I - GENERIC HUMAN HEALTH BASED SOIL REMEDIATION VALUES

The model concept for the calculation of human health based soil remediation values (HHB-SRVs) assumes a homogeneous soil profile, both with regard to soil properties as with regard to contamination. Only the default land use types with their corresponding scenarios are available:

- agricultural land use (type II)
- residential land use (type III)
- recreational land use (day recreation indoor and outdoor – type IV)
- industrial land use (light industry – type Va and heavy industry – type Vb).

The user needs to fill in the contaminant properties or use the built-in chemical property data base and specify the required land use type.

Then the soil remediation value is calculated for the specified land use type and each endpoint (risk metric, concentration in environmental compartments) and reported. As a default, the soil remediation value is calculated for a standard soil. The soil remediation value can also be calculated for other soil types or for varying soil properties (organic carbon, clay content, pH, CEC). Other parameters are not accessible in this application.

In the calculation of generic soil remediation values, the direct use of groundwater is only accounted for in the agricultural land use scenario. In that scenario, leaching from groundwater and subsequent use of groundwater for cattle is considered. For the other land uses only the soil compartment is taken into account. As leaching to groundwater is calculated for all land uses under the option of generic soil remediation values, groundwater could theoretically contribute to the volatilization pathways. Groundwater remediation values taken up in the Walloon legislation are based on conditions for drinking-water consumption, they are calculated outside S-Risk. If site-specific groundwater remediation values are required (e.g. no drinking-water use, but volatilization could be of concern), then application III can be used.

1.2.2. APPLICATION II- CALCULATION OF SITE-SPECIFIC HUMAN HEALTH RISKS

Site-specific human health risks can be calculated simultaneously for a series of contaminants specified by the user. The user can use default chemicals, modify these chemicals or create new records for own-defined chemicals.

The user can base its calculations on the default scenarios provided with the model or can define its own scenarios based on these built-in scenarios. Exposure pathways and exposure parameters can be modified. Default scenarios are:

- agricultural area: residence with garden in agricultural area;
- residential area with vegetable garden;
- residential area with garden;
- residential area without garden;
- day recreation mainly outdoors (incl. sport);
- day recreation mainly indoors (incl. sport);
- light industry (offices, shops, …);
- heavy industry with outside activity.

A flexible soil profile can be specified by the user. Soil properties have to be filled in for each soil layer, allowing a combination of selecting built-in soil types and user-defined values. The user also needs to give in soil concentrations for each defined soil layer. The groundwater concentration is a user input or can be predicted by the model (simple on-site dilution model). The depth of the groundwater table needs to be specified.

Specific information with regard to site conditions can be filled in, exposure patterns can be modified.

Human health risk is calculated from the specified input data. The ratio between concentrations in environmental compartments and reference values is given.

1.2.3. APPLICATION III - CALCULATION OF SITE-SPECIFIC REMEDIATION GOALS

This option allows automatic calculation of site-specific remediation goals by initializing an iterative process. It keeps the flexibility of application II. The model still allows the use of a soil profile and concentrations by soil layer. The layer for which the remediation value is calculated (layer for iteration) should be specified. Fixed concentrations can be filled in for the other layers and for groundwater. Similarly, if the soil concentrations are held fixed, a groundwater remediation goal can be calculated.

The output of the calculations is comparable with that from the calculation of soil remediation values.

CHAPTER 2 CHEMICAL PROPERTIES AND THEIR ESTIMATION

2.1. CHEMICAL PROPERTIES

The model offers a database of chemical-specific properties. New chemicals can be added or can be based on modifications of chemicals present in the database. The properties of the chemicals provided with the model can not be changed. These are the official values used for deriving soil remediation values. However, if one wants to change these fixed values, he can customize the chemical and save it with a user-defined name.

This chapter describes the required physico-chemical properties for the chemicals. Other chemical-specific information is addressed under the respective fate, transfer and exposure headings. The required physico-chemical properties for organic contaminants are listed in Table 1; the required properties for inorganic contaminants are listed in Table 2.

Table 1: Required physico-chemical properties for organic contaminants

Abbr.	Name	Unit	Default value
Name	Name of the chemical	-	-
Type	Type of chemical: organic	-	-
CAS nr.	Chemical Abstracts Service number	-	-
M	Molecular weight	g/mol	-
T_S	Temperature for S	°C	20
S	Water solubility	mg/l	-
T_P	Temperature for P	°C	20
P	Vapour pressure	Pa	-
T_H	Temperature for H (only required if H is filled in)	°C	20
H	Henry coefficient – if not filled in, H is calculated	Pa.m³/mol	- (calculated)
K_{ow}	Octanol-water partition coefficient	-	-
K_{oc}	Organic carbon-water partition coefficient – calculated if no value is filled in – choice of equations	l/kg	-
K_{oa}	Octanol-air partition coefficient – if not filled in, the value is calculated	-	- (calculated)
D_{pe}	Permeation organic substance through PE drinking-water service pipe	m²/d	-
D_{pvc}	Permeation organic substance through PVC drinking-water service pipe – if not filled in for organics, the value is set at D_{pe} / 1000	m²/d	- (calculated)
D_a	Diffusion for organic substance in air – if not filled in, the value is calculated	m²/d	- (calculated)
D_w	Diffusion for organic substance in water – if not filled in, the value is calculated	m²/d	- (calculated)
K_{oc} class	classification for calculation of Koc (only if Koc is not filled in): ▪ hydrophobic or non-hydrophobic (choice of equations) ▪ organic acid ▪ organic base	-	-
pKa	Acid dissociation constant (only required if organic acid or organic base)	-	-

The values for vapour pressure and solubility are preferably determined at the same temperature.

The solubility of inorganic contaminants is generally set at a high value (1.10^6 mg/l as a default value) because of the use of the K_d concept throughout the whole concentration range. For this reason, it is required to fill in a value for the Henry-coefficient (disabling the possibility to have it calculated from vapour pressure and solubility). For non-volatile inorganics, H will equal zero.

Table 2: Required physical-chemical properties for inorganic contaminants

Abbr.	Name	Unit	Default value
Name	Name of the chemical	-	-
Type	Type of chemical: inorganic	-	-
CAS nr.	Chemical Abstracts Service number	-	-
M	Molecular weight	g/mol	-
P	vapour pressure	Pa	0 (default)
S	solubility	mg/l	1.10^{50} (default)
H	Henry coefficient	Pa.m³/mol	0 (default)
K_d	Soil-water partition coefficient: ▪ value ▪ regression equation	l/kg	-
D_{pe}	Permeation through PE drinking-water service pipe	m²/d	0 (fixed)
D_{pvc}	Permeation through PVC drinking-water service pipe	m²/d	0 (fixed)

2.2. ESTIMATION OF PROPERTIES

2.2.1. KD VALUES

The sorption coefficient Kd gives the ratio between the concentration on the soil solid phase and in the soil water phase. It is used to calculate the distribution of the chemical over the soil phases.

→ **Inorganic chemicals**

For inorganic chemicals, the sorption coefficient Kd is a required input parameter. The sorption coefficient can be a single value or an equation, specifying the relation between the sorption coefficient and soil properties or soil concentration. If the input is a regression (on log Kd), then Kd = $10^{(\log Kd)}$.

If the option for a regression is chosen, the user is required to fill in the arguments of a function of form:

(eq. 1)

$$\log K_d = a + b \times \log CL + c \times \log C + d \times \log CEC + e \times \log OM + f \times pH - CaCl_2$$

Where

Abbr.	Name	Unit	From
K_d	soil-water sorption coefficient	l/kg	contaminant properties
CL	soil clay content	%	soil properties
C	total soil concentration	mg/kg dm	user input
CEC	cation exchange capacity	meq/100 g	soil properties
OM	organic matter content	%	soil properties
pH-$CaCl_2$	soil pH determined with $CaCl_2$	-	soil properties, calculated using (eq. 1)

→ **Organic chemicals**

For organic chemicals, either an organic carbon – water coefficient (K_{oc}) is filled in or a K_{oc} is derived from the octanol – water coefficient (Kow). We further distinguish between non-dissociating and dissociating organic chemicals.

Non-dissociating chemicals

For non-dissociating chemicals, there is a general K_{oc} equation for predominantly hydrophobic chemicals and a general K_{oc} equation for non-hydrophobic chemicals. In addition, K_{oc} equations are provided for specific chemical groups. These QSAR equations are taken from Sabljic and Gusten (1995) and are given in Table 3.

(eq. 2)

$$K_{oc} = 10^{\log K_{oc}}$$

Table 3: QSARs for estimating the Koc of organic chemicals (from ECB (2003))

Chemical class	Equation
predominantly hydrophobic chemicals*	$\log K_{oc} = 0.81 \log K_{ow} + 0.1$
non-hydrophobic chemicals**	$\log K_{oc} = 0.52 \log K_{ow} + 1.02$
acetanilides	$\log K_{oc} = 0.40 \log K_{ow} + 1.12$
alcohols	$\log K_{oc} = 0.39 \log K_{ow} + 0.50$
amides	$\log K_{oc} = 0.33 \log K_{ow} + 1.25$
anilines	$\log K_{oc} = 0.62 \log K_{ow} + 0.85$
carbamates	$\log K_{oc} = 0.37 \log K_{ow} + 1.14$
dinitroanilines	$\log K_{oc} = 0.38 \log K_{ow} + 1.92$
esters	$\log K_{oc} = 0.49 \log K_{ow} + 1.05$
nitrobenzenes	$\log K_{oc} = 0.77 \log K_{ow} + 0.55$
organic acids	$\log K_{oc} = 0.60 \log K_{ow} + 0.32$
phenols, benzonitriles	$\log K_{oc} = 0.57 \log K_{ow} + 1.08$
phenylureas	$\log K_{oc} = 0.49 \log K_{ow} + 1.05$
phosphates	$\log K_{oc} = 0.49 \log K_{ow} + 1.17$
triazines	$\log K_{oc} = 0.30 \log K_{ow} + 1.50$
triazoles	$\log K_{oc} = 0.47 \log K_{ow} + 1.41$

*: Hydrophobic chemicals are: all chemicals with only C, H, F, Cl, Br and I atoms

** : Non-hydrophobic chemicals are: all chemicals that are not classified as hydrophobics

Where

Abbr.	Name	Unit	From
K_{oc}	Organic carbon-water partition coefficient	l/kg	(eq. 2)
K_{ow}	Octanol-water partition coefficient	-	Table 1

Dissociating chemicals

For dissociating chemicals, the K_d is calculated from the K_{ow} and a correction factor for the dissociated fraction (Bintein and Devillers, 1994). The latter is a function of the soil pH (water based). (note: there was an error in this equation in the earlier versions of the report)

(eq. 3)

$$\log K_d = 0.25 + 0.93 \times \log K_{ow} + 1.09 \times \log OC + 0.32 \times Cf_a - 0.55 \times Cf_b$$

The correction factors are calculated from the pKa and the soil pH. For organic acids, Cf_b equals 0; for organic bases; Cf_a equals 0.

(eq. 4)

$Cf_a = -\log\left(1 + 10^{(pH - pKa)}\right)$ in case of an organic acid;
or $Cf_a = 0$ in case of an organic base

(eq. 5)

$Cf_b = -\log\left(1 + 10^{(pKa - pH - 2)}\right)$ in case of an organic base;
or $Cf_b = 0$ in case of an organic acid

For organic bases, the pH of the soil solution is corrected as it was shown that the pH at the soil exchange sites is lower than the pH in the soil solution. Anionic species are mostly located in the soil solution and no correction is needed.

Where

Abbr.	Name	Unit	From
K_d	Organic carbon-water partition coefficient	l/kg	(eq. 3)
K_{ow}	Octanol-water partition coefficient	-	chemical properties
OC	Fraction organic carbon	-	
			(eq. 8)
Cf_a	Correction factor for organic acids	-	(eq. 4)
Cf_b	Correction factor for organic bases	-	(eq. 5)
pH	Soil pH (pH-H_2O)	-	(eq. 15)
pKa	Acid dissociation constant	-	Chemical properties

The sorption coefficient Kd is then calculated as the product between the organic carbon – water coefficient and the fraction organic carbon in the soil.

(eq. 6)

$$K_d = OC \times K_{oc}$$

For dissociating chemicals, the sorption coefficient Kd is calculated as

(eq. 7)

$$K_d = 10^{log(K_d)}$$

The organic carbon content OC can be calculated from the soil organic matter content.

(eq. 8)

$$OC = \frac{OM}{100} \times 0.58$$

Where

Abbr.	Name	Unit	From
K_d	Soil-water distribution coefficient	l/kg	(eq. 6)
OC	Fraction organic carbon	-	(eq. 8) or Table 4
K_{oc}	Organic carbon-water partition coefficient	l/kg	Chemical properties Table 1 or calculated
OM	Organic matter content	%	Table 4

2.2.2. HENRY COEFFICIENT

The partioning of a chemical between soil pore water and soil air is calculated by the dimensionless Henry coefficient. The dimensionless Henry coefficient is calculated within the model from the Henry coefficient. If the Henry coefficient is not known, it can be calculated from the vapour pressure and the solubility of a chemical.

(eq. 9)

$$H' = \frac{H}{R_g \times T_H}$$

(eq. 10)

$$H = \frac{P}{S'}$$

(eq. 11)

$$S' = \frac{S}{M}$$

Where

Abbr.	Name	Unit	From
H’	Dimensionless Henry coefficient	-	(eq. 9)
H	Henry coefficient	Pa.m³/mol	Chemical properties or (eq. 10)

Abbr.	Name	Unit	From
R_g	Universal gas constant	Pa.m³/mol.K	8.3144
T_H	Temperature for H	K	Chemical properties
P	Vapour pressure at T_P	Pa	Chemical properties
S	Water solubility at T_S	mg/l	Chemical properties
S'	Water solubility at T_S	mol/m³	(eq. 11)
M	Molecular weight	g/mol	Chemical properties

The Henry coefficient depends upon the temperature. In most cases, the Henry coefficient or the vapour pressure and water solubility will not be available at soil temperature. Therefore the Henry coefficient is transformed to its value at soil temperature, using a simplification of the Clausius-Clapeyron equation (ECETOC, 1992). The Clausius-Clapeyron equation requires knowledge of the enthalpy of vaporization. The empirical temperature correction factor is an average for a large number of chemicals and is derived by Wolff and van der Heijde (1982). A calculator for the temperature dependence of Henry's law coefficient is also available at http://www.epa.gov/athens/learn2model/part-two/onsite/esthenry.html.

(eq. 12)

$$H(T_B) = H(T_H) \times e^{(0.024 \times (T_B - T_H))}$$

Where

Abbr.	Name	Unit	From
H (T_B)	Henry coefficient at soil temperature	Pa.m³/mol	(eq. 12)
H (T_H)	Henry coefficient at specified temperature	Pa.m³/mol	Chemical properties
T_B	Soil temperature	K	283
T_H	Temperature for H	K	Chemical properties

The soil temperature (T_B) is equal for all soil depths. The temperature of the Henry coefficient is either the value filled in the database or the value at which vapour pressure is determined (if the Henry coefficient is calculated from vapour pressure and solubility). It is therefore recommended to have the same reference temperatures of vapour pressure and solubility. As well, the reference temperature for the Henry coefficient (or vapour pressure) should be as close as possible to the soil temperature.

2.2.3. DIFFUSION COEFFICIENT IN AIR AND WATER

The coefficient for gas diffusion in air D_a can be estimated from the molecular weight (M) by

(eq. 13)

$$D_a = 0.036 \times 24 \times \sqrt{\frac{76}{M}}$$

The coefficient for gas diffusion in water D_w can be estimated from the molecular weight (M) by

(eq. 14)

$$D_w = 3.6 \times 10^{-6} \times 24 \times \sqrt{\frac{76}{M}}$$

Where

Abbr.	Name	Unit	From
D_a	Constant for gas diffusion in air	m^2/d	chemical properties or (eq. 13)
D_w	Constant for gas diffusion in water	m^2/d	Chemical properties or (eq. 14)
M	Molecular weight	g/mol	Chemical properties

A variety of more complex models is available to estimate air and water diffusion coefficients. A calculator is available at the US-EPA website for Site assessment calculations (http://www.epa.gov/athens/learn2model/part-two/onsite/estdiffusion.htm).

CHAPTER 3 DISTRIBUTION IN SOIL

This part of the model calculates the distribution of the contaminant concentration over the solid, the water and the air phases of the soil. Calculation starts from the measured total soil concentration (mg/kg dm). As each soil layer is described by its soil type and associated soil properties, the distribution over the soil phases is calculated per soil layer of the unsaturated zone.

3.1. SOIL PROPERTIES W

The required soil properties and their default values for a standard soil and soil types according to the Belgian soil classification are given in Table 4. The values are based on the database Aardewerk (Van Orshoven & al., 1988 – 1993) and on a version adapted for Wallonia by Legrain (2005). Background to the data and equations to estimate soil properties from organic matter content and particle size distribution are given in Bah & al (2015) and summarized in Annex B3 of the GRER part B v.03. Organic matter content can be filled in as percentage organic matter or as fraction organic carbon. If the percentage organic matter is filled in, the fraction organic carbon is calculated automatically according to (eq. 8). When organic matter and clay content are modified by the user to reflect site-specific estimates, the other soil profile parameters should be adapted as well. The data for the standard soil except the generic soil layer and standard remblai are median values of all data points in the Walloon version of the Aardewerk database. The selection of the parameters of the generic soil is detailed in Bah & al (2015) and ISSeP (2015). The data used (organic matter, clay content and pH) for standard remblai are explained in SPAQuE (2015).

Table 4: Default soil properties per soil type ***W***

Soil class	Name	OM (%)	OC (-)	ρ_s (kg/m³)	θ_w (-)	θ_a (-)	θ_s (-)	CL (%)	CEC (meq/100g)	pH-KCl	$\theta_{w,cz}$ (-)	L_{cz} (m)	k_v (m²)
Ge	Generic	2,3	0,0133	1236	0,287	0,247	0,534	9,0	11,0	3,9	0,391	1,2	1,4E-13
A	Loam	2,5	0,0147	1220	0,345	0,202	0,547	14,0	12,0	5,8	0,401	8,1	2,3E-14
E	Clay	4,4	0,0254	1111	0,395	0,190	0,584	24,6	19,3	5,5	0,443	3,8	2,5E-14
L	Sandy loam	2,8	0,0160	1127	0,341	0,243	0,584	12,0	12,9	5,4	0,415	2,3	4,8E-14
P	Light sandy loam	2,2	0,0130	1239	0,283	0,254	0,537	8,0	10,4	5,1	0,389	1,2	1,4E-13
S	Loamy sand	2,8	0,0160	1303	0,253	0,262	0,514	6,0	10,9	4,4	0,376	1,0	2,2E-13
U	Heavy clay	6,8	0,0398	965	0,469	0,158	0,627	40,0	28,6	5,6	0,490	7,3	1,3E-14
Z	Sand	3,3	0,0189	1266	0,209	0,319	0,528	2,0	8,3	3,4	0,365	0,8	3,8E-13
G	Loamy-stony	6,0	0,0348	948	0,401	0,243	0,644	18,1	15,3	4,3	0,452	3,4	2,7E-14
R	Remblai	7,1	0,0412	1236	0,287	0,247	0,534	5,8	11,0	7,5	0,391	1,2	1,4E-13

Abbr.	Name	Unit	From
OM	organic matter content	%	Table 4 or user input
OC	organic carbon fraction	-	Table 4 or user input or calculated from OM
ρ_s	soil dry bulk density	kg/m^3	Table 4 or user input
θ_w^*	volumetric water content	m^3/m^3	Table 4 or user input
θ_a^*	volumetric air content	m^3/m^3	Table 4 or user input
θ_s^*	soil porosity	m^3/m^3	Table 4 or user input
CL	clay content	%	Table 4 or user input
CEC	Cation Exchange Capacity	meq/100 g	Table 4 or user input
pH-KCl	acidity of the soil (KCl)	-	Table 4 or user input
$\theta_{w,cz}$	water-filled porosity in the capillary zone	-	Table 4 or user input
L_{cz}	height of the capillary zone	m	Table 4 or user input
k_v	soil air permeability	m²	Table 4 or user input

The model requires the input of a pH-KCl value as this is the routinely used method for pH measurements in soil. Some model equations need pH values based on H_2O or $CaCl_2$, and therefore the model converts the KCl value to a H_2O based value and a $CaCl_2$ based value (Smolders, et al., 2007).

(eq. 15)

$$pH - H_2O = 1.90 + 0.79 \times pH - KCl$$

(eq. 16)

$$pH - CaCl_2 = 0.79 + 0.89 \times pH - KCl$$

Abbr.	Name	Unit	From
pH-H_2O	pH water base	-	(eq. 15)
pH-KCl	pH KCl base	-	Table 4 or user input
pH-$CaCl_2$	pH $CaCl_2$ base	-	(eq. 16)

3.2. CONNECTING CONCENTRATIONS TO SOIL PROFILE AND SOIL PROPERTIES

For site-specific assessments, the user needs to specify a soil profile (giving values for the soil properties) and concentrations. Concentrations are given for the layers of the soil profile and are automatically linked to transfer/exposure routes as clarified in Table 5.

Table 5: Linkages between contaminant concentrations and soil profile

Route	Layer	Linkage
soil resuspension	top soil	independent from soil properties
soil ingestion	top soil	independent from soil properties
plant uptake	0 – 30 cm	depth-weighted average of soil properties
permeation through drinking-water pipes	depth specified by user	properties of soil layer at corresponding depth
volatilization from unsaturated zone	depth profile specified by user	concentration connected to top of each concentration layer; properties of soil layer at corresponding depth
volatilization from groundwater	depth of groundwater table specified by user	concentration at groundwater table, transfer through capillary zone and unsaturated zone

3.3. SOIL PARTITIONING

The concentration on the solid phase is calculated from the total concentration, the air and water filled porosity, the bulk density of the soil and the distribution coefficients of the contaminant.

(eq. 17)

$$C_s = \frac{C \times \rho_s}{\frac{(\theta_w + \theta_a \times H')}{K_d} \times 1000 + \rho_s}$$

Where

Abbr.	Name	Unit	From
C_s	soil solid phase concentration	mg/kg dm	(eq. 17)
C	Measured concentration in soil	mg/kg dm	user input
ρ_s	Soil dry bulk density	kg/m^3	Table 4 or user input
θ_w	Volumetric soil water content	m^3/m^3	Table 4 or user input
θ_a	Volumetric soil air content	m^3/m^3	Table 4 or user input
H’	Dimensionless Henry coefficient or water-air distribution coefficient (at soil temperature)	-	(eq. 12)
K_d	Soil-water distribution coefficient	l/kg	(eq. 6) or Table 2

The concentration in soil pore water is calculated from the concentration on the solid phase and the soil-water distribution coefficient. For organic contaminants, the maximum concentration in soil water equals water solubility.

(eq. 18)

$$C_w = \frac{C_s}{K_d} \times 1000$$

and, for organic contaminants

(eq. 19)

$$C_w(max) = S$$

Where

Abbr.	Name	Unit	From
C_w	soil pore water concentration	mg/m^3	(eq. 18)
C_s	soil solid phase concentration	mg/kg dm	(eq. 17)
K_d	Soil-water distribution coefficient	l/kg	(eq. 6) or Table 2
C_w(max)	maximum soil pore water concentration for organic contaminants	mg/m^3	(eq. 19)
S	water solubility at soil temperature	mg/m^3	Chemical properties

The concentration in soil air is calculated from the concentration in soil pore water and the dimensionless Henry coefficient.

(eq. 20)

$$C_{sa} = H' \times C_w$$

Where

Abbr.	Name	Unit	Source
C_{sa}	soil air phase concentration	mg/m³	(eq. 20)
H’	Dimensionless Henry coefficient or water-air distribution coefficient	-	(eq. 12) and (eq. 9)
C_w	soil pore water concentration	mg/m³	(eq. 18) or (eq. 19)

CHAPTER 4 CONCENTRATION IN GROUNDWATER AND DRINKING-WATER

4.1. INTRODUCTION

The model allows the calculation of a concentration in groundwater from the concentration in soil due to leaching, or the use of a groundwater concentration specified by the user. This concentration can be either a measured concentration, or a concentration calculated by an external model.

If a plastic drinking-water pipe is located in a contaminated zone, the model calculates the concentration in the water pipe due to permeation through the pipe wall. Permeation is only taken into account for organic contaminants.

The concentration in drinking-water is then based on the concentration in groundwater and the concentration in the water pipe, weighted by the fraction of groundwater being used as drinking-water.

4.2. MIGRATION TO GROUNDWATER

The concentration in groundwater is calculated from the concentration in soil pore water by means of a dilution factor. The calculation is run for each soil layer and the final groundwater concentration is the highest value of the separate concentrations. The calculations allow to account for paved, less permeable, areas on the site.

(eq. 21)

$$C_{gw} = \max_i \frac{C_{w,i}}{DF_{gw}}$$

Where

Abbr.	Name	Unit	Source
C_{gw}	Concentration in groundwater	mg/m^3	(eq. 21)
DF_{gw}	Dilution factor from pore water to groundwater	-	(eq. 22)
$C_{w,i}$	Concentration in soil pore water of layer i	mg/m^3	(eq. 18) or (eq. 19)

(eq. 22)

$$DF_{gw} = \frac{k \times i \times M_z + L_{leach} \times (q_u \times f_u + q_p \times f_p)}{L_{leach} \times (q_u \times f_u + q_p \times f_p)}$$

(eq. 23)

$$f_p = 1 - f_u$$

Where

Abbr.	Name	Unit	Source
DF_{gw}	Dilution factor for pore water to groundwater	-	(eq. 22)
k	Hydraulic conductivity of the phreatic groundwater layer	m/y	Table 7
i	Hydraulic gradient	m/m	Table 7
M_Z	thickness of the mixing zone	m	(eq. 24)
L_{leach}	Length of the source area	m	Table 7
q_u	Infiltration in the vadose zone, unpaved area	m/y	Table 7
q_p	infiltration in the vadose zone, paved area	m/y	user input
f_u	fraction unpaved	-	Table 7
f_p	fraction paved	-	(eq. 23)

(eq. 24)

$$M_z = min\left[\sqrt{0.0112 \times L_{leach}^2} + d_a \times \left(1 - e^{\left(-\frac{L_{leach} \times (q_u + q_p)}{k \times i \times d_a}\right)}\right), d_a\right]$$

Where

Abbr.	Name	Unit	Reference
M_Z	thickness of the mixing zone	m	(eq. 24)
L_{leach}	Length of the source area	m	Table 7
d_a	Thickness of the phreatic groundwater layer	m	Table 7
k	Hydraulic conductivity of the phreatic groundwater layer	m/yr	Table 7
i	Hydraulic gradient	m/m	Table 7
q_u	Infiltration in the vadose zone, unpaved area	m/yr	Table 7
q_p	infiltration in the vadose zone, paved area	m/yr	user input

Under the default values of application I, the dilution factor DF_{gw} equals 1.73.

4.3. PERMEATION THROUGH DRINKING-WATER PIPES

Organic contaminants can permeate through plastic drinking-water pipes. Three different processes can be distinguished:

- dissolution of the organic contaminant in the outside polymer of the pipe.
- diffusion of the contaminant through the polymer.
- dissolution of the contaminant from the polymer into the water present inside the pipe.

As a default, the assumed material of the supply water pipe in the soil is polyethylene (PE). The user can choose between a drinking-water pipe of polyethylene, PVC or other material. A user-defined permeation coefficient (contaminant-specific) is needed for a polyethylene (PE) drinking-water pipe.

The permeation coefficient for PVC is estimated to be 1/1000 of the permeation coefficient of PE. For other materials, the permeation coefficient is set at 0.

The concentration of a contaminant in drinking-water following permeation is calculated according to Vonk (1985).

(eq. 25)

$$C_{wp} = \frac{2 \times (D_p \times C_w \times \frac{dt}{24})}{r \times d_e} \times \frac{(\pi \times r^2 \times L_p)}{Q_{dw}}$$

Where

Abbr.	Name	Unit	Source
C_{wp}	Water concentration in a pipe as a result of permeation	mg/m³	(eq. 25)
D_p	Permeation coefficient	m²/d	Table 6
C_w	soil pore water concentration at depth of the drinking-water pipe	mg/m³	(eq. 18)
dt	Standard stagnation time in pipe	h/d	Table 7
r	Internal radius of the pipe	M	Table 7
d_e	Thickness of the drinking-water pipe wall	M	Table 7
L_p	Total pipe length through the contaminated area	M	Table 7
Q_{dw}	Daily drinking-water use (water use per house)	m³/d	Table 7

Table 6: Values for the permeation coefficient through drinking-water pipes D_p (m²/d)

Pipe material	D_p
polyethylene (PE)	chemical properties
polyvinylchloride (PVC)	chemical properties or D_p (PE)/1000
other material	0

4.4. CONCENTRATION IN DRINKING-WATER

The final concentration in drinking-water results from the contribution of the concentration after permeation and the concentration in groundwater, allowing for local use of groundwater as drinking-water.

(eq. 26)

$$C_{dw} = C_{wp} \times (1 - f_g) + C_{gw} \times f_g$$

Where

Abbr.	Name	Unit	Source
C_{dw}	Drinking-water concentration	mg/m³	(eq. 26)
C_{wp}	Concentration as a result of permeation	mg/m³	(eq. 25)
f_g	Fraction of groundwater used as drinking-water	-	Table 45
C_{gw}	Concentration in groundwater	mg/m³	

(eq. 21)

Table 7: Default water properties for use in application I

Abbr.	Name	Unit	Value
k	Hydraulic conductivity of the phreatic groundwater layer	m/yr	365
i	Hydraulic gradient	m/m	0.001
L_{leach}	Length of source area	m	50
q_u	Infiltration in the vadose zone, unpaved area	m/yr	0.265
f_u	fraction unpaved	-	1
d_a	thickness of the phreatic groundwater layer	m	30
dt	stagnation time in drinking-water pipe	h/d	24
r	Internal radius of the drinking-water pipe	m	0.0098
d_e	Thickness of the drinking-water pipe wall	m	0.0027
L_p	Total length of drinking-water pipe through the contaminated area	m	50
Q_{dw}	Daily drinking-water use per house	m^3/d	0.5

CHAPTER 5 CONCENTRATION IN AMBIENT AIR

5.1. INTRODUCTION

The concentration in ambient air is the result of volatilization of a contaminant present in soil or groundwater and subsequent dilution in outdoor air, and of soil resuspension. The latter process is only relevant if contaminants are present at the soil surface (topsoil).

The concentration in each soil layer is attributed to the top of that soil layer. The ambient air concentration due to volatilization is calculated for each soil layer and for groundwater and the highest resulting value is taken as the ambient air concentration due to volatilization. The ambient air concentration due to soil resuspension is added to the volatilization concentration.

The concentration in outdoor air due to volatilization is the result of two processes:

- Contaminant flux (diffusion) from soil or groundwater to the soil surface;
- Dilution of the soil flux by the wind.

Volatilization from top soil is calculated following the equations given in US-EPA (1996b) – part 2, which are based on the Jury et al. (1984) model for infinite sources. Modifications were introduced as S-Risk starts the calculations from a soil air concentration, whereas US-EPA (1996a) starts from the total soil concentration. The topsoil calculations use the properties of the topsoil layer. For contamination present in subsurface soil or in deeper layers, the concentration in ambient air is calculated from the diffusion flux according to Fick's first law and is similar to the equation in the RBCA Toolkit (GSI, 2007). The diffusion coefficient is calculated from the properties of the above layers. For groundwater, the height of the capillary fringe is calculated and diffusion is assumed to take place from the groundwater table, through the capillary fringe and the unsaturated zone.

If a paved area is present over the contamination, one could define a surrogate top soil layer with the thickness and the porosity of this pavement to include diffusion through that layer.

The flux coming from the contaminated area is diluted in a box, assumed to have the same dimensions of the contaminated area and a height, given by the required height at which the concentration should be available (breathing zone of adult or child, height of plant). The calculations assume that the initial concentration in ambient air entering the box equals zero.

Soil resuspension follows the impact of soil by larger sand particles. The process of soil resuspension can be described following a mechanistic approach. In that case, the saltation flux of sand particles is calculated first and then the vertical flux of fine soil particles is calculated from the strength of the saltation flux and from soil properties. This vertical flux is then the input of the same dilution box model as used for volatile contaminants, to calculate the concentration of PM_{10} in air due to soil resuspension. As this mechanistic approach still needs more validation, it is not available in the model yet. The default approach is empirical and starts from a given concentration of PM_{10}, which is assumed to be of soil origin. The concentration of the contaminant due to soil resuspension is then calculated from that PM_{10} concentration, the concentration in soil and an enrichment factor for differences in particle size between soil and PM_{10}.

The final concentration in ambient air is the sum of the concentration due to volatilization and the concentration due to soil resuspension.

5.2. CONCENTRATION IN AMBIENT AIR DUE TO VOLATILIZATION

The concentration in ambient air is the result of a diffusion flux from soil and a dilution flux in ambient air. As the diffusion flux is dependent on the concentration in ambient air, the dilution flux is not explicitly calculated, but the concentration in ambient air is calculated directly from the concentration in soil (see 5.2.2). The equations require knowledge of the dilution rate in ambient air, which is calculated according to the equations described in 5.2.1 The concentration in ambient air is calculated at three heights: child, adult, and vegetation and serves as input for the corresponding exposure or transfer equations (inhalation child, adult and gas-phase transfer to plants).

The model does not take into account background levels in air.

5.2.1. DILUTION RATE

(eq. 27)

$$V_f = V_g \times \frac{S_z}{L}$$

Where

Abbr.	Name	Unit	Source
V_f	Dilution rate at height Y	m/d	(eq. 27)
V_g	Average air velocity	m/d	(eq. 28)
S_z	Pasquill dispersion coefficient	m	(eq. 32)
L	Length of the contaminated area (in dominant wind direction)	m	Table 9

(eq. 28)

$$V_g = \frac{V_y + V^*}{2}$$

Where

Abbr.	Name	Unit	Source
V_g	Average air velocity	m/d	(eq. 28)
V_y	Wind velocity at height Y	m/d	(eq. 29)
V^*	Friction velocity	m/d	(eq. 30)

The wind velocity V_Y is calculated, taking into account the roughness length (*Zo_r*) of the site. If the *Zo_r* is greater than Y (height at which the dilution rate is calculated), then V_Y equals 0; otherwise, V_Y is calculated.

(eq. 29)

If $Zo_r > Y$, then $V_Y = 0$
else

$$V_y = ln\left(\frac{Y}{Zo_r}\right) \times \frac{V^*}{k_{karman}}$$

Where

Abbr.	Name	Unit	Source
V_y	wind velocity at height Y	m/d	(eq. 29)
Y	breathing height	m	Table 9
Zo_r	terrain roughness length	m	Table 46 or user input
V^*	friction velocity	m/d	(eq. 30)
k_{karman}	von Karman constant	-	Table 9

(eq. 30)

$$V^* = \frac{k_{karman} \times V_h}{ln\left(\frac{h}{Zo_r}\right)}$$

Where

Abbr.	Name	Unit	Source
V^*	Friction velocity	m/d	(eq. 30)
k_{karman}	von Karman constant	-	Table 9
V_h	Wind velocity at height h	m/d	Table 9 or site-specific value (eq. 31)
h	Height for wind velocity V_h	m	Table 9

Zo_r	Terrain roughness length	m	Table 46 or user input

The value of V_h is the average wind speed at the meteorological station of Deurne (near Antwerp). A site-specific value can be calculated as a function of the Lambert X coordinate of the site (only applicable within Flanders).

(eq. 31*) is not implemented in the software. The default value is provided and the user can change the value according to own data or calculations with the equation given below.*

(eq. 31)

$$V_h = \left(-3.10^{-5} \times X + 18.915\right) \times 24000$$

Where

Abbr.	Name	Unit	Source
V_h	Wind velocity at height h	m/d	(eq. 31)
X	Lambert X coordinate	m	user input

(eq. 32)

$$S_z = C_o \times 0.2 \times L^{0.76}$$

Where

Abbr.	Name	Unit	Source
S_z	Pasquill dispersion coefficient	m	(eq. 32)
C_o	Correction factor for terrain roughness length	-	(eq. 33)
L	Length of the contaminated area in dominant wind direction	m	user input

(eq. 33)

$$C_o = (10 \times Zo_r)^{0.53 \times L^{-0.22}}$$

Where

Abbr.	Name	Unit	Source
C_0	Correction factor for terrain roughness length	-	(eq. 33)
Zo_r	Terrain roughness length	m	Table 46 or user input
L	Length of the contaminated area in dominant wind direction	m	user input

Scenario-specific defaults for Zo_r are given in Table 46. Possible values for modification of the defaults are given in Table 8. Default values for the scenarios are given in bold in the latter table.
The length of the site in the dominant wind direction is a user input value. For application I, the value is set at 50 m in line with the default of the first Tier of the leaching methodology (OVAM, 2005) and the F-Leach model.

Table 8: Roughness length for a series of land cover (source:EC (1993)) (default values are marked in bold and are taken up in Table 46)

Land use	Soil cover	Zo_r (m)
residential area	continuous urban area	**1.100**
	discontinuous urban area	**0.600**
	green urban area	0.100
industrial area	industrial or commercial area	**0.600**
	roads and railroads	0.100
	port	0.600
	airport	0.100
	mines	0.100
	landfills	0.600
	construction sites	0.600
recreation	sport and recreation	**0.100**
agriculture	non-irrigated agricultural area	0.600
	fruit trees and orchards	0.034
	pasture	**0.100**
	complex cultivated land	0.100
	agricultural area with natural vegetation	1.200

Land use	Soil cover	Zo_r (m)
nature	deciduous wood	1.200
	pine wood	1.200
	mixed woods	0.034
	natural grass land	0.034
	heathland	0.300
	bushes	0.010
	sand, dunes	0.010
	limited vegetation	0.010
	fenland	0.010
	water areas	0.001

5.2.2. CONCENTRATION IN AMBIENT AIR

→ **Contaminant present in topsoil**

For contaminants present in the topsoil layer, the simplified solution of the Jury model for an infinite source is used (US-EPA, 1996b).

The concentration in outdoor air relates to the concentration in the topsoil layer as follows

(eq. 34)

$$C_{ao,Y,v} = \sqrt{\frac{4 \times D_{eff}^{sa}}{\pi \times T}} \cdot \frac{1}{V_f} \cdot C_{sa,t}$$

Where

Abbr.	Name	Unit	Source
$C_{ao,Y,v}$	concentration in ambient air at height Y due to volatilization	mg/m³	(eq. 34)
D^{sa}_{eff}	Effective diffusion coefficient in air in soil air	m²/d	(eq. 36)
$C_{sa,t}$	concentration in topsoil air	mg/m³	
			(eq. 20)
V_f	dilution rate at height Y	m/d	(eq. 27)
T	Averaging time	d	*

* Averaging time is the time period over which exposure takes place; at the moment the values are fixed, but this should be linked to the exposure averaging time (which is, in turn, linked to toxicity calculations):

Agricultural and Residential areas: 6yrs * 365 (child);
Recreational areas: 6yrs * 365
Industrial areas: 45yrs * 365

→ **Contaminant present in subsurface soil**

The flux calculations from subsurface soil follow Fick's first law of diffusion and are generally described as $J = D/L \cdot (C\_2 - C\_1)$, where D is the diffusion coefficient, L is the distance over which diffusion occurs (diffusion length) and the difference between C_2 and C_1 reflects the concentration gradient over the diffusion length. The concentration in ambient air is calculated according to the general equation $C = (J \times L)/(V\_f \times Y)$. The presence of a stagnant air boundary layer is not accounted for.

Two variables are unknown: the concentration in soil air at the soil surface and the concentration in ambient air. By substitution, the concentration in ambient air is calculated directly from the concentration in soil air. The ambient air concentration is calculated for each subsurface soil layer.

(eq. 35)

$$C_{ao,Y,v} = \frac{1}{1 + \frac{L_{T,s,o} \times V_f}{D^{sa}_{eff,o}}} \times C_{sa}$$

Where

Abbr.	Name	Unit	Source
$C_{ao,Y,v}$	concentration in ambient air at height Y due to volatilization	mg/m³	(eq. 35)
C_{sa}	concentration in soil air	mg/m³	(eq. 20)
$L_{T,s,o}$	thickness of the layer between soil surface and top of the contamination	m	to be calculated from contaminant profile
$D^{sa}_{eff,o}$	effective diffusion coefficient in soil for ambient air calculations	m²/d	(eq. 37)
V_f	dilution rate at height Y	m/d	(eq. 27)

The effective diffusion coefficient in a layer is calculated using the Millington-Quirk relationship. The effective diffusion coefficient for a series of soil layers is calculated from the effective diffusion coefficients of the separate layers

(eq. 36)

$$D^{sa}_{eff} = D_a \times \left(\frac{\theta_a^{\frac{10}{3}}}{\theta_s^2} \right) + D_w \times \frac{1}{H'} \times \left(\frac{\theta_w^{\frac{10}{3}}}{\theta_s^2} \right)$$

(eq. 37)

$$D^{sa}_{eff,o} = \frac{L_{T,s,o}}{\sum_n \frac{L_{i,o}}{D^{sa}_{eff,i}}}$$

Where

Abbr.	Name	Unit	Reference
D^{sa}_{eff}	effective diffusion coefficient in soil air	m²/d	(eq. 36)
D_a	diffusion coefficient in air	m²/d	chemical properties or (eq. 13)
D_w	diffusion coefficient in water	m²/d	chemical properties or (eq. 14)

Abbr.	Name	Unit	Reference
$D^{sa}_{eff,o}$	effective diffusion coefficient in soil air for a series of soil layers, outdoor air concentration	m²/d	(eq. 37)
$L_{T,s,o}$	Thickness of soil layers between the top of the contamination and the soil surface	m	calculated from soil profile
$L_{i,o}$	thickness of the soil layer	m	user input
H'	dimensionless Henry coefficient	-	(eq. 9)
θ_w	water-filled porosity	-	Table 4 or user input
θ_a	air-filled porosity	-	Table 4 or user input
θ_s	total soil porosity	-	Table 4 or user input

→ **Contaminant present in groundwater**

The concentration in soil air at the groundwater table is calculated from the concentration in groundwater. This concentration is then used to calculate the flux through the capillary zone and the unsaturated zone. The equations used are similar to those of a subsurface contamination.

(eq. 38)

$$C_{ao,Y,v} = \frac{1}{\left(1 + \frac{L_{T,gw,o} \times V_f}{D^{gw}_{eff,o}}\right)} \times C_{sa,g}$$

(eq. 39)

$$C_{sa,g} = C_{gw} \times H'$$

Where

Abbr.	Name	Unit	Reference
$C_{ao,Y,v}$	concentration in ambient air at height Y due to volatilization	mg/m³	(eq. 38)
$C_{sa,g}$	concentration in soil air due to volatilization from groundwater	mg/m³	(eq. 39)
$D^{gw}_{eff,o}$	effective diffusion coefficient in soil air for transfer from groundwater to topsoil	m²/d	(eq. 40)
$L_{T,gw,o}$	thickness of soil layers between the top of the groundwater layer and the soil surface	m	calculated from soil profile
C_{gw}	concentration in groundwater	mg/m³	calculated or user input
H'	dimensionless Henry coefficient	-	(eq. 9)
V_f	dilution rate at height Y	m/d	(eq. 27)

The overall effective diffusion coefficient is given by the effective diffusion coefficients of the capillary zone and the soil layers between the top of the capillary zone and the soil surface.

(eq. 40)

$$D_{eff,o}^{gw} = \frac{L_{T,gw,o}}{\frac{L_{cz}}{D_{eff}^{cz}} + \sum_i \frac{L_{i,o}}{D_{eff,i}^{sa}}}$$

(eq. 41)

$$\theta_{a,cz} = \theta_s - \theta_{w,cz}$$

Where

Abbr.	Name	Unit	Reference
$D^{gw}_{eff,o}$	effective diffusion coefficient in soil air for transfer from groundwater to topsoil	m²/d	(eq. 40)
$L_{T,gw,o}$	Thickness of soil layers between the top of the groundwater layer and the soil surface	m	calculated from soil profile
L_{cz}	height of the capillary zone	m	Table 4 or user input
$L_{i,o}$	thickness of the soil layer	m	user input
D^{cz}_{eff}	effective diffusion coefficient in the capillary zone	m²/d	(eq. 36): θ_w replaced by $\theta_{w,cz}$
$\theta_{a,cz}$	air-filled porosity in the capillary zone	-	(eq. 41)
$\theta_{w,cz}$	water-filled porosity in the capillary zone	-	Table 4 or user input

The height and the water-filled porosity of the capillary zone were calculated according to the method provided in the Johnson & Ettinger user's guide (US-EPA, 2004b).

→ **Overall ambient air concentration due to volatilization**

The final ambient air concentration is the maximum value of the concentrations calculated from the concentration in topsoil, in each of the subsurface layers and in groundwater.

(eq. 42)

$$C_{ao,Y,vf} = max\left(C_{ao,Y,v,i}\right)$$

Where

Abbr.	Name	Unit	Reference
$C_{ao,Y,vf}$	final ambient air concentration at height Y due to volatilization	mg/m³	(eq. 42)
$C_{ao,Y,v,i}$	ambient air concentration at height Y due to volatilization from layer i	mg/m³	(eq. 34), (eq. 35) or (eq. 38)

The volatilization models assume an infinite source. For volatile contaminants, the concentration in soil will be depleted over time. Mass balance models could be used to account for the finite concentration present in soil. The F-Leach model (in Dutch, available from the OVAM website: www.ovam.be) allows the calculation of the evolution of the soil concentration over time and provides an indication of the speed at which the concentration in soil will be depleted. A simple mass balance approximation can be used the estimate the average ambient air concentration that would result from total volatilization of the contamination from a soil layer assuming constant flux over the exposure period. This equation is not programmed in S-Risk.

(eq. 43)

$$C_{ao,Y,v}(finite) = \frac{1}{V_f} \times \frac{\rho_s \times L_{io}}{T} \times C$$

Where

Abbr.	Name	Unit	Reference
$C_{ao,Y,v}$ (finite)	average finite source ambient air concentration at height Y due to volatilization	mg/m³	(eq. 43)
V_f	dilution rate at height Y	m/d	(eq. 27)
ρ_s	soil bulk density	kg/m³	Table 4 or user input
$L_{i,o}$	thickness of the soil layer	m	user input
T	averaging time	d	*
C	Measured concentration in soil	mg/kg dm	user input

* Averaging time is the time period over which exposure takes place; at the moment the values are fixed, but this should be linked to the exposure averaging time (which is, in turn, linked to toxicity calculations):

Agricultural and Residential areas: 6yrs * 365 (child);
Recreational areas: 6yrs * 365
Industrial areas: 45yrs * 365

5.3. CONCENTRATION IN AMBIENT AIR DUE TO SOIL RESUSPENSION

The concentration in ambient air due to soil resuspension is calculated from the concentration of suspended particles (PM_{10} fraction) that is assumed to be soil-derived, the concentration in soil and an enrichment factor from total soil concentration to PM_{10} concentration. The concentration in the gas phase of the soil is not accounted for in soil resuspension.

(eq. 44)

$$C_{PM10,o} = PM_{10}^{soil} * EF_{PM10} * C_{s+w} * CF_{PM10}$$

Where

Abbr.	Name	Unit	Source
$C_{PM10,o}$	Concentration in outdoor air (on PM10) as a result of soil quality	mg/m³	(eq. 44)
PM_{10}^{soil}	Concentration of PM_{10} resulting from soil	µg/m³	Table 9
EF_{PM10}	enrichment factor from soil to PM_{10}	-	Table 9
C_{s+w}	Concentration in the soil solid + water phase from top soil	mg/kg dm	(eq. 45)
CF_{PM10}	Conversion factor from µg/m³ to kg/m³	kg/µg	Table 9

(eq. 45)

$$C_{s+w} = C_s + C_w \times \frac{\theta_w}{\rho_s}$$

Where

Abbr.	Name	Unit	Source
C_{s+w}	Concentration in the soil solid + water phase	mg/kg dm	

			(eq. 45)
C_s	Concentration in the soil solid phase	mg/kg dm	(eq. 17)
C_w	Concentration in soil pore water	mg/m^3	(eq. 18)
θ_w	Volumetric soil water content	m^3/m^3	Table 4 or user input
ρ_s	Soil dry bulk density	kg/m^3	Table 4 or user input

5.4. TOTAL CONCENTRATION IN AMBIENT AIR

The total concentration in ambient air due to local volatilization and soil particle emission is given by

(eq. 46)

$$C_{ao,Y} = C_{ao,Y,vf} + C_{PM10,0}$$

Where

Abbr.	Name	Unit	Reference
$C_{ao,Y}$	concentration in ambient air at height Y	mg/m^3	(eq. 46)
$C_{ao,Y,vf}$	concentration in ambient air due to volatilization at height Y	mg/m^3	(eq. 42)
$C_{PM10,o}$	concentration in ambient air due to soil resuspension	mg/m^3	(eq. 44)

Table 9: Properties for ambient air calculations, including application I defaults

Abbr	Name	unit	value
k_{karman}	von Karman constant	-	0.4 (fixed)
V_h	wind velocity at height h	m/d	288000
h	height for wind velocity V_h	m	10 (fixed)
PM_{10}^{soil}	concentration of PM_{10} resulting from soil resuspension	µg/m^3	5
EF_{PM10}	enrichment factor from soil to PM_{10}	-	2
CF_{PM10}	conversion factor from µg/m^3 to kg/m^3	kg/µg	1E-9 (fixed)
L	length of the contaminated area in dominant wind direction	m	50
Y	breathing height	m	
	adult		1.5 (fixed)
	child		1 (fixed)
	vegetation		0.5 (fixed)

CHAPTER 6 CONCENTRATION IN INDOOR AIR AND SETTLED DUST

The concentration in indoor air is the result of two processes:

- Vapour intrusion from soil or groundwater into the building;
- Particle intrusion from ambient air into the building.

Separately, the model also considers the evaporation in bathroom air due to volatilization of contaminants from water during showering.

The concentration in settled dust is calculated from the concentration in soil.

6.1. CONCENTRATION IN INDOOR AIR DUE TO VAPOUR INTRUSION

Seen the high concentrations resulting from initial default assumptions for soil remediation value calculations (application I), the final default scenario for soil remediation values is the result of discussions with RIVM and within the steering committee of the S-Risk project. Final decisions with regard to default values were made, taking into account the opinion that current remediation values for volatile compounds are already rather stringent and that a further decrease of these values would not be in line with reality.

The concentration in indoor air due to vapour intrusion from soil or groundwater into the building is calculated according to the Volasoil model as described in Bakker et al. (2008a). The model distinguishes three building types (Figure 2):

- *Building with basement*: the contaminant is transported through the floor and the walls of the basement; complete mixing is assumed within the building (including the basement).
- *Building with a crawl space*: the contaminant is transported from soil into the crawl space, and through the crawl space walls, followed by transport from the crawl space through the building floor into the living area of the building; within the building complete mixing takes place;
- *Building with slab-on-grade*: the contaminant is transported from soil through the floor into the building; complete mixing takes place within the building;

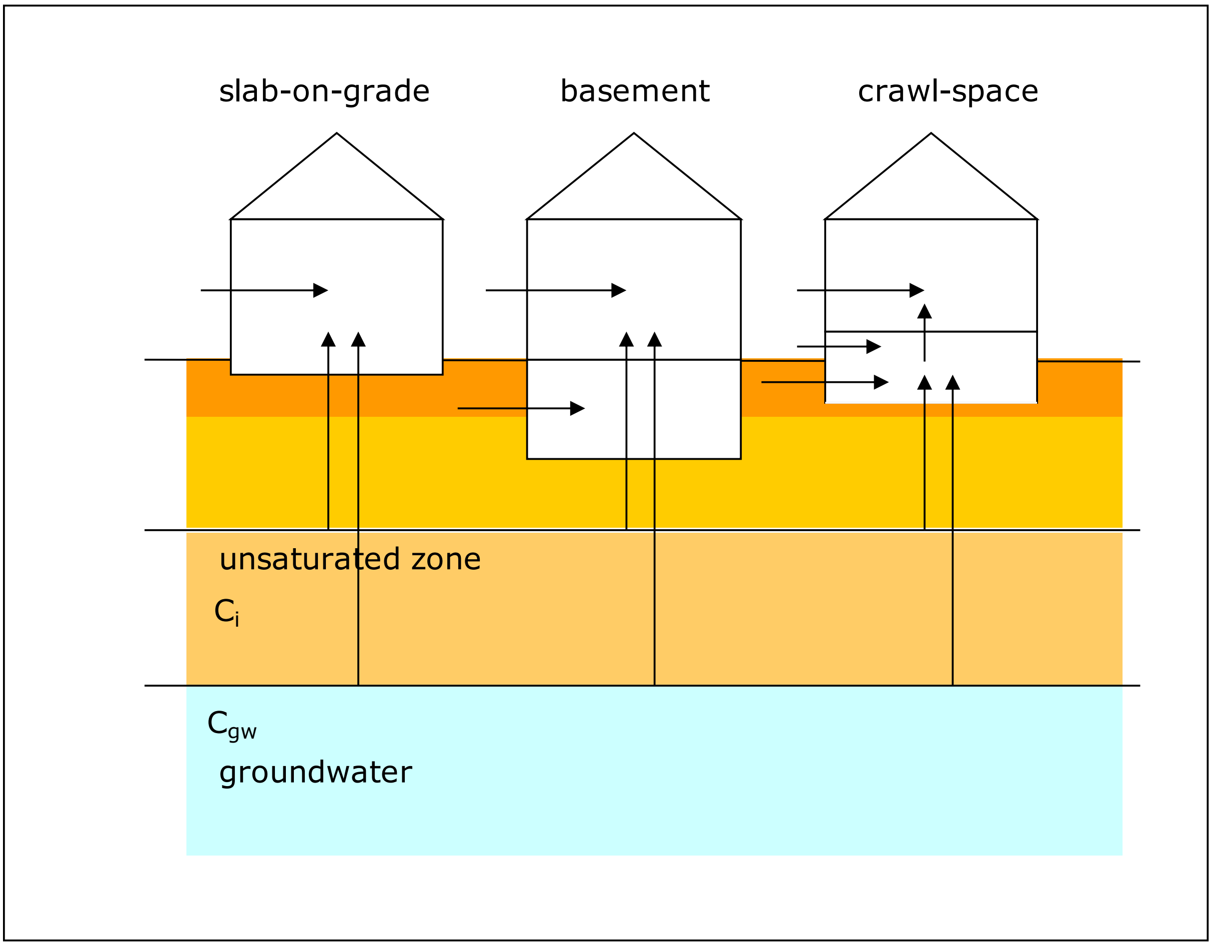

Figure 2: Schematic representation of the building types considered for modeling indoor air concentrations due to vapour intrusion from soil or groundwater

The model assumes parallel diffusion and convection over the whole soil profile. The model allows the specification of different soil layers (soil profile). The effective diffusion coefficient for the whole distance between top of the contamination and the floor of the building is calculated as a length-weighted value of the effective diffusion coefficients in the separate layers. The same approach is followed for the calculation of soil air permeability, which is used for the convective flow. This is illustrated in Figure 3 for a contaminant present in the unsaturated zone and in groundwater. In the latter case, transport first takes place through the capillary zone and then through the soil layers above the capillary zone.

The pressure difference causing convective transport is in reality limited to some meters below the building/basement floor (3 – 5 m); the depth of the influence zone is u.o. dependent on soil type. If the top of contamination is present at a greater depth, preference should be given to measured soil air concentrations at a depth of maximum 3 - 5 m as input for the vapour intrusion model.

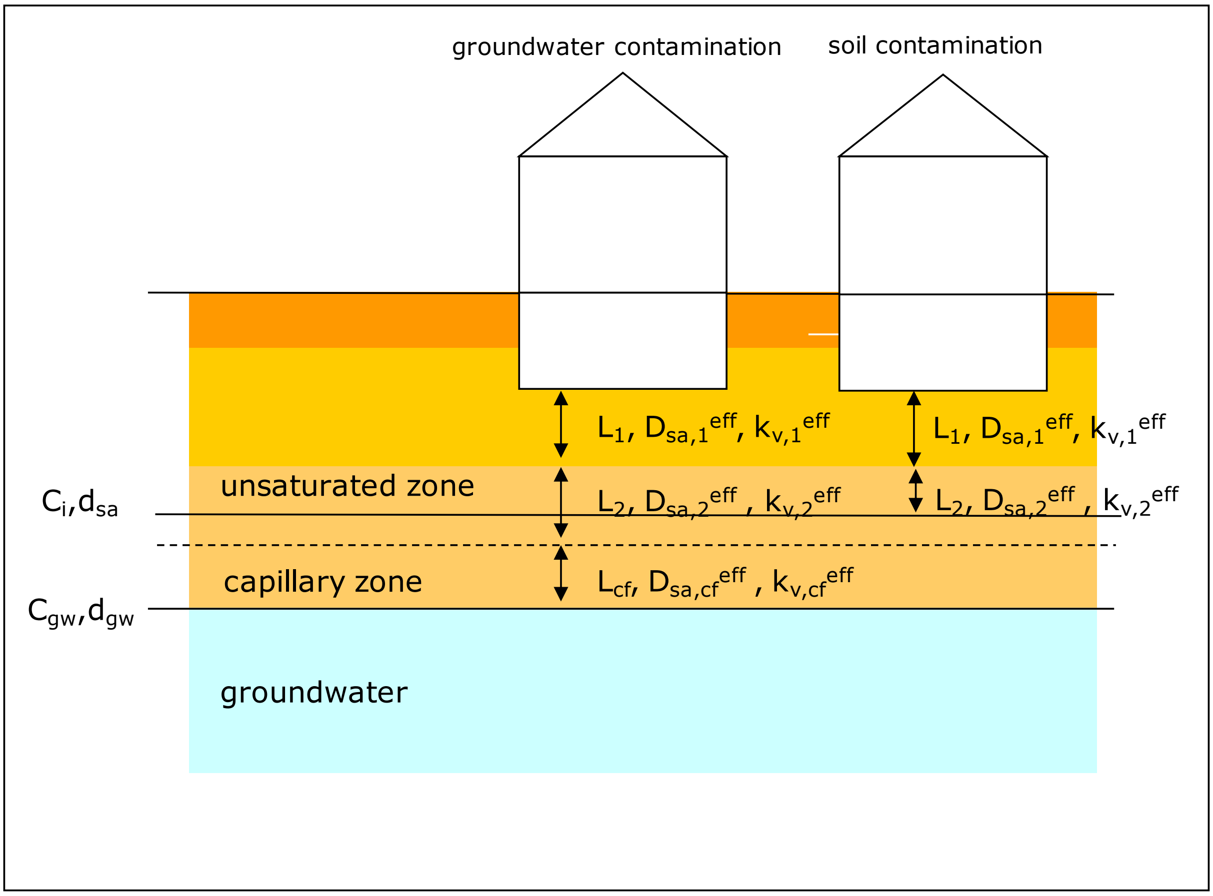

Figure 3: Illustration of the approach for incorporation of the soil profile in the diffusion calculations

Similar to the ambient air concentration model, the concentration in each specified layer is assigned to the top of that layer, except when the basement, slab-on-grade or crawl space is within the contaminated layer. The indoor air concentration is calculated from each soil (and groundwater) layer and its associated concentration, taking into account the soil properties of the layers between the top of contamination and the bottom of the building and of all layers above the top of the contamination in case of transfer through the walls. The final indoor air concentration is the maximum value of the separate concentrations.

The way the contaminant fluxes are calculated for different contamination types (depth of soil layer compared to situation of basement) is illustrated in Figure 4 for a basement. The system is similar for a crawl space. For a slab-on-grade, only the flux through the floor applies.

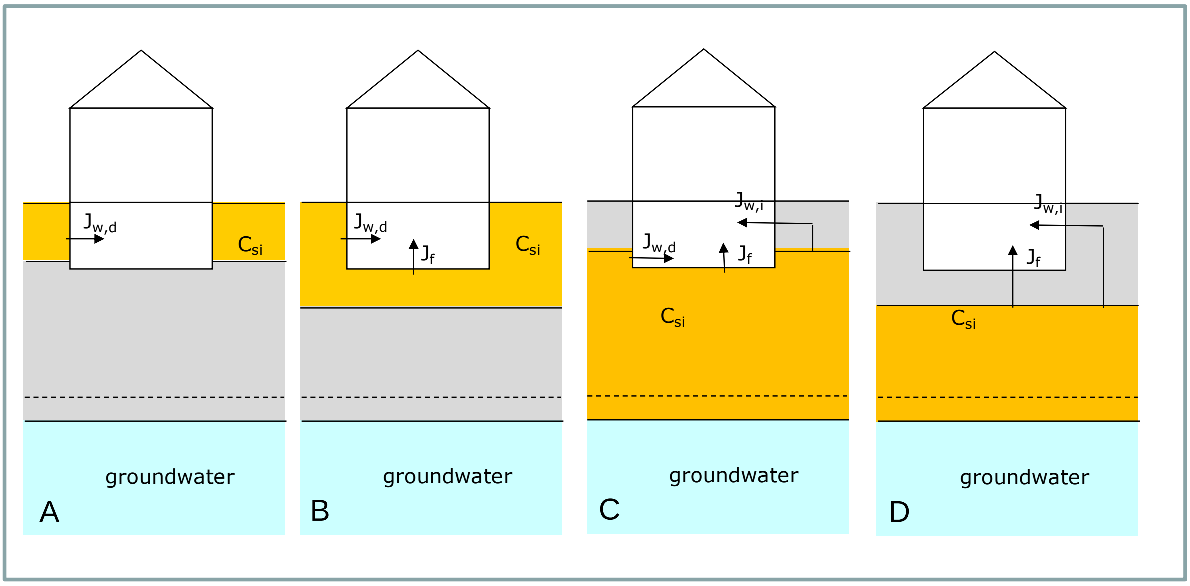

Figure 4: Illustration of indoor contaminant fluxes for typical situations in case of a basement ($J_{w,d}$: direct wall flux; $J_{w,i}$: indirect wall flux; J_f: floor flux)

Situation A – the bottom of a contaminated topsoil layer is above the floor of the basement:

Only a direct flux through the wall applies; the distance over which transport to the building takes place is set at a minimum value (buffer space). The total area for this flux is calculated from the wall length times the height over which there is contact between the contaminated layer and the basement walls.

Situation B – the bottom of a contaminated topsoil layer is at or below the floor of the basement:

A direct flux through the wall is calculated; the distance over which transport to the building takes place is set at a minimum value (buffer space). The area over which the direct wall flux takes place is the total basement wall area. A flux through the basement floor is calculated; the distance over which transport to the building takes place is set at a minimum value (buffer space).

Situation C – the top of a contaminated subsurface layer is above the floor of the basement and the bottom of the contaminated layer is below the floor of the basement:

A direct flux through the wall is calculated; the distance over which transport to the building takes place is set at a minimum value (buffer space). The total area for this flux is calculated from the wall length times the height over which there is contact between the contaminated layer and the basement walls. A flux through the basement floor is calculated; the distance over which transport to the building takes place is set at a minimum value (buffer space). An indirect flux from the top of the contamination through the basement walls is calculated. The distance over which transport takes place is set at half the distance between top of contamination and soil surface.

Situation D – the top of a contaminated subsurface layer is at or below the floor of the basement and the bottom of the contaminated layer is below the floor of the basement:

A flux through the basement floor is calculated; the distance over which transport to the building takes place is the distance between top of contamination and basement floor. An indirect flux from the top of the contamination through the basement walls is calculated. The distance over which transport takes place is set at the distance for the floor flux plus half the basement depth.

For a basement floor and a slab-on-grade, two calculation options are available: floor with gaps and holes and intact floor. Basement and crawl space walls are modelled according to an intact wall. In case of an intact floor or wall, transport takes only place through the (connected) pores of the building material (called open porosity).

Under application I, the default building type is a basement with a floor characterized by cracks and holes. The default soil profile is a uniformly contaminated layer from 0 m till 3 m depth. The groundwater table is at 3 m depth.

The top of the groundwater layer should be below the bottom of the basement, crawl-space or slab-on-grade. The minimum distance is specified by the buffer space.

The so-called buffer space is a critical parameter in the indoor vapour intrusion model. It represents a virtual minimum distance (without contamination) between contamination and building envelope to enable the calculation of "realistic" contaminant fluxes. This minimum distance is set at 0.10 m after consultation with the authors of the Volasoil model (Johannes Lijzen, personal communication). The buffer space condition is automatically applied in S-Risk.
However, the Vlier-Humaan model assumes a fixed diffusion length of 0.75 m, independent of the real soil profile (it converts the soil profile data to a weighted concentration at 0.75 m). Consequently, this assumption alsoholds in case of a uniformly contaminated profile in direct contact with the basement. Due to the unrealistically high predicted indoor air concentrations of the vapour intrusion model implemented in S-Risk under the default soil profile for application I and with buffer space 0.10 m, it was decided to set the buffer space for application I at 0.75 m. For application II and III the buffer space remains at 0.10 m.

6.1.1. BUILDING WITHOUT A BASEMENT (SLAB-ON-GRADE)

The building is constructed on top of a concrete foundation. No basement or crawl space is present. Two options are included:

- Intact floor (no gaps or cracks): applies to a new building;
- Floor with gaps and holes: applies to older buildings and buildings with pipes through the floor.

→ **Intact concrete slab**

(eq. 47)

$$J_{si} = \frac{-F_{si} \times C_{sa}}{exp\left(-\frac{F_{si} \times L_s}{D_{eff,f}^{sa}}\right) \times \exp\left(-\frac{F_{si} \times L_f}{D_{eff}^{fa}}\right) - 1}$$

(eq. 48)

$$F_{si} = \frac{\Delta P_{si}}{\frac{L_s}{K_{sa}} + \frac{L_f}{K_f}}$$

(eq. 49)

$$D_{eff,f}^{sa} = \frac{\sum L_i}{\sum \frac{L_i}{D_{eff,i}^{sa}}}$$

(eq. 50)

$$K_{sa} = \frac{k_{v,eff}}{\eta}$$

The effective air permeability coefficient $k_{v,eff}$ is calculated from the coefficients of all layers between the top of contamination and the floor of the building and their corresponding thicknesses.

(eq. 51)

$$k_{v,eff} = \frac{\sum L_i}{\sum_n \frac{L_i}{k_{v,i}}}$$

In this equation, the sum of all L_i equals L_s

(eq. 52)

$$K_f = \frac{k_{v,f}}{\eta}$$

(eq. 53)

$$L_s = \max(d_{sa} - d, L_{bs})$$

The length of the soil column L_s should be at least some cm to prevent unrealistic high flow rates. This minimal distance is called the buffer space (L_{bs}) The Volasoil documentation (Bakker, Lijzen, and van Wijnen, 2008b) specifies a buffer space of 0.01 m, after discussion with RIVM (Johannes Lijzen, personal communication), we set the buffer space at 0.05 m.

(eq. 54)

$$D_{eff}^{fa} = \frac{\left(\varepsilon_{v,f}\right)^{\frac{10}{3}}}{\left(\varepsilon_{T,f}\right)^{2}} \times D_a$$

(eq. 55)

$$\varepsilon_{T,f} = 2 \times \varepsilon_{v,f}$$

Where

Abbr.	Name	Unit	Source
J_{si}	contaminant flux from soil to indoor air through floor	mg/m².d	(eq. 47)

Abbr.	Name	Unit	Source
F_{si}	air flux from soil to indoor air through floor	m³/m².d	(eq. 48)
C_{sa}	concentration in soil air	mg/m³	(eq. 20)
L_s	length of the zone between top of the contamination and bottom of the building floor	m	(eq. 53)
L_f	thickness of the floor	m	Table 14
L_i	thickness of the ith soil layer	m	contaminant profile
L_{bs}	thickness of buffer space	m	Table 15
d	depth of the floor of the concrete slab below soil surface	m	Table 14
$D^{sa}_{eff,f}$	effective diffusion coefficient in soil for vapour intrusion through floor of building, basement or bottom of crawl space	m²/d	(eq. 49)
D^{fa}_{eff}	effective diffusion coefficient in the floor	m²/d	(eq. 54)
d_{sa}	depth of the top of the contamination	m	calculated from contaminant profile
K_{sa}	air conductivity of the soil layer	m²/Pa.d	(eq. 50)
K_f	air conductivity of the floor	m²/Pa.d	(eq. 52)
$k_{v,i}$	air permeability of the soil layer	m²	Table 4
$k_{v,eff}$	effective air permeability of the soil for vapour intrusion	m²	(eq. 51)
$k_{v,f}$	air permeability of the floor, intact floor	m²	Table 15 or Table 10
ΔP_{si}	pressure difference between indoor space and soil	Pa	Table 15
η	dynamic viscosity of air	Pa.d	Table 15
$\varepsilon_{v,f}$	air-filled porosity of a concrete floor, intact floor	-	Table 15 or Table 10
$\varepsilon_{T,f}$	total porosity of a concrete floor, intact floor	-	(eq. 55)

Values of air permeability and air-filled porosity of an intact concrete floor are given in Table 10. The default value (Table 15) is marked in bold.

→ **Floor with gaps and holes**

(eq. 56)

$$J_{si} = \frac{-F_{si} \times C_{sa}}{exp\left(-\frac{F_{gap} \times L_f}{D^{sa,u}_{eff}}\right) \times \exp\left(-\frac{F_{si} \times L_s}{D^{sa}_{eff,f}}\right) - 1}$$

Holes are assumed to be filled with soil of the underlying soil layer, so that the effective diffusion coefficient in the gaps equals the effective diffusion coefficient of the soil layer below the floor.

(eq. 57)

$$F_{si} = \frac{\Delta P_{si}}{\frac{L_s}{K_{sa}} + \frac{L_f}{K_f}}$$

(eq. 58)

$$K_f = \frac{f_{of}^2}{n_f \times \pi \times 8 \times \eta}$$

(eq. 59)

$$F_{gap} = \frac{F_{si}}{f_{of}}$$

Where

Abbr.	Name	Unit	Source
J_{si}	contaminant flux from soil to indoor air	mg/m².d	(eq. 56)
F_{si}	air flux from soil to indoor air	m³/m².d	(eq. 57)
F_{gap}	air flux through gaps in the floor (per area of holes)	m³/m².d	(eq. 59)
C_{sa}	concentration in soil air	mg/m³	(eq. 20)
L_s	length of the zone between top of the contamination and bottom of the building floor	m	(eq. 53)
L_f	thickness of the floor	m	Table 14
d	depth of the floor of the concrete slab below soil surface	m	Table 14
$D^{sa}_{eff,f}$	effective diffusion coefficient in soil for vapour intrusion through floor of building, basement or bottom of crawl space	m²/d	(eq. 49)
$D^{sa,u}_{eff}$	effective diffusion coefficient in soil air for the soil layer below the floor of the building	m²/d	(eq. 36)
K_{sa}	air conductivity of the soil layer	m²/Pa.d	(eq. 50)
K_f	air conductivity of the gaps	m²/Pa.d	(eq. 58)
ΔP_{si}	pressure difference between indoor space and soil	Pa	Table 15
f_{of}	fraction of openings in the floor	m²/m²	Table 15
n_f	number of openings per floor area	m^{-2}	Table 15
η	dynamic viscosity of air	Pa.d	Table 15

Values of fraction of openings in the floor are given in Table 11. The default value (Table 15) is marked in bold.

→ **Concentration in indoor air (slab-on-grade)**

The concentration in indoor air is then calculated as

(eq. 60)

$$vv_i = vv_{i,b} + \frac{F_{si} \times A_f}{V_i}$$

(eq. 61)

$$C_{ia} = \frac{J_{si} \times A_f}{V_i \times vv_i}$$

Where

Abbr.	Name	Unit	Reference
J_{si}	contaminant flux from soil to indoor air	mg/m².d	(eq. 47) or (eq. 56)
F_{si}	air flux from soil to indoor air	m³/m².d	(eq. 48) or (eq. 57)
vv_i	air exchange rate for indoor space	1/d	(eq. 60)
$vv_{i,b}$	basic air exchange rate for indoor space	1/d	Table 15
A_f	area of the floor	m²	Table 14 or user input
V_i	volume of the indoor space	m³	Table 14 or user input
C_{ia}	concentration in indoor air	mg/m³	(eq. 61)

6.1.2. BUILDING WITH A BASEMENT

The contaminant flux $J_{si,f}$ through the basement floor is calculated according to equations (eq. 47) or (eq. 56) for an intact basement floor or a basement floor with gaps and holes, respectively.

The contaminant flux through the basement walls is calculated assuming an intact porous wall. Two fluxes are possible, depending upon the depth and thickness of the contaminated soil layer relative to the basement depth (see Figure 4): a direct flux when there is contact between the contaminated layer and the basement walls, and an indirect flux to that part of the basement walls that is above the contaminated layer.

(eq. 62)

$$J_{si,w} = \frac{-F_{si,w} \times C_{sa}}{\exp\left(\frac{-F_{si,w} \times L_{s,w}}{D^{sa}_{eff,w}}\right) \times exp\left(\frac{-F_{si,w} \times L_{bw}}{D^{wa}_{eff}}\right) - 1}$$

(eq. 63)

$$D^{sa}_{eff,w} = \frac{\sum L_i}{\sum \frac{L_i}{D^{sa}_{eff,i}}}$$

For the direct flux through the walls, the effective diffusion coefficient of the profile is equal to the effective diffusion coefficient of the contaminated layer in contact with the basement walls. For the indirect flux through the walls, the sum of all L_i is equal to d_{sa}.

(eq. 64)

$$F_{si,w} = \frac{\Delta P_{si}}{\frac{L_{s,w}}{K_{sa,w}} + \frac{L_{bw}}{K_{bw}}}$$

(eq. 65)

$$K_{sa,w} = \frac{k_{v,eff,w}}{\eta}$$

For the direct flux through the basement wall, $k_{v,eff,w}$ is equal to k_v of the contaminated soil layer in contact with the basement wall. For the indirect flux through the basement wall, $k_{v,eff,w}$ is calculated as in (eq. 51). The sum of all L_i equals d_{sa}.

(eq. 66)

$$L_{s,w,d} = L_{bs}$$

(eq. 67)

$$L_{sw,i} = L_s + \frac{(d_{sa} - L_s)}{2}$$

(eq. 68)

$$D_{eff}^{wa} = \frac{\left(\varepsilon_{v,w}\right)^{\frac{10}{3}}}{\left(\varepsilon_{T,w}\right)^{2}} \times D_a$$

(eq. 69)

$$\varepsilon_{T,w} = 2 \times \varepsilon_{v,w}$$

(eq. 70)

$$K_{bw} = \frac{k_{v,w}}{\eta}$$

(eq. 71)

$$vv_i = vv_{i,b} + \frac{F_{si,f} \times A_f + F_{si,w,d} \times A_{w,d} + F_{si,w,i} \times A_{w,i}}{V_i + V_b}$$

(eq. 72)

$$C_{ia} = \frac{J_{si,f} \times A_f + J_{si,w,d} \times A_{w,d} + J_{si,w,i} \times A_{w,i}}{(V_i + V_b) \times vv_i}$$

(eq. 73)

$$A_{w,d} = A_w \times \frac{d - d_{sa}}{d} \text{ when } d_{sa} < d$$

(eq. 74)

$$A_{w,i} = A_w \times \frac{d_{sa} - L_s}{d}$$

where

Abbr.	Name	Unit	Reference
$J_{si,f}$	contaminant flux from soil to indoor air through the basement floor	mg/m².d	(eq. 47)or (eq. 56)
$J_{si,w}$	contaminant flux from soil to indoor air through basement walls	mg/m².d	(eq. 62)
$J_{si,w,d}$	direct contaminant flux from soil to indoor air through basement walls	mg/m².d	(eq. 62)
$J_{si,w,i}$	indirect contaminant flux from soil to indoor air through basement walls	mg/m².d	(eq. 62)
$F_{si,f}$	air flux from soil to indoor air through the basement floor	m³/m².d	(eq. 48) or (eq. 57)
$F_{si,w}$	air flux from soil to indoor air through basement walls	m³/m².d	(eq. 64)
$F_{si,w,d}$	direct air flux from soil to indoor air through basement walls	m³/m².d	(eq. 64)
$F_{si,w,i}$	indirect air flux from soil to indoor air through basement walls	m³/m².d	(eq. 64)
C_{sa}	concentration in soil air	mg/m³	
$L_{s,w}$	transfer distance for wall flux	m	(eq. 20) (eq. 66) or (eq. 67)
$L_{s,w,d}$	transfer distance for direct wall flux	m	(eq. 66)
$L_{s,w,i}$	transfer distance for indirect wall flux	m	(eq. 67)
L_i	thickness of the soil layer	m	soil profile
L_{bw}	thickness of the basement walls	m	Table 14 or user input
L_s	length of the zone between top of the contamination and bottom of the building floor	m	(eq. 53)
L_{bs}	thickness of buffer space	m	Table 15
$D^{sa}_{eff,w}$	effective diffusion coefficient in soil for walls	m²/d	(eq. 63)
$D^{sa}_{eff,i}$	effective diffusion coefficient of a soil layer	m²/d	(eq. 36)
D^{wa}_{eff}	effective diffusion coefficient in the basement wall	m²/d	(eq. 68)
$K_{sa,w}$	air conductivity of the soil profile for basement walls	m²/Pa.d	(eq. 65)
$\varepsilon_{v,w}$	air-filled porosity of the basement wall	-	Table 15 or Table 12

Abbr.	Name	Unit	Reference
$\varepsilon_{T,w}$	total porosity of the basement wall	-	(eq. 69)
			(eq. 68)
d_{sa}	depth of the top of the contamination	m	calculated from contamination profile
d	depth of the basement floor below soil surface	m	Table 14
K_{bw}	air conductivity of an intact basement wall	m^2/Pa.d	
			(eq. 70)
$k_{v,eff,w}$	effective air permeability of the soil profile for basement walls	m^2	(eq. 51)
$k_{v,w}$	air permeability of the basement wall	m^2	Table 15 or Table 12
η	dynamic viscosity of air	Pa.d	Table 15
ΔP_{si}	pressure difference between indoor space and soil	Pa	Table 15
A_f	surface area of the floor of the basement	m^2	Table 14 or user input
A_w	surface area of the basement walls	m^2	Table 14 or user input
$A_{w,d}$	surface area of the basement walls for direct flux	m^2	(eq. 73)
$A_{w,i}$	surface area of the basement walls for indirect flux	m^2	(eq. 74)
vv_i	air exchange rate for indoor space	1/d	
			(eq. 71)
$vv_{i,b}$	basic air exchange rate for indoor space	1/d	Table 15
V_i	volume of the indoor space	m^3	Table 14 or user input
V_b	volume of the basement	m^3	Table 14 or user input
C_{ia}	concentration in indoor air	mg/m^3	(eq. 72)

6.1.3. BUILDING WITH A CRAWL SPACE

In the situation of a crawl space, two fluxes are calculated: a flux from soil to the crawl space, and a flux from the crawl space to indoor air. The design of the crawl space assumes that there is no crawl space floor, i.e. there is direct contact between the soil and the indoor air of the crawl space. In case a crawl space with a concrete floor is present, the concentration in indoor air can be simulated by first assuming a building with a basement and setting the building dimensions as it was only a basement. The calculated indoor air concentration can then be used as if it was a measured crawl space concentration. The contaminant flux through the crawl space walls is calculated as for a basement. The contaminant flux from soil to crawl space is given by

(eq. 75)

$$J_{sc} = \frac{-F_{sc} \times C_{sa}}{exp\left(-F_{sc} \times \frac{L_s}{D_{eff}^{sa}}\right) - 1}$$

The air flux from soil to the crawl space as a result of convection is given by

(eq. 76)

$$F_{sc} = K_{sa} \times \frac{\Delta P_{sc}}{L_s}$$

(eq. 77)

$$L_s = \max(d_{sa} - d_c, L_{bs})$$

The effective diffusion coefficient is calculated from the depth of the soil layers above the top of the contamination and their corresponding effective diffusion coefficient.

The flux from the crawl space into the building assumes only convective transport through the floor between crawl space and building.

(eq. 78)

$$F_{ci} = K_f \times \frac{\Delta P_{ci}}{L_f}$$

(eq. 79)

$$K_f = \frac{f_{of}^2}{n_f \times \pi \times 8 \times \eta}$$

(eq. 80)

$$J_{ci} = F_{ci} \times C_{ca}$$

(eq. 81)

$$vv_c = vv_{c,b} + \frac{F_{sc} \times A_f + F_{sc,w,d} \times A_{w,d} + F_{sc,w,i} \times A_{w,i}}{V_c}$$

(eq. 82)

$$C_{ca} = \frac{J_{sc} \times A_f + J_{sc,w,d} \times A_{w,d} + J_{sc,w,i} \times A_{w,i}}{V_c \times vv_c}$$

(eq. 83)

$$vv_i = vv_{i,b} + \frac{F_{ci} \times A_f}{V_i}$$

(eq. 84)

$$C_{ia} = \frac{J_{ci} \times A_f}{V_i \times vv_i}$$

Where

Abbr.	Name	Unit	Source
J_{sc}	contaminant flux from soil to crawl space	mg/m².d	(eq. 75)

Abbr.	Name	Unit	Source
F_{sc}	air flux from soil to the crawl space	m³/m².d	(eq. 76)
C_{sa}	concentration in soil air	mg/m³	(eq. 20)
L_s	length of the zone between top of the contamination and bottom of the crawl space	m	(eq. 77)
$D^{sa}_{eff,f}$	effective diffusion coefficient in soil for vapour intrusion through floor of building, basement or bottom of crawl space	m²/d	(eq. 49)
d_{sa}	depth of the top of the contamination	m	calculated from contaminant profile
d_c	depth of the crawl space beneath soil surface	m	Table 14
F_{ci}	air flux from crawl space to indoor space	m³/m².d	(eq. 78)
K_{sa}	air conductivity of the soil layer	m²/Pa.d	(eq. 50)
K_f	air conductivity of the floor	m²/Pa.d	(eq. 79)
ΔP_{sc}	pressure difference between crawl space and soil	Pa	Table 15
ΔP_{ci}	pressure difference between indoor space and crawl space	Pa	Table 15
L_f	thickness of the floor	m	Table 14
f_{of}	fraction of openings in floor	m²/m²	Table 15 or Table 11
L_{bs}	thickness of buffer space	m	Table 15
n_f	number of openings per floor area	m^{-2}	Table 15
η	dynamic viscosity of air	Pa.d	Table 15
J_{ci}	contaminant flux from crawl space to indoor space	mg/m².d	(eq. 80)
C_{ca}	concentration in crawl space	mg/m³	(eq. 82)
vv_c	air exchange rate for crawl space	1/d	(eq. 81)
$vv_{c,b}$	basic air exchange rate for crawl space	1/d	Table 15
$F_{sc,w,d}$	direct air flux through crawl space walls	m³/m².d	(eq. 64)
$F_{sc,w,i}$	indirect air flux through crawl space walls	m³/m².d	(eq. 64)
A_f	surface area of the floor of the crawl space	m²	Table 14 or user input
$A_{w,d}$	surface area of the crawl space walls for direct flux	m²	(eq. 73)
$A_{w,i}$	surface area of the crawl space walls for indirect flux	m²	(eq. 74)
V_c	volume of the crawl space	m³	Table 14 or user input
vv_i	air exchange rate for indoor space with crawl space	1/d	(eq. 83)
$vv_{i,b}$	basic air exchange rate for indoor space	1/d	Table 15
V_i	volume of the indoor space	m³	Table 14 or user input
C_{ia}	concentration in indoor air	mg/m³	(eq. 84)

6.1.4. FINAL CONCENTRATION IN INDOOR AIR DUE TO VOLATILIZATION

The final gas-phase concentration in indoor air equals the maximum of the indoor and the outdoor air concentration.

(eq. 85)

$$C_{ai,v} = max\left(C_{ia}, C_{ao,ch,vf}\right)$$

Where

Abbr.	Name	Unit	Reference
$C_{ai,v}$	final concentration in the gas phase of indoor air	mg/m³	(eq. 85)
$C_{ao,ch,vf}$	concentration in outdoor air due to volatilization at child's height	mg/m³	(eq. 42)
C_{ia}	concentration in indoor air due to vapour intrusion	mg/m³	(eq. 84) or (eq. 61) or (eq. 72)

The values for air permeability and air-filled porosity of concrete floors are taken from Bakker et al. (2008b). They are only used for the floors of basement and slab-on-grade. For the floor between crawl-space and indoor space, a gaps and holes scenario is assumed where air permeability and air-filled porosity do not apply.

Table 10: Air permeability and air-filled porosity of an intact concrete floor

Quality of the floor	Air permeability ($k_{v,f}$, m²)	Air-filled porosity ($\varepsilon_{v,f}$, -)*
bad	$10^{-15.0}$	0.135
average	$\mathbf{10^{-16.5}}$	**0.045**
good	$10^{-17.5}$	0.015
very good	$10^{-18.5}$	0.006

*: air-filled porosity represents open porosity

The values for the fraction of openings in the floor are taken from Bakker et al. (2008b). These values are applied to the floor between crawl-space and indoor space and for the bottom floor of a basement or slab-on-grade in case of gaps and holes. The fraction of openings represents the area of the gaps and holes in 1 m² floor. It is related to the number of openings per m² (n) by the diameter (surface area) of a single pore.

Table 11: Fraction of openings in the floor (ground floor), default value marked in bold

Quality of the floor	Description	Fraction of openings (f_{of}, m²/m²)
very bad	wooden floor	2E-4
bad	concrete / 1985 - 1993	1E-4
normal	**concrete / 1985 - 2000**	**1E-5**
good	concrete / newer than 2000	1E-6
very good	concrete / newer than 2000	1E-7

Air permeability of basement walls is taken from Bakker et al. (2008b). The authors did not provide values for the air-filled (open) porosity of basement walls. An overview of values from the literature is given in Appendix II.

Table 12: Air permeability and air-filled porosity of basement walls

Quality of the wall	Example	Air permeability (m^2) ($k_{v,w}$)	Air-filled porosity ($\varepsilon_{v,f}$, -)*
very bad		1E-7	0.25
bad	uncoated hollow wall	1E-9	0.20
average	uncoated hollow cement-block	1E-11	0.12
good	**sealed hollow cement block**	**1E-13**	**0.07**
very good	hollow cement block filled with cement and outside asphalt sealing	1E-15	0.045

*: air-filled porosity represents open porosity

Bakker et al. (2008b) recommended the indoor air exchange rates ($vv_{i,b}$) given in Table 13 for residential buildings. A search for Flemish/Belgian data was undertaken and is documented in Appendix III. The overview from Appendix III has lead to the default values for application I as given in Table 15, being 24 d^{-1} for a residential building (land uses I – IV) and 48 d^{-1} for an industrial or commercial building (land uses V).

Table 13: Basic air exchange rate $vv_{i,b}$ in the building (based on residences) as given by Bakker et al. (2008b)

Ventilation characteristics	Ventilation rate (m^3/h)	Exchange rate (1/h)*	Exchange rate (1/d)
very low	25	0.17	4.08
low	50	0.33	7.92
average	75	0.5	12
high	100	0.67	16.08
very high	150	1	24

*: calculated from a floor surface of 50 m² and a height of 3 m

Table 14: Default values for buildings and basements

Parameter	Unit	Crawl space	Basement	No basement
depth below soil surface (d, d_c)	m	0.4	2	0.1
thickness of floor (L_f)	m	0.1	0.1	0.1
thickness of walls (L_{bw})	m	0.15	0.15	na
area of the floor (A_f)	m^2	50	50	50
volume of crawl space or basement (V_c, V_b)	m^3	25	100	na
area of basement/crawl space walls (A_w)	m^2	12	60	na
volume of indoor space (V_i)	m^3	150	150	150

na: not applicable

6.2. CONCENTRATION IN SETTLED DUST AND INDOOR AIR DUE TO INTRUSION OF SUSPENDED PARTICLES

The concentration of contaminants on particulate matter in both settled dust and indoor air results from a combination of processes: intrusion of particles due to intrusion of outdoor air (ventilation, air leakage in the house), deposition onto floors and objects, soil entrainment with shoes and clothing, resuspension from floors and objects, removal by cleaning. Although part of these processes can be described, the concentrations in settled dust and indoor PM_{10} are estimated using empirical relationships.

6.2.1. CONCENTRATION IN SETTLED DUST

The concentration in settled dust is calculated from the concentration in soil and an enrichment factor.

(eq. 86)

$$C_{settled\_dust} = F_{soil/settled\_dust} \times EF_{soil/settled\_dust} \times C_{s+w}$$

Where

Abbr.	Name	Unit	Reference
$C_{settled\_dust}$	Concentration in settled dust indoors from soil	mg/kg dm	(eq. 86)
$F_{soil/settled\_dust}$	Fraction soil in indoor settled dust	-	Table 46
$EF_{soil/settled\_dust}$	Enrichment factor from soil to settled indoor dust	-	Table 15
C_{s+w}	Concentration in the soil solid + water phase	mg/kg dm	(eq. 45)

6.2.2. CONCENTRATION IN INDOOR PM_{10}

The concentration in PM_{10} in indoor air is calculated from the concentration on PM_{10} in outdoor air.

(eq. 87)

$$C_{PM10,i} = F_{out/in} \times C_{PM10,0}$$

Where

Abbr.	Name	Unit	Reference
$C_{PM10,i}$	Concentration in indoor air (on PM10) as a result of soil quality	mg/m^3	(eq. 87)
$C_{PM10,o}$	Concentration in outdoor air (on PM10) as a result of soil quality	mg/m^3	(eq. 44)
$F_{out/in}$	contribution of the concentration on ambient PM_{10} to the concentration on indoor PM_{10}	-	Table 15

6.3. TOTAL CONCENTRATION IN INDOOR AIR

The overall concentration in indoor air is the sum of the concentration in the gas-phase and the concentration in the particle phase.

(eq. 88)

$$C_{ia,t} = C_{ia,v} + C_{PM10,i}$$

Where

Abbr.	Name	Unit	Source
$C_{ia,t}$	total concentration in indoor air	mg/m³	(eq. 88)
$C_{ia,v}$	gas-phase concentration in indoor air	mg/m³	(eq. 85)
$C_{PM10,i}$	concentration in indoor air on PM_{10} as a result of soil quality	mg/m³	(eq. 87)

Table 15: Default values for indoor air parameters

Abbr	Name	Unit	Value
ΔP_{sc}	pressure difference between crawl space and soil air	Pa	1 (default)
ΔP_{ic}	pressure difference between indoor space and crawl space	Pa	1 (default)
ΔP_{si}	pressure difference between indoor space and soil (slab-on-grade / basement)	Pa	1 (default)
f_{of}	fraction of openings in floor	m²/m²	1E-5
n_f	number of openings per floor area	m^{-2}	0.2 (default)
η	dynamic viscosity of air	Pa.d	2.30E-10 (fixed, at 20°C)
$vv_{c,b}$	basic air exchange rate for crawl space	1/d	19.2 (default)
$vv_{i,b}$	basic air exchange rate for indoor space	1/d	24 (agricultural, residential and recreational areas) 48 (commercial and industrial areas)
$k_{v,f}$	air permeability of a concrete floor, intact floor	m²	$10^{-16.5}$
$k_{v,w}$	air permeability of the wall	m²	10^{-13}
$\varepsilon_{v,f}$	air-filled porosity of a concrete floor, intact floor	-	0.045
$\varepsilon_{v,w}$	air-filled porosity of the wall	-	0.07
L_{bs}	thickness of the buffer space	m	0.75 (application I) 0.10 (application II and III) (fixed values)
$EF_{soil/settled\_dust}$	Enrichment factor from soil to indoor settled dust	-	1.5 (default)
$F_{out/in}$	contribution of the concentration on ambient PM_{10} to the concentration on indoor PM_{10}	-	1 (default)

6.4. CONCENTRATION IN BATHROOM AIR

If volatile contaminants are present in drinking-water, volatilization can take place during showering. A two-step approach is followed. First the concentration in the shower stall is calculated. A simple mass balance model is used, assuming that the mass of contaminant emitted during showering, accumulates in the volume of the shower stall and that no air exchange takes place with bathroom air. Secondly, it is assumed that after showering, the air from the shower stall mixes with the air in the bathroom. Ventilation of the bathroom is accounted for.

The average concentration in the air of the shower stall during showering is given by (assuming the initial concentration in air equals 0).

(eq. 89)

$$C_{sh} = \frac{k_{wa} \times V_w \times C_{dw} \times t_{sh}}{2 \times V_{sh}}$$

The degree of volatilization (or transfer efficiency) expressed as a weight fraction is still calculated following the equations of ECETOC (1992), which are based on Andelman (1985). The equations for this part of the model have not been reviewed and are the same as in Vlier-Humaan.

(eq. 90)

$$k_{wa} = \frac{H_{sh}}{R_g \times T_{sh}} \times k_L \times k_G \times \frac{t_f \times \frac{3}{r_d}}{\frac{H_{sh}}{R_g \times T_{sh}} \times k_G + k_L}$$

(eq. 91)

$$H_{sh} = H(T_H) \times e^{\left(0.024 \times (T_{sh} - T_H)\right)}$$

Where

Abbr.	Name	Unit	Source
$C_{sh,a}$	Concentration in the shower stall air	mg/m³	(eq. 89)
k_{wa}	Degree of volatilization (weight fraction)	-	(eq. 90)
V_w	water use during showering	m³/h	Table 16
C_{dw}	Drinking-water concentration	mg/m³	(eq. 26)
t_{sh}	duration of shower	h	Table 33
V_{sh}	Volume of the shower stall	m³	Table 16
H_{sh}	Henry coefficient at shower temperature	Pa.m³/mol	(eq. 91)
$H(T_H)$	Henry coefficient at specified temperature	Pa.m³/mol	chemical properties or calculated
T_H	temperature for H	K	chemical properties
T_{sh}	Shower temperature	K	Table 16
R_g	Universal gas constant	Pa.m³/mol. K	8.3144
k_L	Fluid mass transfer coefficient	m/h	(eq. 92)
k_G	gas phase mass transfer coefficient	m/h	(eq. 93)
t_f	Time of fall for a drop	h	Table 16
r_d	Diameter of a drop	m	Table 16

The mass transfer coefficient for the liquid and the gas phase are calculated from the liquid transfer coefficient of CO_2 and the gas phase transfer coefficient of water.

(eq. 92)

$$k_L = K_l \times \sqrt{\frac{44}{M}}$$

(eq. 93)

$$k_G = K_g \times \sqrt{\frac{18}{M}}$$

Where

Abbr.	Name	Unit	Source
k_L	Fluid mass transfer coefficient	m/h	(eq. 92)
K_l	Liquid phase mass transfer coefficient of CO_2	m/h	Table 16
M	Molecular weight	g/mol	chemical properties
k_G	Gas phase mass transfer coefficient	m/h	(eq. 93)
K_g	Gas phase mass transfer coefficient of H_2O	m/h	Table 16

After showering, the mass of contaminant present in the shower stall dilutes in the bathroom air. Further decrease in concentration results from ventilation of the bathroom. The average concentration in bathroom air is given by

(eq. 94)

$$C_{br,a} = \frac{C_{br,a,0}}{vv_{br} \times t_{br}} \times \exp\left(-vv_{br} \times t_{br}\right)$$

(eq. 95)

$$C_{br,a,0} = C_{sh,a} \times \frac{V_{sh}}{V_{br}}$$

Where

Abbr.	Name	Unit	Source
$C_{br,a}$	Concentration in bathroom air	mg/m^3	(eq. 94)
$C_{br,a,0}$	Concentration in bathroom air at start	mg/m^3	(eq. 95)
vv_{br}	ventilation rate in the bathroom	1/h	Table 16
t_{br}	time spent in the bathroom after showering	h	Table 33
V_{sh}	Volume of the shower stall	m^3	Table 16
V_{br}	volume of the bathroom	m^3	Table 16

Table 16: Values for bathroom air parameters

Abbr	Name	Unit	Value
V_w	water use during showering	m^3/h	0.5 (fixed value)
V_{sh}	Volume of the shower stall	m^3	2 (default value)
T_{sh}	Shower temperature	K	313 (fixed)
t_f	Time of fall for a drop	h	2.78 E-4 (fixed)
r_d	Diameter of a drop	m	0.0005 (fixed)
K_l	Liquid phase mass transfer coefficient of CO_2	m/h	0.2 (fixed)
K_g	Gas phase mass transfer coefficient of H_2O	m/h	29.88 (fixed)
vv_{br}	ventilation rate in the bathroom	1/h	3.3 (default value)
V_{br}	volume of the bathroom	m^3	15 (default value)

The air exchange rate in bathroom air is based on the minimum requirements of the Belgian legislation.

CHAPTER 7 UPTAKE OF CONTAMINANTS BY PLANTS

Plants and crops can be contaminated via the environment by the following processes (Figure 5):

- transfer of chemicals from the soil to the plant via the roots and further translocation to aboveground plant parts;
- transfer of chemicals from air via the gas phase;
- transfer of chemicals from air via particle deposition;
- transfer of chemicals from soil particles that splash up and stick on the leaf.

Uptake modeling is dependent upon the type of chemical (organic or inorganic) and on the type of plant (root or foliar). Uptake of dissociating chemicals and salts is not modeled.

Uptake by the roots from soil is considered to take place from the upper 30 cm of the soil. If the soil profile 0 – 30 cm consists of more than one layer, depth-weighted average soil properties are used. Soil splash results from the top soil layer. Concentrations in air due to volatilization and soil resuspension that are used for above-ground uptake processes, are the concentrations calculated in chapters 5.2 and 5.3 and thus solely account for contaminant levels arising from soil.

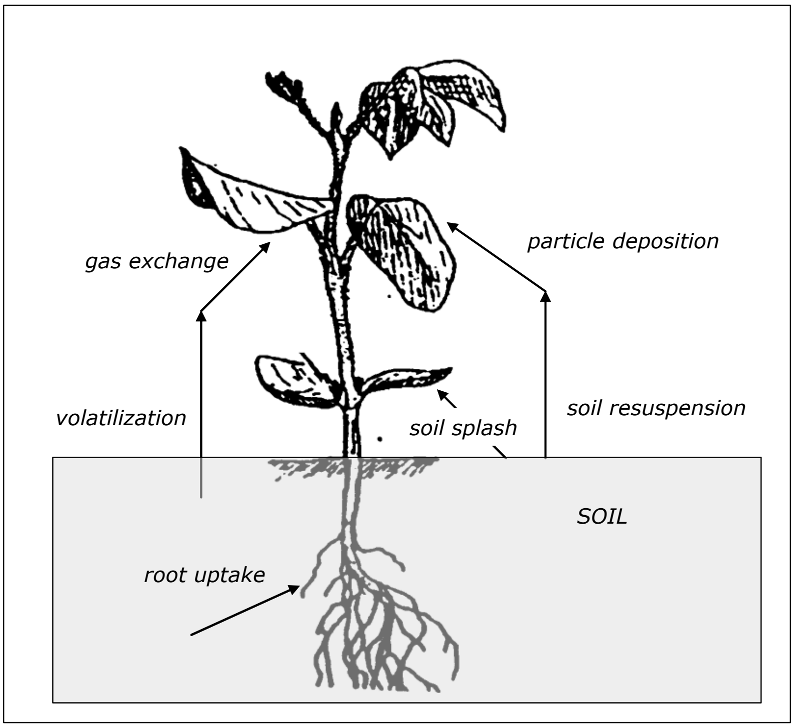

Figure 5: Schematic representation of contaminant uptake by plants

7.1. PLANT UPTAKE OF ORGANIC CHEMICALS

7.1.1. PLANT UPTAKE IN ROOT PLANTS

The concentration in the core of root plants is calculated according to Trapp (2002), assuming steady-state. The model applies to non-ionizing chemicals with a log Kow > 1. The concentration in root plants is solely determined by soil – plant transfer.

(eq. 96)

$$C_v = C_{v,s}$$

If a user-defined bioconcentration factor (BCF) is filled in, the concentration is root plants is calculated from that BCF. Otherwise, the concentration in root plants is predicted from chemical and plant properties. The user-defined BCF for organic chemicals is expressed in mg/kg dm per mg/m³ in pore water, which makes it consistent with the units of the predicted BCF, which also starts from pore water.

(eq. 97)

$$C_{v,s} = BCF_{org} \times C_w \times \frac{dm}{100}$$

(eq. 98)

$$C_{v,s} = \frac{Q_{transp}}{\frac{Q\times 1000}{K_{RW}} + (a_{growth} + a_{metabolism}) \times V_r \times \rho_r} \times C_w$$

Where

Abbr.	Name	Unit	Source
C_v	Total plant concentration for organic chemicals	mg/kg fw	(eq. 96)
$C_{v,s}$	Plant concentration due to soil – plant transfer	mg/kg fw	(eq. 97) or (eq. 98)
Q_{transp}	Transpiration rate	$m^3/m^2.d$	Table 19
K_{RW}	Partition factor plant tissue – pore water	l/kg fw	(eq. 99)
a_{growth}	Chemical elimination via growth	1/d	Table 20
$a_{metabolism}$	loss due to metabolization in the plant	1/d	Table 25
V_r	Root volume	m^3/m^2	Table 20
C_w	concentration in topsoil pore water	mg/m^3	(eq. 18)
ρ_r	Density of the root	kg fw/m^3	Table 20
BCF_{org}	bioconcentration factor for organic contaminants	(mg/kg dm) /(mg/m^3)	Table 25
dm	Dry matter content of the plant	%	Table 20

(eq. 99)

$$K_{RW} = W + L_{plant} \times a_1 \times K_{ow}{}^{b1}$$

Where

Abbr.	Name	Unit	Source
K_{RW}	Partition factor plant tissue – pore water	l/kg	(eq. 99)
W	Water content of the plant	kg/kg*	(eq. 100)
L_{plant}	Lipid content of the plant	kg/kg	Table 20
a_1	Correction factor for the difference in density between water and n-octanol ($1/\rho_{octanol}$)	-	Table 19
K_{ow}	Octanol-water partition coefficient	-	chemical properties
b_1	Briggs factor for root plants	-	Table 19

*: assuming the density of water being equal to 1

Water content of the plant is calculated from the dry matter content.

(eq. 100)

$$W = 1 - \frac{dm}{100}$$

Abbr.	Name	Unit	Source
W	Water content of the plant	kg/kg	
			(eq. 100)
dm	Dry matter content of the plant	%	Table 20

The model is parameterized for a surface area of 1m², assuming that the ratio of transpiration / root mass is constant during growth. Values for Q_{transp} and V_r are therefore taken from Trapp (2002).

7.1.2. PLANT UPTAKE IN POTATOES (TUBERS)

The concentration in potato plants is calculated according to Trapp et al. (2007), assuming steady-state. A modification is applied to make use of a soil concentration on dry weight basis instead of a soil concentration on wet weight basis as used in the publication. The model applies to non-ionizing lipophilic chemicals with a log Kow > 1.

(eq. 101)

$$C_v = C_p$$

If a user-defined bioconcentration factor (BCF) is filled in, then the concentration in root plants is calculated from that BCF. Otherwise, the concentration in root plants is predicted from chemical and plant properties.

(eq. 102)

$$C_p = BCF_{org} \times C_w \times \frac{dm}{100}$$

(eq. 103)

$$C_p = \frac{k_1}{k_2 + \left(a_{growth} + a_{metabolism}\right)} \times C_w$$

(eq. 104)

$$k_2 = \frac{23 \times D_{p,p}}{{r_p}^2}$$

(eq. 105)

$$D_{p,p} = \frac{D_w \times W^{7/3}}{K_{PW}}$$

Where

Abbr.	Name	Unit	
C_v	Total plant concentration for organic chemicals	mg/kg fw	(eq. 101)
C_w	Concentration in the soil pore water	mg/m³	

Abbr.	Name	Unit	
			(eq. 18)
BCF_{org}	bioconcentration factor for organic contaminants	(mg/kg dm)/ (mg/m³)	Table 25
dm	Dry matter content of the plant	%	Table 20
C_p	Concentration in the potato	mg/kg fw	(eq. 102) or (eq. 103)
k_1	Uptake rate in the potato	1/d	(eq. 107)
k_2	depuration rate from the potato	1/d	(eq. 104)
a_{growth}	Chemical elimination via growth	1/d	Table 20
$a_{metabolism}$	loss due to metabolization in the plant	1/d	Table 25
$D_{p,p}$	effective diffusion coefficient in the potato	m²/d	(eq. 105)
r_p	radius of the potato	m	Table 20
ρ_w	density of water	kg/m³	Table 19
K_{PW}	partition coefficient between potato and water	l/kg fw	
			(eq. 106)
D_w	diffusion coefficient in water	m²/d	chemical properties or (eq. 14)

The equation for K_{PW} is comparable to the equation for K_{RW}, but includes an additional term for the carbohydrate content of the potato.

(eq. 106)

$$K_{PW} = W + L_{plant} \times a_1 \times K_{ow}{}^{b1} + f_{ch} \times K_{ch}$$

Where

Abbr.	Name	Unit	Source
K_{PW}	partition coefficient between potato and water	l/kg fw	
			(eq. 106)
f_{CH}	fraction of carbohydrates in potato	kg/kg	Table 20*
L_{plant}	Lipid content of the plant	kg/kg	Table 20
a_1	Correction factor for the difference in density between water and n-octanol ($1/\rho_{octanol}$)	-	Table 19
b_1	Briggs factor for root plants	-	Table 19
K_{CH}	partition coefficient between carbohydrates and water	l/kg fw	
			Table 17

*: this value is not the same as in Trapp et al. (2007)

Table 17: Values for K_{CH} as a function of log K_{OW} (Chiou, et al., 2001)

Log K_{OW}	K_{CH}
< 0	0.1
≥ 0 - < 1	0.2
≥ 1 - < 2	0.5
≥ 2 - < 3	1
≥ 3 - < 4	2
≥ 4	3

(eq. 107)

$$k_1 = \frac{k_2 \times K_{pw}}{1000}$$

Where

Abbr.	Name	Unit	Source
k_1	Uptake rate in the potato	1/d	(eq. 107)
k_2	depuration rate from the potato	1/d	(eq. 104)
K_{PW}	partition coefficient between potato and water	l/kg fw	(eq. 106)

7.1.3. PLANT UPTAKE IN ABOVE-GROUND PLANTS

The concentration of contaminants in above-ground plant parts is the results of three processes:

- Uptake by the roots and subsequent translocation to aboveground plant parts and gas phase exchange;
- Atmospheric deposition on aboveground plant parts;
- Splashing soil particles.

(eq. 108)

$$C_v = C_{v,sg} + C_{v,p} + C_{v,sp}$$

Where

Abbr.	Name	Unit	Source
C_v	Total plant concentration	mg/kg fw	(eq. 108)
$C_{v,sg}$	Plant concentration as a result of translocation from the root to the stem and leaves and gas phase exchange	mg/kg fw	(eq. 109) or (eq. 110)
$C_{v,p}$	Plant concentration as a result of wet and dry deposition	mg/kg fw	(eq. 117)
$C_{v,sp}$	Plant concentration as a result of splashed soil particles	mg/kg fw	(eq. 122)

→ Translocation and gas deposition between root and stem

The processes are described according to Trapp and Matthies (1995). The model is again parameterized for a surface area of 1 m². Chemicals are assumed to be taken up from the soil and from the atmosphere and to disappear due to evaporation from and transformation within the plant.

If a user-defined BCF is filled in, then the concentration in root plants is calculated from that BCF. Otherwise, the concentration in root plants is predicted from chemical and plant properties.

(eq. 109)

$$C_{v,sg} = BCF_{org} \times C_w \times \frac{dm}{100}$$

(eq. 110)

$$C_{v,sg} = \frac{b_s}{a \times \rho} \times (1 - e^{-a \times t})$$

Where

Abbr.	Name	Unit	Source
$C_{v,sg}$	Plant concentration as a result of gas exchange and translocation from the root to the stem and leaves	mg/kg fw	(eq. 109) or (eq. 110)
C_w	Concentration in the soil pore water	mg/m³	(eq. 18)
BCF_{org}	bioconcentration factor for organic contaminants	(mg/kg dm)/ (mg/m³)	Table 25
dm	Dry matter content of the plant	%	Table 20
t	Growth period of plant	d	Table 20
a	Total chemical elimination constant for removal out of the plant	1/d	(eq. 111)
b_s	Source term which describes transfer from soil and gas deposition	mg/m³.d	(eq. 115)
ρ	Density of the plant	kg fw/m³	Table 20

The chemical elimination constant consists of loss by metabolisation, photo-degradation, volatilization and growth and is described in the following equation.

(eq. 111)

$$a = \sum a_i = a_{metabolism} + a_{photo\text{-}degradation} + a_{volatilization} + a_{growth}$$

Where

Abbr.	Name	Unit	Source
a	Total chemical elimination constant for removal out of the plant	1/d	(eq. 111)
$a_{metabolism}$	Chemical elimination via metabolisation	1/d	Table 25
$a_{photodegradation}$	Chemical elimination via photo-degradation	1/d	Table 25
$a_{volatilization}$	Chemical elimination via volatilization	1/d	(eq. 112)
a_{growth}	Chemical elimination via growth	1/d	Table 20

(eq. 112)

$$a_{volatilization} = \frac{A \times g}{V \times K_{PA}}$$

Where

Abbr.	Name	Unit	Source
$a_{volatilization}$	Chemical elimination via volatilization	1/d	(eq. 112)
A	Surface area of aboveground plant parts	m^2/m^2	Table 20
g	Conductance of the leaf	m/d	Table 18
V	Volume of the aboveground plant parts	m^3/m^2	Table 20
K_{PA}	Gas-plant partition coefficient	m^3/m^3	(eq. 113)

Table 18: Conductance (g) of the leaf (from Trapp and Matthies (1995))

Condition	g (m/d)	Reference
$(\log K_{ow} - \log H') \leq 5$	47.5	Riederer (1995)
$(\log K_{ow} - \log H') > 5 - \leq 7.5$	173	Average of interpolated range
$(\log K_{ow} - \log H') > 7.5 - \leq 10$	346	Average of interpolated range
$(\log K_{ow} - \log H') > 10$	432	Thompson (1983)

The volumetric gas-plant partition coefficient K_{PA} depends upon the chemical and the plant species. The value is estimated from the octanol-air partition coefficient.

(eq. 113)

$$K_{PA} = m \times (K_{oa})^n$$

Where

Abbr.	Name	Unit	Source
K_{PA}	Gas-plant partition coefficient	m^3/m^3	(eq. 113)
m	Regression constant	-	Table 19
n	Regression constant	-	Table 19
K_{oa}	Octanol-air partition coefficient	-	(eq. 114)

The regression constants m and n are plant specific (and temperature dependent). No values for vegetables are available. The values for m and n are those for ryegrass at 25 °C (Komp and McLachlan, 1997a, 1997b).

K_{oa} is calculated from Kow and H'.

(eq. 114)

$$K_{oa} = \frac{K_{ow}}{H'}$$

Where

Abbr.	Name	Unit	Source
K_{oa}	Octanol-air partition coefficient	-	(eq. 114)
K_{ow}	Octanol-water partition coefficient	-	chemical properties
H'	Dimensionless Henry coefficient	-	(eq. 9)

(eq. 115)

$$b_s = C_w \times \frac{TSCF \times Q_{transp}}{V} + C_{ao,pl,vf} \times \frac{g \times A}{V}$$

Where

Abbr.	Name	Unit	Source
b_s	Source term which describes transfer from soil and gas deposition	mg/m³.d	(eq. 115)
C_w	Concentration in the soil pore water	mg/m³	(eq. 18)
TSCF	Transpiration stream concentration factor	-	(eq. 116)
Q_{transp}	Transpiration rate	m³/m².d	Table 20
V	Volume of the aboveground plant parts	m³/m²	Table 20
$C_{ao,pl,vf}$	Concentration in the gas phase in ambient air at plant height	mg/m³	(eq. 42)
g	Conductance of the leaf	m/d	Table 18
A	Surface area of the aboveground plant parts	m²/m²	Table 20

TSCF is calculated according to the publication of Briggs et al. (1982).

(eq. 116)

If $\log K_{ow} \leq 4.5$ $$TSCF = 0.784 \times \exp\left[-\frac{(\log K_{ow} - 1.78)^2}{2.44}\right]$$

If $\log K_{ow} > 4.5$ $$TSCF = 0.038$$

→ Plant concentration as a result of particle deposition

The concentration in the plant as a result of wet and dry deposition can be calculated from the particle concentration in air (Meneses, Schuhmacher, and Domingo, 2002).

(eq. 117)

$$C_{v,p} = \frac{C_{PM10,o} \times I_V \times \left((V_d) + (R_n \times R_w \times W_c)\right) \times \left(1 - \exp[-k_w \times t]\right)}{k_w \times Y_V}$$

Where

Abbr.	Name	Unit	Source
$C_{v,p}$	Plant concentration due to particle deposition	mg/kg fw	(eq. 117)
$C_{PM10,o}$	Concentration in outdoor air as a result of soil quality	mg/m³	(eq. 44)
I_V	Fraction of particles intercepted	-	(eq. 118) or (eq. 119) or (eq. 120) or (eq. 121)
V_d	Dry particle deposition rate	m/d	Table 19
R_n	Annual rainfall	m/d	Table 19
R_w	Fraction retained after rainfall	-	Table 19
W_c	Volumetric washout factor for particles	-	Table 25
k_w	Plant weathering constant	1/d	Table 19
t	Growth period of the plant	d	Table 20
Y_V	Plant yield	kg fw/m²	Table 20

The fraction of the particles deposited on the plant (I_V) is calculated according to Baes et al. (1984). The plant weathering constant is taken from Lorber, Cleverly et al. (1994) and Douben, Alcock et al. (1997). The volumetric washout factor for particles W_c is the ratio between the concentration in precipitation and the concentration in the atmosphere. The value is chemical-specific, but a default value of 5.10^5 is provided (Aurora model, PM_{10}, (Mensink, Colles, Janssen, and Cornelis, 2003)).

The relation between yield and interception for grasses was derived by Baes et al. (1984) from experimental studies. It can thus be considered a rather reliable relationship. The relationship for silage (corn) is based on theoretical calculations by Baes et al. (1984), taking into account assumptions of exposed plant area and plant distances. The relationship for foliar or leafy vegetables and for produce (called here other vegetables) is again based on theoretical calculations. The group of leafy vegetables also included cabbage and onion. The category other produce consisted of various fruits and vegetables such as tomato, cucumber, asparagus. A consumption-weighted averaging of crop-specific calculations was done for leafy vegetables and for produce. The theoretical equations assume that interception will increase with yield. Although this holds true for grasses, it does not completely hold true for the other classes as in later stages growth biomass will increase, but leaf area will level off and even decrease (Pröhl, 2009). We should therefore consider the relationshiop as not really plant-specific except for grass and silage.

(eq. 118)

$$I_v = 1 - exp\left(-2.88 \times Y_{v,grass} \times \frac{dm}{100}\right)$$

(eq. 119)

$$I_v = 1 - \exp\left(-0.769 \times Y_{v,silage} \times \frac{dm}{100}\right)$$

(eq. 120)

$$I_v = 1 - \exp(-0.0846 \times Y_{v,foliar})$$

(eq. 121)

$$I_v = 1 - \exp(-0.0324 \times Y_{v,other})$$

Where

Abbr.	Name	Unit	Source
I_V	Fraction of particles intercepted	-	(eq. 118) or (eq. 119) or (eq. 120) or (eq. 121)
Y_V	Plant yield	kg fw/m²	Table 20

→ **Concentration in the plant as a result of splashed soil particles**

The concentration in the plant due to transfer from splashed soil particles is calculated according to Samsoe-Petersen (2002). Calculations only apply to aboveground leafy vegetables and grass (growing close to the soil surface).

(eq. 122)

$$C_{v,sp} = TF_{net} \times C_{s+w}$$

Where

Abbr.	Name	Unit	Source
$C_{v,sp}$	Plant concentration as a result of splashed soil particles	mg/kg fw	(eq. 122)
TF_{net}	Net transfer factor of particles to the plant	-	(eq. 123)
C_{s+w}	Concentration in the soil solid and water phase	mg/kg dm	(eq. 45)

(eq. 123)

$$TF_{net} = f_{eff} \times \frac{R}{1-R}$$

Where

Abbr.	Name	Unit	Source
TF_{net}	Net transfer factor of particles to the plant	-	(eq. 123)
f_{eff}	Fraction of soil particles taken up by the plant	-	Table 19
R	Ratio of the particles on the leaves (weight) to the total weight of the plant	g/g fw	Table 19

7.2. PLANT UPTAKE FOR INORGANIC CHEMICALS

For inorganic chemicals, only root uptake and atmospheric particle deposition are considered.

The model offers the possibility to fill in user-defined BCF values or BCF relationships. These relationships express the BCF value or the concentration in the plant as a function of soil properties and the concentration in the soil.

7.2.1. PLANT UPTAKE IN ROOT PLANTS

The concentration of inorganic chemicals in root plants is the result of uptake from soil.

(eq. 124)

$$C_v = C_{v,s}$$

Where

Abbr.	Name	Unit	Source
C_v	Total plant concentration	mg/kg fw	(eq. 124)
$C_{v,s}$	Plant concentration due to soil – plant transfer	mg/kg fw	(eq. 125)

(eq. 125)

$$C_{v,s} = BCF_{inorg} \times C \times \frac{dm}{100}$$

Where

Abbr.	Name	Unit	Source
$C_{v,s}$	Plant concentration due to soil – plant transfer	mg/kg fw	(eq. 125)
BCF_{inorg}	Bioconcentration factor for inorganic contaminants	(mg/kg plant dm)/ (mg/kg soil dm)	Table 25
C	Total soil concentration	mg/kg dm	user input

dm	Dry matter content	%	Table 20

7.2.2. PLANT UPTAKE IN ABOVE-GROUND PLANTS

The concentration of inorganic chemicals in above-ground plant parts is the result of uptake from soil and subsequent translocation, and of deposition.

(eq. 126)

$$C_v = C_{v,s} + C_{v,p}$$

Where

Abbr.	Name	Unit	Source
C_v	Total plant concentration	mg/kg fw	(eq. 126)
$C_{v,s}$	Plant concentration due to soil – plant transfer	mg/kg fw	(eq. 125)
$C_{v,p}$	Plant concentration as a result of deposition	mg/kg fw	(eq. 117)

→ **Translocation between root and stem**

The calculation of the $C_{v,s}$ for foliar plants is as for root plants.

→ **Plant concentration as a result of particle deposition**

The calculation of the $C_{v,p}$ for foliar plants is the same as for organic chemicals.

Table 19: Fixed parameter values for the plant uptake models

Parameter	Value	Unit
a_1 (correction factor for the difference in density between water and n-octanol)	1.22	-
b_1 (Briggs factor for root plants)	0.77	-
ρ_w (density of water)	1000	kg/m³
m (regression constant)	0.003	-
n (regression constant)	1.0928	-
V_d (dry particle deposition rate)	865	m/d
R_n (annual rainfall)	0.0022	m/d
R_w (fraction retained after rainfall)	1.0	-
k_w (plant weathering constant)	0.049	1/d
f_{eff} (fraction of soil particles taken up by the plant)	1.0	-
R (ratio of particle weight on plant leaves to total plant weight)	0.005	g/g fw

Table 20: Plant characteristics

Plant	Type	Q_{transp} ($m^3/m^2.d$)	a_{growth} (1/d)	L_{plant} (kg/kg)	f_{CH} (kg/kg)	t (d)	ρ / ρ_r (kg/m^3)	V / V_r (m^3/m^2)	A (m^2/m2)	Y_V (kg fw/m^2)	dm (%)	r_p (m)
Potato	tuber	n.a.	0.139	0.0015	0.19	128	1020	0.0038	n.a.	3.897	20	0.04
Carrot	Root	0.000778	0.1	0.025	n.a.	120	1020	0.0051	n.a.	5.2	11	n.a.
Radish	Root	0.001292	0.1	0.025	n.a.	29	820	0.0024	n.a.	2	5	n.a.
Scorzonera	Root	0.000271	0.1	0.025	n.a.	120	1020	0.0025	n.a.	2.5	9	n.a.
Onion	Foliar	0.001008	0.035	0.025	n.a.	55	800	0.0043	5	3.4	11	n.a.
Leek	Foliar	0.001563	0.035	0.025	n.a.	179	800	0.0046	5	3	13	n.a.
Tomatoes	aboveground non-foliar	0.000658	0.035	0.025	n.a.	150	800	0.0496	5	39.7	5	n.a.
Cucumber	aboveground non-foliar	0.000658	0.035	0.025	n.a.	150	800	0.0423	5	33.8	4	n.a.
Paprika	aboveground non-foliar	0.000658	0.035	0.025	n.a.	150	800	0.0203	5	16.2	9	n.a.
cabbage	aboveground non-foliar	0.000658	0.035	0.025	n.a.	91	800	0.0069	5	5.5	8	n.a.
Cauliflower	aboveground non-foliar	0.001	0.035	0.025	n.a.	91	800	0.00300	5	2.4	8.1	n.a.
Sprout	aboveground non-foliar	0.000512	0.035	0.025	n.a.	117	800	0.0023	5	1.8	17	n.a.
Lettuce	Foliar	0.001225	0.035	0.025	n.a.	69	610	0.0072	5	4.4	4	n.a.
Lamb's lettuce	Foliar	0.000442	0.035	0.025	n.a.	69	650	0.0015	5	1	4	n.a.
Endive	Foliar	0.000925	0.035	0.025	n.a.	69	735	0.0068	5	5	6.2	n.a.
Spinach	Foliar	0.001225	0.035	0.025	n.a.	69	630	0.0032	5	2	8	n.a.
Chicory	Foliar	0.000563	0.035	0.025	n.a.	73	700	0.0021	5	1.5	6	n.a.
Celery	Foliar	0.000392	0.035	0.025	n.a.	120	800	0.0079	5	6.3	8	n.a.
Beans	aboveground non-foliar	0.000392	0.035	0.025	n.a.	77	800	0.0031	5	2.5	11	n.a.
Peas	aboveground non-foliar	0.000533	0.035	0.025	n.a.	95	800	0.0010	5	0.8	18	n.a.
Grass	Foliar	0.001563	0.035	0.025	n.a.	30	820	0.002	5	5.93	35	n.a.
maize	aboveground non-foliar	0.0012	0.035	0.054	n.a.	183	800	0.0057	5	4.53	25	n.a.

n.a.: not applicable

V: equals Yv/ρ; Q_{transp}: transpiration rate is expressed per m² of soil and assumes that Q_{transp}/mass of plant is constant during the growth season; Q_{transp} is calculated from E_0 (reference transpiration, Ukkel) at harvest, multiplied by crop specific factors at the end of the growing season (Allen, Pereira, Raes, and Smith, 1998); these values replace the default of 0.001 m³/day given by Trapp et al.(2002);

k: growth rate is taken from the publications of Trapp et al. (2002; 2007; 1995);

A: horizontal surface area of the aboveground plant per m² of soil

CHAPTER 8 TRANSFER OF CONTAMINANTS TO MEAT, MILK AND EGGS

8.1. INTRODUCTION

The model predicts concentrations of contaminants in meat of beef cattle and sheep, in milk and in eggs of free-ranging chicken. For organic contaminants biotransfer factors (BTFs) for meat and milk are calculated, or chemical dependent BTFs can be put in the chemicals database. For inorganic contaminants BTFs are required input parameters for meat and milk. For eggs, biotransfer factors are always required input parameters.

A biotransfer factor relates the concentration in animal products to the contaminant intake. S-RISK assumes equilibrium between intake and output in the animal products (meat, milk, etc.). At shorter exposure periods (animals slaughtered at young ages), this assumption of equilibrium does not hold true for accumulating chemicals.

Intake calculations are limited to intake via soil, feed and water. Inhalation and dermal contact are considered less important for the transfer to animal products.

The model allows to take into account both the local contribution as well as potential contribution from non-local feed (e.g. concentrate for beef, commercial feed mixtures for chicken).

8.2. EXPOSURE

8.2.1. EXPOSURE OF CATTLE

Intake of contaminants occurs through the intake of feed (grass, fodder crops and concentrates), water, soil particles and concentrate. Concentrates are considered although levels in concentrates are not of local (contaminated) origin. A distinction is made between the summer and winter diet of the animals. The total amount of contaminant that is taken in by the cattle is given by:

(eq. 127)

$$J_{f,summer} = RBA_{c,soil} \times J_{soil,summer} + J_{pasture,summer} + J_{grass\ silage,summer} + J_{maize,summer} + J_{water,summer} + J_{concentrate,summer}$$

(eq. 128)

$$J_{f,winter} = RBA_{c,soil} \times J_{soil,winter} + J_{pasture,winter} + J_{grass\ silage,winter} + J_{maize,winter} + J_{water,winter} + J_{concentrate,winter} +$$

(eq. 129)

$$J_{f,year} = J_{f,summer} \times t_{f,summer} + J_{f,winter} \times t_{f,winter}$$

(eq. 130)

$$t_{f,summer} = 1 - t_{f,winter}$$

Where

Abbr.	Name	Unit	Source
J_f	daily contaminant intake in summer or winter	mg/d	(eq. 127) or (eq. 128)
$J_{f,year}$	daily contaminant intake on yearly basis	mg/d	(eq. 129)
J_{soil}	daily contaminant intake via soil	mg/d	(eq. 131)
$J_{pasture}$	daily contaminant intake via pasture	mg/d	(eq. 132)
$J_{grass,silage}$	daily contaminant intake via silage grass	mg/d	(eq. 133)
J_{maize}	daily contaminant intake via maize	mg/d	(eq. 134)
J_{water}	daily contaminant intake via water	mg/d	(eq. 135)
$J_{concentrate}$	daily contaminant intake via concentrate	mg/d	(eq. 137)
$RBA_{c,soil}$	relative bioavailability of contaminants in soil versus food, cattle	-	Table 25
$t_{f,summer}$	time fraction for summer diet	-	(eq. 130)
$t_{f,winter}$	time fraction for winter diet	-	Table 23

(eq. 131)

$$J_{soil} = q_{soil} \times C$$

(eq. 132)

$$J_{pasture} = q_{grass} \times \left[f_{local}^{pasture} \times C'_{grass} + \left(1 - f_{local}^{pasture}\right) \times C'_{background,pasture} \right]$$

(eq. 133)

$$J_{grass,silage} = q_{grass,silage} \times \left[f_{local}^{grass,silage} \times C'_{grass} + \left(1 - f_{local}^{grass,silage}\right) \times C'_{background,grass,silage} \right]$$

(eq. 134)

$$J_{maize} = q_{maize} \times \left[f_{local}^{maize} \times C'_{maize} + \left(1 - f_{local}^{maize}\right) \times C'_{background,maize} \right]$$

(eq. 135)

$$J_{water} = q_{water} \times C_{c,water}$$

(eq. 136)

$$J_{concentrate} = q_{concentrate} \times C'_{concentrate}$$

Where

Abbr.	Name	Unit	Source
J_{soil}	daily contaminant intake via soil	mg/d	(eq. 131)
q_{soil}	daily intake of soil particles	kg dm/d	Table 23
C	contaminant concentration in total soil top layer	mg/kg dm	user input
$J_{pasture}$	daily contaminant intake via pasture	mg/d	(eq. 132)
$J_{grass,silage}$	daily contaminant intake via silage grass	mg/d	(eq. 133)
J_{maize}	daily contaminant intake via maize	mg/d	(eq. 134)
$J_{concentrate}$	daily contaminant intake via concentrate	mg/d	
			(eq. 136)
$q_{pasture}$	daily consumption of grass	kg dm/d	Table 23
$q_{grass,silage}$	daily consumption of silage grass	kg dm/d	Table 23
q_{maize}	daily consumption of silage maize	kg dm/d	Table 23
q_{water}	daily intake of water	m³/d	Table 23
$q_{concentrate}$	daily intake of concentrate	kg dm/d	Table 23
C'_{grass}	concentration in grass	mg/kg dm	
			(eq. 137)
C'_{maize}	concentration in maize	mg/kg dm	
			(eq. 138)
$C_{c,water}$	concentration in water for cattle	mg/m³	
			(eq. 139)
$C'_{concentrate}$	concentration in concentrate	mg/kg dm	chem.prop.
$C'_{background,pasture}$	background concentration in pasture grass	mg/kg dm	chem.prop.
$C'_{background, grass,silage}$	background concentration in silage grass	mg/kg dm	chem.prop.
$C'_{background, maize}$	background concentration in maize	mg/kg dm	chem.prop.
f_{local}	fraction of pasture grass, silage grass or maize coming from contaminated area	-	Table 23

(eq. 137)

$$C'_{grass} = \frac{C_{grass}}{dm_{grass}} * 100$$

(eq. 138)

$$C'_{maize} = \frac{C_{maize}}{dm_{maize}} * 100$$

(eq. 139)

$$C_{c,water} = C_{gw} \times f_{c,water,gw} + C_{wp} \times f_{c,water,wp} + C_{water,other} \times f_{c,water,other}$$

(eq. 140)

$$f_{c,water,other} = 1 - \left(f_{c,water,gw} + f_{c,water,wp} \right)$$

Where

Abbr.	Name	Unit	Source
C'_{grass}	concentration in grass dry weight basis	mg/kg dm	(eq. 137)
C'_{maize}	concentration in maize dry weight basis	mg/kg dm	(eq. 138)
$C_{c,water}$	concentration in water for cattle	mg/m³	(eq. 139)
C_{grass}	concentration in grass fresh weight basis	mg/kg fw	(eq. 108) or (eq. 126)
C_{maize}	concentration in maize fresh weight basis	mg/kg fw	(eq. 108) or (eq. 126)
dm	dry matter content of the plant	%	Table 20
C_{gw}	concentration in groundwater	mg/m³	(eq. 21) or user input
C_{wp}	concentration in drinking-water	mg/m³	(eq. 25)
$C_{water,other}$	concentration in other water	mg/m³	user input
$f_{c,water,gw}$	fraction of groundwater for cattle (summer / winter)	-	Table 23
$f_{c,water,wp}$	fraction of drinking-water for cattle (summer / winter)	-	Table 23
$f_{c,water,other}$	fraction of other water for cattle (summer / winter)	-	(eq. 140)

8.2.2. EXPOSURE OF CHICKEN

Exposure of chicken results from the intake of grass and soil (from the free-range area) and other feed components (with non-local origin) and from the intake of water.

(eq. 141)

$$J_{f,chicken} = f_{free-range} \times J_{grass,chicken} + J_{mixture,chicken} + J_{water,chicken}$$

(eq. 142)

$$J_{grass,chicken} = q_{grass,chicken} \times C'_{grass}$$

(eq. 143)

$$J_{mixture,chicken} = q_{mixture,chicken} \times C'_{mixture}$$

(eq. 144)

$$J_{water,chicken} = q_{water,chicken} \times C_{ch,water}$$

(eq. 145)

$$C_{ch,water} = C_{gw} \times f_{ch,water,gw} + C_{wp} \times f_{ch,water,wp} + C_{water,other} \times f_{ch,water,other}$$

(eq. 146)

$$f_{ch,water,other} = 1 - \left(f_{ch,water,gw} + f_{ch,water,wp}\right)$$

(eq. 147)

$$J_{soil,chicken} = f_{free-range} \times q_{soil,chicken} \times C$$

Where

Abbr.	Name	Unit	source
$J_{f,chicken}$	daily contaminant intake via feed	mg/d	(eq. 141)
$J_{grass,chicken}$	daily contaminant intake via grass	mg/d	(eq. 142)
$J_{mixture,chicken}$	daily contaminant intake via feed mixture	mg/d	(eq. 143)
$q_{grass,chicken}$	daily consumption of grass	kg dm/d	Table 24
$q_{mixture,chicken}$	daily consumption of feed mixture	kg dm/d	Table 24
$q_{water,chicken}$	daily intake of water	m^3/d	Table 24
$f_{free-range}$	fraction of free-range	-	Table 24
C'_{grass}	concentration in grass	mg/kg dm	(eq. 137)
$C'_{mixture}$	concentration in feed mixture for chicken	mg/kg dm	background levels database
$C_{ch,water}$	concentration in water for chicken	mg/m^3	(eq. 145)
C_{gw}	concentration in groundwater	mg/m^3	(eq. 21) or user input
C_{wp}	concentration in drinking-water	mg/m^3	(eq. 25)
$C_{water,other}$	concentration in other water	mg/m^3	user input
$f_{ch,water,gw}$	fraction of groundwater for chicken	-	Table 24
$f_{ch,water,wp}$	fraction of drinking-water for chicken	-	Table 24
$f_{ch,water,other}$	fraction of other water for chicken	-	(eq. 140)
$J_{soil,chicken}$	daily contaminant intake via soil	mg/d	(eq. 147)
$q_{soil,chicken}$	daily intake of soil by chicken	kg dm/d	Table 24
C	concentration in soil	mg/kg dm	user input

The intake of soil by free-range chicken is dependent on the area available per chicken and on the coverage of the soil. A maximum value for low area per chicken and no coverage is given as a default. If additional information is available, the amount of soil intake can be modified according to Table 21.

Table 21: Soil intake (kg/day) by free-range chicken as a function of area and soil coverage (Waegeneers, De Steur, De Temmerman, Van Steenwinkel, and Viaene, 2009)

	Surface area per chicken		
Soil coverage (%)	**≤6 m²**	**6 – 50 m²**	**> 50 m²**

0 - < 20	30.10^{-3}	30.10^{-3}	30.10^{-3}
20 - < 50	25.10^{-3}	20.10^{-3}	15.10^{-3}
50 - < 75	20.10^{-3}	15.10^{-3}	10.10^{-3}
75 - < 90	15.10^{-3}	10.10^{-3}	5.10^{-3}
90 - < 95	10.10^{-3}	5.10^{-3}	2.10^{-3}
≥ 95	5.10^{-3}	2.10^{-3}	2.10^{-3}

8.3. CONCENTRATION IN ANIMAL PRODUCTS

8.3.1. CONCENTRATION IN MEAT AND MILK

If the BTF for organic contaminants needs to be estimated, the Travis and Arms (1988) equations are used. However, the BTF is limited to a maximum value of 10^{-1} for meat and $10^{-1.8}$ for milk, in accordance with experimental observations (Birak, et al., 2001). If the biotransfer factor is available from the biological properties database, a distinction can be made between meat, liver and kidney. If the biotransfer factor is estimated, then no distinction is made between these food items in terms of biotransfer. Similarly, if the biotransfer factor for organics is estimated, then no distinction is made between beef and sheep, whereas the biological properties database allows for this distinction.

(eq. 148)

$$\log BTF_{meat,org} = \min(-1; -7.7 + 1.03 \times \log K_{ow})$$

(eq. 149)

$$\log BTF_{milk,org} = \min(-1.8; -8.056 + 0.992 \times \log K_{ow})$$

(eq. 150)

$$BTF = 10^{\log BTF}$$

Where

Abbr.	Name	Unit	Source
$BTF_{meat,org}$	biotransfer factor to meat for organic contaminants	(mg/kg fw)/ (mg/d)	(eq. 148)
$BTF_{milk,org}$	biotransfer factor to milk for organic contaminants	(mg/kg fw)/ (mg/d)	(eq. 149)
K_{ow}	octanol-water partition coefficient	-	chemical properties

(eq. 151)

$$C_{meat} = BTF_{meat} * J_{f,year}$$

(eq. 152)

$$C_{milk} = BTF_{milk} * J_{f,year}$$

(eq. 153)

$$C_{liver} = BTF_{liver} * J_{f,year}$$

(eq. 154)

$$C_{kidney} = BTF_{kidney} * J_{f,year}$$

The concentration in butter is – for organic contaminants - calculated from the concentration in milk, by using the ratio of fat contents. For inorganic contaminants, the concentration in butter is the same as the concentration in milk.

(eq. 155)

organic contaminants: $C_{butter} = C_{milk} \times \frac{f_{f,butter}}{f_{f,milk}}$

(eq. 156)

inorganic contaminants: $C_{butter} = C_{milk}$

Where

Abbr.	Name	Unit	Source
C_{meat}	concentration in meat (beef or sheep)	mg/kg fw	(eq. 151)
C_{milk}	concentration in milk	mg/kg fw	(eq. 152)
C_{liver}	concentration in liver	mg/kg fw	(eq. 153)
C_{kidney}	concentration in kidney	mg/kg fw	(eq. 154)
BTF_{meat}	biotransfer factor to meat	(mg/kg fw)/(mg/d)	(eq. 148) or Table 25
BTF_{milk}	biotransfer factor to milk	(mg/kg fw)/(mg/d)	(eq. 149) or Table 25
BTF_{liver}	biotransfer factor to liver	(mg/kg fw)/(mg/d)	(eq. 148) or Table 25
BTF_{kidney}	biotransfer factor to kidney	(mg/kg fw)/(mg/d)	(eq. 148) or Table 25
$J_{f,year}$	yearly contaminant intake (cattle or sheep)	mg/d	(eq. 129)
C_{butter}	concentration in butter	mg/kg fw	(eq. 155) or (eq. 156)
$f_{f,butter}$	fat content of butter	-	Table 22
$f_{f,milk}$	fat content of milk	-	Table 22

The values for fat content of butter and milk are those for typical full-fat products.

Table 22: Fat content of animal products

Abbr.	Name	Unit	Default value
$f_{f,butter}$	fat content of butter	-	0.85
$f_{f,milk}$	fat content of milk	-	0.04

The feed intake rates for cattle are based on Van Raamsdonk et al. (2007) en DLV (2007, 2008). For chicken we used the data of Van Raamsdonk et al. (2007) and Waegeneers et al. (2009). Soil ingestion for cattle is taken from the XtraFood model (Seuntjens, Steurbaut, and Vangronsveld, 2006a), while soil ingestion for sheep is taken as 2 % of feed intake (Römkens, et al., 2007).

Table 23: Cattle and sheep properties (references, see text)

Parameter	Unit	Beef cattle	Milk cattle	Sheep
$t_{f,winter}$	-	0.54	0.54	0.33
$q_{soil,summer}$	kg dm/d	0.6	0.6	0.175
$q_{soil,winter}$	kg dm/d	0	0	0.175
$q_{pasture,summer}$	kg dm/d	0	7.918	1.8
$q_{pasture,winter}$	kg dm/d	0	0	1.8
$q_{grass,silage,summer}$	kg dm/d	0	4.298	0
$q_{grass,silage,winter}$	kg dm/d	0	7.537	0
$q_{maize,summer}$	kg dm/d	4.745	2.217	0
$q_{maize,winter}$	kg dm/d	3.811	4.358	0
$q_{water,summer}$	m^3/d	0.067	0.067	0.006
$q_{water,winter}$	m^3/d	0.067	0.067	0.006
$q_{concentrate,summer}$	kg dm/d	2.61	0.257	0
$q_{concentrate,winter}$	kg dm/d	3.314	2.346	0.63
$f_{c,water,gw,summer}$	-	1	1	1
$f_{c,water,wp,summer}$	-	0	0	0
$f_{c,water,gw,winter}$	-	1	1	1
$f_{c,water,wp,winter}$	-	0	0	0
$f_{local}^{pasture}$	-	1	1	1
$f_{local}^{grass,silage}$	-	1	1	1
f_{local}^{maize}	-	1	1	1

Table 24: Chicken properties (references see text)

Parameter	Unit	Chicken
$f_{free\text{-}range}$	-	1 (can be 0 or 1)
$q_{grass,chicken}$	kg dm/d	0.007
$q_{water,chicken}$	m^3/d	0.0002
$q_{mixture,chicken}$	kg dm/d	0.123
$q_{soil,chicken}$	kg dm/d	3.10^{-2}
$f_{ch,water,gw}$	-	1
$f_{ch,water,wp}$	-	0

8.3.2. CONCENTRATION IN EGGS

(eq. 157)

$$C_{egg} = BTF_{soil,egg} * J_{soil,chicken} + BTF_{feed,egg} \times J_{f,chicken}$$

Where

Abbr.	Name	Unit	Source
C_{egg}	contaminant concentration in eggs	mg/kg fw	(eq. 157)
$J_{soil,chikcen}$	daily contaminant intake via soil	mg/d	(eq. 147)
$J_{f,chicken}$	daily contaminant intake via feed	mg/d	(eq. 141)
$BTF_{soil,egg}$	biotransfer factor from soil to egg	(mg/kg fw)/(mg/d)	Table 25
$BTF_{feed,egg}$	biotransfer factor from feed to egg	(mg/kg fw)/(mg/d)	Table 25

Table 25: Chemical-specific biological parameters

Abbr.	Name	Unit	Default value
W_c	volumetric washout factor particles	-	5.10^5
$a_{metabolism}$	metabolisation rate in plants	1/d	0
$a_{photodegradation}$	photodegradation rate in aboveground plants	1/d	0
BCF_{inorg}*	bioconcentration factor for inorganics: ▪ Veg categories; ▪ List of vegetables	(mg/kg dm)/ (mg/kg dm)	-
BCF_{org}**	bioconcentration factor for organics: ▪ Veg categories; ▪ List of vegetables	(mg/kg dm)/ (mg/m³)	-
$RBA_{c,soil}$	relative bioavailability of contaminants in soil versus food, cattle	-	1
$BTF_{meat,beef}$	biotransferfactor to beef meat	(mg/kg fw)/ (mg/d)	-
$BTF_{meat,sheep}$	biotransferfactor to sheep meat	(mg/kg fw)/ (mg/d)	-
BTF_{liver}	biotransfer factor to liver	(mg/kg fw)/ (mg/d)	-
BTF_{kidney}	biotransfer factor to kidney	(mg/kg fw)/ (mg/d)	-
BTF_{milk}	biotransfer factor to milk	(mg/kg fw)/ (mg/d)	-
$BTF_{soil,egg}$	biotransfer factor from soil to egg	(mg/kg fw)/ (mg/d)	-
$BTF_{feed,egg}$	biotransfer factor from feed to egg	(mg/kg fw)/ (mg/d)	-

*: Bioconcentration factors have to be filled in; either at the level of vegetable categories (see exposure) or at the level of vegetables;

**: bioconcentrations factors can optionally be filled in; either at the level of vegetable categories (see exposure) or at the level of vegetables

CHAPTER 9 HUMAN EXPOSURE

9.1. INTRODUCTION

Human exposure is calculated through the oral, dermal and inhalation route. Following exposure pathways are considered:

- Oral:
  - Ingestion of soil and indoor settled dust;
  - Intake of vegetables from local production (home-grown);
  - Intake of meat and milk from local production;
  - Intake of water (drinking-water or groundwater);
- Dermal:
  - Absorption from soil and indoor settled dust;
  - Absorption from water during showering and bathing;
- Inhalation:
  - Inhalation of outdoor air (gas-phase + particles);
  - Inhalation of indoor air (gas-phase + particles);
  - Inhalation during showering (gas-phase).

The model is provided with a series of default scenarios, which specify the exposure pathways considered and the scenario dependent exposure parameters. The default scenarios and their characteristics are given in Table 26. These scenarios are designed under the assumption that exposure is resulting from one scenario only. If a regional contamination occurs and more than one scenario applies per individual (e.g. residential and sport), the user should define the appropriate scenarios and combine the results of the exposure calculations. Table 26 also presents how these scenarios are connected to the derivation of soil remediation values. For recreational and industrial areas, more than one scenario is used for the calculation of soil remediation values. The applicable exposure pathways per scenario are given in Table 27.

Scenarios are considered to be "hierarchical" with less exposure pathways active when going from agriculture to industry. User-defined scenarios can be created based on available scenarios, both by deselecting or selecting default exposure pathways (not by adding a new exposure pathways) and by modifying exposure parameters.
Compared to the Flanders version, the scenario REC-stay (holiday resort - recreational) is not taken into account in the Walloon version (***W***).

Table 26: Default scenarios of the S-Risk model

Full name	Abbreviation	SRV
Residence with vegetable garden in agricultural area	AGR	agricultural
Residential area with vegetable garden	RES-veg	residential
Residential with garden	RES	
Residential without garden	RES-ng	
Day recreation (incl. sport)	REC-dayout	recreational
Day recreation indoor sport scenario	REC-dayin	recreational
Light industry (adults)	IND-l	Industrial
Heavy industry with outside activity (adults)	IND-h	Industrial

Table 27: Exposure pathways by scenario

	AGR	RES-veg	RES	RES-ng	REC-dayout	REC-dayin	IND-I	IND-h
Oral								
Ingestion of soil	X	X	X	X	X		X	X
Ingestion of indoor settled dust	X	X	X	X		X	X	X
Intake of vegetables from local production	X	X						
Intake of meat and milk from local production	X							
Intake of eggs from local origin								
Intake of water (drinking-water or groundwater)	X	X	X	X			X	X
Dermal								
Absorption from soil	X	X	X	X	X		X	X
absorption from indoor settled dust	X	X	X	X		X	X	X
Absorption from water during showering and bathing	X	X	X	X				
Inhalation								
Inhalation of outdoor air (gas-phase + particles)	X	X	X	X	X		X	X
Inhalation of indoor air (gas-phase + particles)	X	X	X	X		X	X	X
Inhalation during showering (gas-phase)	X	X	X	X				

Exposure is calculated for a series of age categories starting at 1 year. The age categories are given in Table 28. Body weight values are averages males and females for the Belgian population (Demarest and Drieskens, 2004; Roelants and Hauspie, 2004).

Table 28: Age categories and body weight (derived from Roelants and Hauspie (2004) Demarest and Drieskens (2004))

Age	Body weight (kg)
1 - < 3 year	12.3
3 - < 6 year	17.6
6 - < 10 year	26.8
10 - < 15 year	44.4
15 - < 21 year	62.5
21 - < 31 year	68.5
31 - < 41 year	70.5
41 - < 51 year	71.0
51 - < 61 year	74.0
≥ 61 years	72.5

Exposure is calculated as an external exposure metric, with the exception of the dermal pathways where an absorbed dose is calculated. The equation for exposure from soil and settled dust allows the use of a relative bioavailability factor. This factor expresses the ratio of the bioavailability of the contaminant in soil or dust to the bioavailability of the contaminant in food or water. Inhalation exposure is calculated as a time-weighted concentration. Weighting factors are applied for inhalation rate differences by age and activity.

Exposure is first calculated as a daily average value, representing exposure on the day of the event. Then the exposure dose is averaged over a one year period, accounting for the number of days per year exposure takes place. This distinction is merely important for the scenarios with intermittent exposure (recreational) and allows the comparison of these short-term exposures with corresponding health limits.

The choice of the values for the exposure parameters is such that a combination of average and high-end values results. For each set of parameter values summary information is given with regard to the conservatism of the value. More detailed information can be found in Cornelis et al. (2008). Time spent on-site has been modified, based on an intermediary analysis of the prototype (Cornelis, et al., 2012). An important change has been made to the residential time pattern, where time spent at school is not accounted for anymore in the age groups older than 3 years.

9.2. ORAL EXPOSURE

Intake from oral routes is expressed as intake equivalent to food intake. Therefore relative bioavailability factors are incorporated in the equations for drinking-water (potential higher bioavailability than in food) and for soil and dust (potential lower bioavailability than in food). As such, intakes from all oral pathways can be summed up for comparison with the adequate toxicological parameter and the relative contribution of the pathways can be assessed in a correct way.

9.2.1. INTAKE FROM SOIL AND INDOOR SETTLED DUST

Intake via soil and indoor settled dust is calculated differently for scenarios with assumed continuous intake over a day and for scenarios with intake limited to some fraction of the day. In the first case, a daily intake value is used, whereas in the latter case an hourly intake value is multiplied by the number of hours present at the site.

For continuous intake, a daily ingestion value for soil and settled dust is provided, together with a factor for the fraction of soil in the ingestion value. Daily ingestion values are P95 approximations (Van Holderbeke, et al., 2008). Hourly ingestion rates are taken from previous work (Cornelis, et al., 2007).

→ **Continuous intake**

(eq. 158)

$$ED_{oral\_soil}^{daily} = \frac{IR_{soil/dust\_daily} \times RBA_{soil} \times F_{oral\_soil} \times C \ \times CF}{BW}$$

(eq. 159)

$$ED_{oral\_dust}^{daily} = \frac{IR_{soil/dust\_daily} * RBA_{dust} * (1 - F_{oral\_soil}) * C_{settled\_dust} * CF}{BW}$$

(eq. 160)

$$ED_{oral\_soil/dust}^{daily} = ED_{oral\_soil}^{daily} + ED_{oral\_dust}^{daily}$$

(eq. 161)

$$ED_{oral\_soil}^{yearly} = \frac{ED_{oral\_soil}^{daily} * EF}{365}$$

(eq. 162)

$$ED_{oral\_dust}^{yearly} = \frac{ED_{oral\_dust}^{daily} * EF}{365}$$

(eq. 163)

$$ED_{oral\_soil/dust}^{yearly} = ED_{oral\_soil}^{yearly} + ED_{oral\_dust}^{yearly}$$

Where

Abbr.	Name	Unit	Source
$ED_{oral\_soil}^{daily}$	Daily average intake via soil	mg/kg.d	(eq. 158)
$IR_{soil/dust\_daily}$	Daily ingestion of soil and dust	mg/d	Table 43
RBA_{soil}	Relative bioavailability of contaminants in soil	-	
			Table 34
F_{oral_soil}	fraction of soil in soil and settled dust ingestion	-	Table 43
C	Total top soil concentration for intake via soil ingestion	mg/kg dm	user input

Abbr.	Name	Unit	Source
CF	Conversion factor from mg/d to kg/d	kg/mg	Table 33
$ED^{daily}_{oral\_dust}$	Daily average intake via settled indoor dust	mg/kg.d	(eq. 159)
RBA_{dust}	Relative bioavailability of contaminants in settled dust	-	Table 34
$C_{settled\_dust}$	concentration in settled indoor dust due to soil contamination	mg/kg dm	(eq. 86)
BW	Body weight	kg	Table 28
$ED^{daily}_{oral\_soil/dust}$	Daily average intake via soil and dust particles	mg/kg.d	(eq. 160)
$ED^{yearly}_{oral\_soil}$	Yearly average intake via soil particles	mg/kg.d	(eq. 161)
$ED^{yearly}_{oral\_dust}$	Yearly average intake via dust particles	mg/kg.d	(eq. 162)
$ED^{yearly}_{oral\_soil/dust}$	Yearly average intake via soil and dust particles	mg/kg.d	(eq. 163)
EF	Exposure frequency	d/y	(eq. 164)

(eq. 164)

$$EF = EF_{week} \times EF_{year}$$

Where

Abbr.	Name	Unit	Reference
EF	Exposure frequency	d/y	(eq. 164)
EF_{week}	Frequency on a weekly basis	d/w	Table 35 or Table 36 or Table 37 or Table 38 or Table 39 or Table 40 or Table 41 or Table 42
EF_{year}	Frequency on a yearly basis	w/y	Table 35 or Table 36 or Table 37 or Table 38 or Table 39 or Table 40 or Table 41 or Table 42

→ **Intermittent intake**

(eq. 165)

$$ED^{daily}_{oral\_soil} = \frac{IR_{soil\_hourly} \times t_{out} \times RBA_{soil} \times C \times CF}{BW}$$

(eq. 166)

$$ED^{daily}_{oral\_dust} = \frac{IR_{dust\_hourly} \times t_{in} \times RBA_{dust} \times C_{settled\_dust} \times CF}{BW}$$

(eq. 167)

$$ED^{daily}_{oral\_soil/dust} = ED^{daily}_{oral\_soil} + ED^{daily}_{oral\_dust}$$

(eq. 168)

$$ED_{oral\_soil}^{yearly} = \frac{ED_{oral\_soil}^{daily} * EF}{365}$$

(eq. 169)

$$ED_{oral\_dust}^{yearly} = \frac{ED_{oral\_dust}^{daily} * EF}{365}$$

(eq. 170)

$$ED_{oral\_soil/dust}^{yearly} = ED_{oral\_soil}^{yearly} + ED_{oral\_dust}^{yearly}$$

Where

Abbr.	Name	Unit	Reference
$ED_{oral\_soil}^{daily}$	Daily average intake via soil particles	mg/kg.d	(eq. 165)
$ED_{oral\_dust}^{daily}$	Daily average intake via dust particles	mg/kg.d	(eq. 166)
$ED_{oral\_soil/dust}^{daily}$	Daily average intake via soil and dust particles	mg/kg.d	(eq. 167)
$ED_{oral\_soil}^{yearly}$	Yearly average intake via soil and dust particles	mg/kg.d	(eq. 168)
$ED_{oral\_dust}^{yearly}$	Yearly average oral intake via dust particles	mg/kg.d	(eq. 169)
$ED_{oral\_soil/dust}^{yearly}$	Yearly average intake via soil and dust particles	mg/kg.d	(eq. 170)
IR_{soil_hourly}	Hourly ingestion of soil	mg/h	Table 44
IR_{dust_hourly}	Hourly ingestion of settled dust	mg/h	Table 44
t_{out}	Time spent outside	h/d	Table 39 or Table 40
t_{in}	Time spent inside	h/d	Table 39 or Table 40
RBA_{soil}	Relative bioavailability of contaminants in soil	-	Table 34
RBA_{dust}	Relative bioavailability of contaminants in settled dust	-	Table 34
C	Top soil concentration for ingestion	mg/kg dm	user input
$C_{settled\_dust}$	Concentration in settled dust indoors from soil	mg/kg dm	(eq. 86)
CF	Conversion factor	kg/mg	Table 33
BW	Body weight	kg	Table 28

9.2.2. INTAKE FROM LOCALLY PRODUCED FOOD

Depending on the scenario, locally grown food contributes to a specified extent to the contaminant intake from the site. Dietary exposure from locally produced food is taken into account for the following food groups:

- Vegetables;
- Meat (beef, organ meat);
- Dairy products (milk, butter);
- Eggs.

While the transfer module calculates concentrations in mutton, contaminant intake through muttons consumption is not accounted for in S-Risk. Exposure is calculated from concentration by using food consumption data and the fraction of the food item or food group that is assumed to be from local production. Intake from locally produced food is only calculated on a yearly basis as this contribution only applies to scenarios with continuous exposure.

→ **Vegetables**

First, a consumption-weighted concentration by vegetable category is calculated. Then this concentration is combined with the intake rate at category level and the fraction home-grown to give the intake by vegetable category.

(eq. 171)

$$C_{veg_{category},j,} = \frac{\sum C_{v,i,j} \times Q_{vegetable,i,j}}{\sum Q_{vegetable,i,j}}$$

Where

Abbr.	Name	Unit	Reference
$C_{veg\_category,j}$	Concentration in vegetable category j	mg/kg fw	(eq. 171)
$C_{v,i,j}$	concentration in vegetable i from vegetable category j	mg/kg fw	(eq. 96) or (eq. 101) or (eq. 108) or (eq. 124) or (eq. 126)
$Q_{vegetable,i,j}$	amount of consumed vegetable i from category j	g fw/d	Table 29

(eq. 172)

$$ED^{yearly}_{veg\_category} = \frac{C_{veg\_category} \times Q_{veg\_category} \times f^{garden}_{veg\_category}}{BW * 1000}$$

(eq. 173)

$$ED^{yearly}_{vegetables} = \sum ED^{yearly}_{veg\_category}$$

Where

Abbr.	Name	Unit	Reference
$ED^{yearly}_{veg\_category}$	Yearly average intake through consumption of locally grown vegetables by vegetable category	mg/kg d	(eq. 172)

$ED_{vegetables}^{yearly}$	yearly average intake through consumption of locally grown vegetables	mg/kg d	(eq. 173)
$C_{veg\_category}$	Concentration in vegetable category	mg/kg fw	(eq. 171)
$Q_{veg\_category}$	Amount of consumed vegetable category	g fw/d	Table 29
$f_{veg\_category}^{garden}$	Fraction of locally grown vegetables by category	-	Table 45
BW	Body weight	kg	Table 28

Vegetable consumption data were taken from the XtraFood model (Seuntjens, Steurbaut, and Vangronsveld, 2006b) and are based on Belgian data with interpolations for lacking age categories or gender. Average intakes were selected from the database. They were compared with the more recent adult data from the Belgian Food Consumption Survey (Devriese, Huybrechts, Moreau, and Van Oyen, 2006). Then, a correction has been made to account for the increase in vegetable consumption for people with an own vegetable garden (Cornelis, et al., 2007). This correction was based on the food frequency questionnaires of the Flemish Human Biomonitoring 2001-2006 and on Dutch data (Swartjes, et al., 2007). Data for children in the age group 1 - < 3yrs are taken from the Netherlands and correspond to data for 18 months old children (Voedingscentrum, 2002).

Table 29: Vegetable consumption data ($Q_{veg,i,j}$ and $Q_{veg\_category,j}$) (g fw/d)

			Root and tuberous plants			**Bulbous plants**			**Fruit vegetables**			
age	potatoes	carrot	Scorzonera and parsnip	Other root vegetables (as parsnip)	**Σ Root and tuberous plants**	Bulbous vegetable (as onion)	leek	**Σ bulbous plants**	cucumber	tomatoes	Other fruit vegetables (as paprika)	**Σ fruit vegetables**
1 - < 3 year	**36.30**	9.12	0.24	0.45	**9.81**	2.23	3.61	**5.84**	1.61	6.40	0.88	**8.89**
3 - < 6 year	**85.35**	14.45	0.38	0.71	**15.54**	3.53	5.73	**9.25**	2.56	10.13	1.39	**14.09**
6 - < 10 year	**100.81**	15.43	0.48	0.81	**16.71**	5.59	5.35	**10.94**	3.70	16.17	1.74	**21.62**
10 - < 15 year	**120.69**	16.68	0.60	0.95	**18.24**	8.25	4.86	**13.10**	5.18	23.93	2.19	**31.30**
15 - < 21 year	**140.21**	21.57	0.79	1.45	**23.81**	11.68	5.04	**16.72**	8.59	36.77	4.41	**49.77**
21 - < 31 year	**129.90**	24.78	0.46	1.70	**26.94**	13.85	5.30	**19.14**	16.98	53.14	9.03	**79.15**
31 - < 41 year	**124.54**	24.78	0.46	1.70	**26.94**	13.85	5.30	**19.14**	16.98	53.14	9.03	**79.15**
41 - < 51 year	**129.29**	24.78	0.46	1.70	**26.94**	13.85	5.30	**19.14**	16.98	53.14	9.03	**79.15**
51 - < 61 year	**134.31**	24.78	0.46	1.70	**26.94**	13.85	5.30	**19.14**	16.98	53.14	9.03	**79.15**
≥ 61 year	**137.19**	24.78	0.46	1.70	**26.94**	13.85	5.30	**19.14**	16.98	53.14	9.03	**79.15**

Table 29: Vegetable consumption data (Qveg,i,j and Qveg_category,j) (g fw/d) (continued)

	Cabbages				**Leafy vegetables**						
age	cabbage	sprouts	Cauliflower and broccoli	**Σ cabbages**	lettuce	spinach	chicory	celery	endive	lamb’s lettuce	**Σ leafy vegetables**
1 - < 3 year	1.74	1.74	3.76	**7.24**	0.50	4.08	2.07	0.90	0.14	0.14	**7.82**
3 - < 6 year	2.76	2.76	5.95	**11.47**	0.79	6.46	3.28	1.42	0.22	0.22	**12.39**
6 - < 10 year	2.40	2.40	6.49	**11.29**	2.90	6.38	4.72	1.58	0.44	0.44	**16.46**
10 - < 15 year	1.93	1.93	7.19	**11.06**	5.62	6.28	6.58	1.88	0.72	0.72	**21.80**
15 - < 21 year	1.50	1.50	10.54	**13.54**	8.45	5.29	8.89	2.08	1.20	1.20	**27.11**
21 - < 31 year	2.50	2.50	13.50	**18.50**	10.56	8.54	9.33	2.43	0.92	0.92	**32.70**
31 - < 41 year	2.50	2.50	13.50	**18.50**	10.56	8.54	9.33	2.43	0.92	0.92	**32.70**
41 - < 51 year	2.50	2.50	13.50	**18.50**	10.56	8.54	9.33	2.43	0.92	0.92	**32.70**
51 - < 61 year	2.50	2.50	13.50	**18.50**	10.56	8.54	9.33	2.43	0.92	0.92	**32.70**
≥ 61 year	2.50	2.50	13.50	**18.50**	10.56	8.54	9.33	2.43	0.92	0.92	**32.70**

Table 29: Vegetable consumption data (Qveg,i,j and Qveg_category,j) (g fw/d) (continued)

	Leguminous vegetables		
age	beans	peas	**Σ leguminous vegetables**
1 - < 3 year	3.47	2.00	**5.47**
3 - < 6 year	5.49	3.17	**8.66**
6 - < 10 year	6.42	3.51	**9.94**
10 - < 15 year	7.63	3.96	**11.59**
15 - < 21 year	9.60	4.19	**13.80**
21 - < 31 year	11.75	3.87	**15.62**
31 - < 41 year	11.75	3.87	**15.62**
41 - < 51 year	11.75	3.87	**15.62**
51 - < 61 year	11.75	3.87	**15.62**
≥ 61 year	11.75	3.87	**15.62**

→ **Animal products**

(eq. 174)

$$ED_{beef}^{yearly} = \frac{C_{beef} \times Q_{beef} \times f_{beef}^{local}}{BW * 1000}$$

(eq. 175)

$$ED_{organ\_meat}^{yearly} = \frac{\left(\frac{C_{kidney} + C_{liver}}{2} \right) \times Q_{organ\_meat} \times f_{organ\_meat}^{local}}{BW * 1000}$$

(eq. 176)

$$ED_{milk}^{yearly} = \frac{C_{milk} \times Q_{milk} \times f_{milk}^{local}}{BW * 1000}$$

(eq. 177)

$$ED_{butter}^{yearly} = \frac{C_{butter} \times Q_{butter} \times f_{butter}^{local}}{BW * 1000}$$

(eq. 178)

$$ED_{eggs}^{yearly} = \frac{C_{eggs} \times Q_{eggs} \times f_{eggs}^{local}}{BW * 1000}$$

Where

Abbr.	Name	Unit	Reference
ED_{beef}^{yearly}	yearly average intake through consumption of locally produced beef	mg/kg d	(eq. 174)
$ED_{organ\_meat}^{yearly}$	yearly average intake through consumption of locally produced organ meat	mg/kg d	(eq. 175)
ED_{milk}^{yearly}	yearly average intake through consumption of locally produced milk	mg/kg d	(eq. 176)
ED_{butter}^{yearly}	yearly average intake through consumption of locally produced butter	mg/kg d	(eq. 177)
ED_{eggs}^{yearly}	yearly average intake through consumption of locally produced eggs	mg/kg d	(eq. 178)
C_{beef}	Concentration in beef	mg/kg fw	(eq. 151)
C_{kidney}	concentration in kidney	mg/kg fw	(eq. 154)
C_{liver}	concentration in liver	mg/kg fw	(eq. 153)
C_{milk}	concentration in milk	mg/kg fw	(eq. 152)

Abbr.	Name	Unit	Reference
C_{butter}	concentration in butter	mg/kg fw	(eq. 155) or (eq. 156)
C_{eggs}	concentration in eggs	mg/kg fw	(eq. 157)
Q_{beef}	Consumption of beef	g/d	Table 30
Q_{organ_meat}	consumption of organ meat	g/d	Table 30
Q_{milk}	consumption of milk	g/d	Table 30
Q_{butter}	consumption of butter	g/d	Table 30
Q_{eggs}	consumption of eggs	g/d	Table 30
$f_{animal\_product}^{local}$	fraction of animal product coming from location	-	Table 45
BW	Body weight	kg	Table 28

(eq. 179)

$$ED_{animal\_products}^{yearly} = ED_{beef}^{yearly} + \mathrm{ED}_{\mathrm{organ\_meat}}^{yearly} + ED_{milk}^{yearly} + ED_{butter}^{yearly} + ED_{eggs}^{yearly}$$

Where

Abbr.	Name	Unit	Reference
$ED_{animal\ products}$	yearly average intake through consumption of locally produced animal products	mg/kg.d	(eq. 179)
ED_{beef}	yearly average intake through consumption of locally produced beef	mg/kg d	(eq. 174)
ED_{organ_meat}	yearly average intake through consumption of locally produced organ meat	mg/kg d	(eq. 175)
ED_{milk}	yearly average intake through consumption of locally produced milk	mg/kg d	(eq. 176)
ED_{butter}	yearly average intake through consumption of locally produced butter	mg/kg d	(eq. 177)
ED_{eggs}	yearly average intake through consumption of locally produced eggs	mg/kg d	(eq. 178)
ED_{beef}	yearly average intake through consumption of locally produced beef	mg/kg d	(eq. 174)

Consumption data for meat and milk products represent averages (Cornelis, et al., 2008). Egg consumption is set at P95.

Table 30: Consumption data for animal products (g/d)

Age	Q_{beef}	Q_{organ_meat}	Q_{milk}	Q_{butter}	Q_{eggs}
1 - < 3 year	10.0	0.00	395	0.40	15
3 - < 6 year	10.0	0.07	387	0.46	29
6 - < 10 year	18.0	0.23	340	0.97	30
10 - < 15 year	30.0	0.46	280	1.6	30
15 - < 21 year	37.0	0.39	229	2.6	33
21 - < 31 year	32.0	0.15	215	3.1	41
31 - < 41 year	36.0	0.28	181	3.4	43
41 - < 51 year	37.0	0.28	186	4.7	45
51 - < 61 year	38.0	0.28	191	6.0	47
≥ 61 years	35.0	0.28	211	7.5	44

The consumption data of eggs do not include the consumption of eggs in processed food, such as pastry. Milk includes milk, yoghurt and white cheese; butter includes full-fat butter. Data for meat, and milk products were taken from the XtraFood model (Seuntjens, et al., 2006a) and correspond to average consumption. Egg consumption is set at P95.

9.2.3. INTAKE FROM DRINKING-WATER

The intake from drinking-water allows to take into account differences in relative bioavailability compared to the bioavailability on which the toxicological criterion is based and a reduction factor because of limited time spent on-site. The reduction factor for drinking-water consumption includes the nature of the activities and time spent on the site. It is assumed that for land use types with residence the reduction factor always equals 1. In other words the total daily drinking-water intake occurs on-site. For the landuse types day recreation it is assumed that no contaminated drinking-water is consumed. For the industrial landuse types the reduction factor equals the ratio between time spent on the job and at home.

(eq. 180)

$$ED^{daily}_{drinking\_water} = \frac{C_{dw} \times RBA_{drinking\_water} \times Q_{drinking\_water} \times RF_{drinking\_water}}{BW * 1000}$$

Where

Abbr.	Name	Unit	Source
$ED^{daily}_{drinking\_water}$	Daily average intake through drinking-water	mg/kg.d	(eq. 180)
C_{dw}	Concentration in drinking-water	mg/m³	(eq. 26)
$RBA_{drinking\_water}$	Relative bioavailability in drinking-water	-	Table 34
$Q_{drinking\_water}$	Consumption of drinking-water	l/d	Table 31
$RF_{drinking\_water}$	Reduction factor for drinking-water consumption	-	Table 45
BW	Body weight	kg	Table 28

(eq. 181)

$$ED^{yearly}_{drinking\_water} = \frac{ED^{daily}_{drinking\_water} \times EF}{365}$$

Where

Abbr.	Name	Unit	Source
$ED^{yearly}_{drinking\_water}$	Yearly average intake via drinking-water	mg/kg d	(eq. 181)
$ED^{daily}_{drinking\_water}$	Daily average intake via drinking-water	mg/kg d	(eq. 180)
EF	Exposure frequency	d/y	(eq. 164)

Table 31: Values for water consumption per age category

Age	$Q_{drinking\_water}$ (l/d)
1 - < 3 year	0.3
3 - < 6 year	0.313
6 - < 10 year	0.381
10 - < 15 year	0.649
15 - < 21 year	0.999
21 - < 31 year	1.759
31 - < 41 year	2.231
41 - < 51 year	2.199
51 - < 61 year	1.798
≥ 61 years	1.590

Water consumption values correspond to the P95 of the sum of water, coffee and tea from the XtraFood database (Seuntjens, et al., 2006b).

9.2.4. TOTAL ORAL DOSE

(eq. 182)

$$ED_{oral}^{daily} = ED_{oral\_soil/dust}^{daily} + ED_{vegetables}^{yearly} + ED_{animal\_products}^{yearly} + ED_{drinking\_water}^{daily}$$

Where

Abbr.	Name	Unit	Reference
ED_{oral}^{daily}	Total daily oral dose	mg/kg d	(eq. 182)
$ED_{oral\_soil/dust}^{daily}$	Daily average intake via soil and dust particles	mg/kg.d	(eq. 167)
$ED_{vegetables}^{yearly}$	Yearly average intake via vegetables	mg/kg d	(eq. 173)
$ED_{animal\_products}^{yearly}$	Yearly average intake via animal products	mg/kg d	(eq. 179)
$ED_{drinking\_water}^{daily}$	Daily average intake via drinking-water	mg/kg.d	(eq. 181)

(eq. 183)

$$ED_{oral}^{yearly} = ED_{oral\_soil/dust}^{yearly} + ED_{vegetables}^{yearly} + ED_{animal\_products}^{yearly} + ED_{drinking\_water}^{yearly}$$

Where

Abbr.	Name	Unit	Source
ED_{oral}^{yearly}	Total yearly oral dose	mg/kg d	(eq. 183)
$ED_{oral_{soil}/dust}^{yearly}$	Yearly average intake via soil and dust particles	mg/kg.d	(eq. 170)

Abbr.	Name	Unit	Source
$ED^{yearly}_{vegetables}$	Yearly average intake via vegetables	mg/kg d	(eq. 173)
$ED^{yearly}_{animal\_products}$	Yearly average intake via animal products	mg/kg d	(eq. 179)
$ED^{yearly}_{drinking\_water}$	Yearly average intake via drinking-water	mg/kg d	(eq. 181)

9.3. DERMAL EXPOSURE

Dermal exposure is calculated as an absorbed dose through the skin. Dermal exposure is modelled according to the approach and equations given in US-EPA (US-EPA, 1997, 2004a). Skin surface area is calculated from body weight and length (Demarest, et al., 2004; Roelants, et al., 2004), using the equation of Gehan and George (1970) given in US-EPA (2004a). The proportion of the various body parts to total body surface area is taken from US-EPA (2004a) and US-EPA (1997).

9.3.1. DERMAL ABSORPTION VIA SOIL AND DUST PARTICLES

The dermal absorbed dose via contact with soil and dust is first calculated as an external amount per skin area and per event, which is then converted to an absorbed daily dose. The number of events per day (which is related to the time between washing of the skin) is hard to estimate and is set to a fixed value of 1 for the outdoor (soil) and indoor (dust) pathway.

(eq. 184)

$$EDE_{dermal\_soil} = C \times AF_{soil\_skin} \times CF$$

(eq. 185)

$$EDE_{dermal\_dust} = C \times AF_{dust\_skin} \times CF$$

Where

Abbr.	Name	Unit	Source
EDE_{dermal_soil}	Intake via dermal contact with soil particles, per event	mg/m².event	(eq. 184)
EDE_{dermal_dust}	Intake via dermal contact with dust particles, per event	mg/m².event	(eq. 185)
C	Concentration in soil / dust	mg/kg dm	user input
AF_{soil_skin}	average soil adherence on skin	mg/m²	Table 47
AF_{dust_skin}	average dust adherence on skin	mg/m²	Table 48
CF	Conversion factor	kg/mg	Table 33

(eq. 186)

$$AD^{daily}_{dermal\_soil} = \frac{EDE_{dermal\_soil} \times ABS_{dermal} \times SA_{out} \times EV_{out}}{BW}$$

(eq. 187)

$$AD^{daily}_{dermal\_dust} = \frac{EDE_{dermal\_dust} \times ABS_{dermal} \times SA_{in} \times EV_{in}}{BW}$$

Where

Abbr.	Name	Unit	Source
$AD_{dermal\_soil}^{daily}$	Daily uptake via dermal contact with soil particles	mg/m².d	(eq. 186)
$AD_{dermal\_dust}^{daily}$	Daily uptake via dermal contact with dust particles	mg/m².d	(eq. 187)
ABS_{dermal}	Dermal absorption factor for soil and dust	-	Table 34
SA_{out}	skin surface area covered with soil during outside activities	m²	Table 49
SA_{in}	skin surface area covered with dust during inside activities	m²	Table 50
EV_{out}	number of "soil" events	events/d	Table 33
EV_{in}	number of "dust" events	events/d	Table 33
BW	body weight	kg	Table 28

Absorption factors for dermal uptake from soil and dust can be found in the literature. A compilation of values can also be found in US-EPA (2004a) and on the RAIS website (http://rais.ornl.gov/).

(eq. 188)

$$AD_{dermal\_soil/dust}^{daily} = AD_{dermal\_soil}^{daily} + AD_{dermal\_dust}^{daily}$$

Where

Abbr.	Name	Unit	Source
$AD_{dermal\_soil/dust}^{daily}$	Total daily uptake via dermal contact with soil and dust	mg/kg.d	(eq. 188)
$AD_{dermal\_soil}^{daily}$	daily uptake via dermal contact with soil (outdoor)	mg/kg.d	(eq. 186)
$AD_{dermal\_dust}^{daily}$	daily uptake via dermal contact with dust (indoor)	mg/kg.d	(eq. 187)

(eq. 189)

$$AD_{dermal\_soil}^{yearly} = \frac{AD_{dermal\_soil}^{daily} \times EF}{365}$$

(eq. 190)

$$AD_{dermal\_dust}^{yearly} = \frac{AD_{dermal\_dust}^{daily} \times EF}{365}$$

(eq. 191)

$$AD_{dermal\_soil/dust}^{yearly} = AD_{dermal\_soil}^{yearly} + AD_{dermal\_dust}^{yearly}$$

Where

Abbr.	Name	Units	Source
$AD^{yearly}_{dermal\_soil}$	Yearly average uptake via dermal contact with soil	mg/kg.d	(eq. 189)
$AD^{daily}_{dermal\_soil}$	Daily uptake via dermal contact with soil	mg/kg.d	(eq. 186)
$AD^{yearly}_{dermal\_dust}$	Yearly average uptake via dermal contact with dust	mg/kg.d	(eq. 190)
$AD^{daily}_{dermal\_dust}$	Daily uptake via dermal contact with dust	mg/kg.d	(eq. 187)
$AD^{yearly}_{dermal\_dust/soil}$	Yearly average uptake via dermal contact with dust and soil	mg/kg.d	(eq. 191)
EF	Exposure frequency	d/y	(eq. 164)

9.3.2. DERMAL ABSORPTION DURING BATHING AND SHOWERING

Dermal uptake during bathing and showering is calculated on an event basis, accounting for duration of the event. The calculations differ between organic contaminants and for inorganic contaminants. The equations used follow the guidance developed by US-EPA (2004a) and updates (checked september 2009).

→ **Absorbed dose per event for organic contaminants**

The equations account for the absence of equilibrium at the beginning of exposure. The time needed to reach an equilibrium state is calculated for each contaminant and different exposure equations apply depending whether event duration is shorter or longer than the time of this transient phase.

The key parameter is the dermal permeability coefficient, which can be calculated or can be user input.

(eq. 192)

$$\log K_p = -2.80 + 0.66 \times \log K_{ow} - 0.0056 \times M$$

Where

Abbr.	Name	Units	Source
K_p	dermal permeability coefficient	cm/h	(eq. 192) or user input
K_{ow}	octanol-water partition coefficient	-	chem. prop.
M	molecular weight	g/mol	chem. prop.

The limits of the application domain are given by following equations

(eq. 193)

$$-0.06831 \leq 5.103 \times 10^{-4} \times M + 0.05616 \times \log K_{ow} \leq 0.5577$$

$$-0.3010 \leq -5.103 \times 10^{-4} \times M + 0.05616 \times \log K_{ow} \leq 0.1758$$

For (highly lipophilic) contaminants outside the application domain, the predicted K_p value is corrected by a factor FA in the exposure equation ((eq. 201) or
(eq. 202)). FA accounts for the epidermal turnover of the skin: the total absorption of the chemical is reduced by desquamation of the outermost skin layer, the *stratum corneum*. The reducting factor FA

can be derived from Figure 6. S-Risk evaluates the condition of the application domain and gives the parameters to read FA from Figure 6.

Experimental values for Kp are preferred for halogenated compounds. Values for Kp can be found in the literature and on the US-EPA website (http://epa.gov/oswer/riskassessment/ragse/index.htm#background).

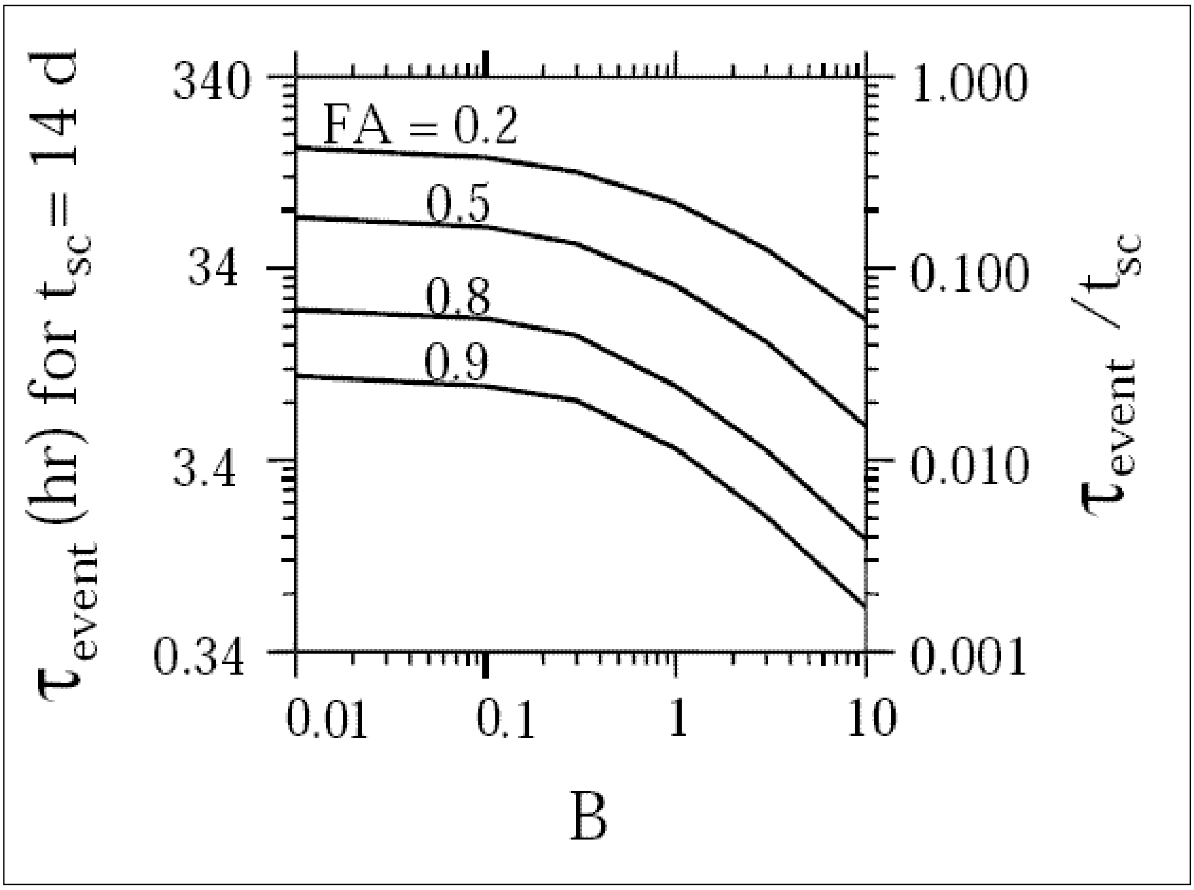

Figure 6:FA as a function of B and τ_{event} (t_{sc} equals the average turnover time of the stratum corneum and has a default value of 14 days)

We first calculate t*, the time needed to reach the equilibrium state.

(eq. 194)

$$t^* = 2.4 * \tau_{event} \quad \text{if } B \leq 0.6$$

(eq. 195)

$$t^* = 6 \times \tau_{event} \times \left(b - \sqrt{b^2 - c^2}\right) \text{ if } B > 0.6$$

(eq. 196)

$$B = K_p \times \frac{\sqrt{M}}{2.6}$$

(eq. 197)

$$b = \frac{2 \times (1 + B)^2}{\pi} - c$$

(eq. 198)

$$c = \frac{1 + 3 \times B + 3 \times B^2}{3 \times (1 + B)}$$

(eq. 199)

$$\tau_{event} = l_{sc} \times \frac{l_{sc}}{6 \times D_{sc}}$$

(eq. 200)

$$\frac{l_{sc}}{D_{sc}} = \frac{1}{10^{(-2.80 - 0.0056 \times MW)}}$$

Where

Abbr.	Name	Units	Source
t*	time to reach steady-state	h	(eq. 194) or (eq. 195)
τ_{event}	lag time per event	h/event	(eq. 199)
b	correlation coefficient	-	(eq. 197)(eq. 198)
c	correlation coefficient	-	(eq. 198)
B	ratio of permeability through stratum corneum versus viable epidermis	-	(eq. 196)
l_{sc}	apparent thickness of the stratum corneum	cm	Table 33
D_{sc}	effective diffusion coefficient for chemical transfer through the stratum corneum	cm²/h	-
M	molecular weight	g/mol	chem. properties
K_p	dermal permeability coefficient	cm/h	(eq. 192) or user input

Then, exposure dose is calculated per event, taking into account event duration. Event duration (t_{event}) equals time under the shower (t_{sh}) or time in the bath ($t_{bathing}$).

If $t_{event} \leq t^*$. Then

(eq. 201)

$$ADE_{dermal\_bathing} = 2 \times FA \times K_p \times C_{dw} \times \sqrt{\frac{6 \times \tau_{event} \times t_{bathing}}{\pi}} \times CF_2$$

(eq. 202)

$$ADE_{dermal\_showering} = 2 \times FA \times K_p \times (1 - k_{wa}) \times C_{dw} \times \sqrt{\frac{6 \times \tau_{event} \times t_{sh}}{\pi}} \times CF_2$$

Where

Abbr.	Name	Unit	Source
$ADE_{dermal\_bathing}$	Absorbed dose via skin contact through bathing	mg/m².event	(eq. 201)
$ADE_{dermal\_showering}$	Absorbed dose via skin contact through showering	mg/m².event	(eq. 202)
FA	Fraction absorbed water	-	1 or from Figure 6
K_p	dermal permeability coefficient	cm/h	(eq. 192) or user input
C_{dw}	concentration in drinking-water	mg/m³	(eq. 26)
τ_{event}	lag time per event	h/event	(eq. 199)
$t_{bathing}$	time in bath	h	Table 33
t_{sh}	duration of shower	h	Table 33
CF_2	unit conversion factor	m/cm	Table 33
k_{wa}	degree of volatilization	-	(eq. 90)

If $t_{event} > t^*$. then

(eq. 203)

$$ADE_{dermal\_bathing} = FA \times K_p \times C_{dw} \times \left[\frac{t_{bathing}}{1+B} + 2 \times \tau_{event} \times \left(\frac{1+3\times B+3\times B^2}{(1+B)^2} \right) \right] \times CF_2$$

(eq. 204)

$$ADE_{dermal\_showering} = FA \times K_p \times (1-k_{wa}) \times C_{dw} \times \left[\frac{t_{sh}}{1+B} + 2 \times \tau_{event} \times \left(\frac{1+3\times B+3\times B^2}{(1+B)^2} \right) \right] \times CF_2$$

Where

Abbr.	Name	Unit	Source
$ADE_{dermal\_bathing}$	Absorbed dose via skin contact through bathing	mg/m².event	(eq. 203)
$ADE_{dermal\_showering}$	Absorbed dose via skin contact through showering	mg/m².event	(eq. 204)
FA	Fraction absorbed water	-	1 or from Figure 6
K_p	dermal permeability coefficient	cm/h	(eq. 192) or user input
C_{dw}	concentration in drinking-water	mg/m³	(eq. 26)
τ_{event}	lag time per event	h/event	(eq. 199)
$t_{bathing}$	time in bath	h	Table 33
t_{sh}	duration of shower	h	Table 33
CF_2	unit conversion factor	m/cm	Table 33
k_{wa}	degree of volatilization	-	(eq. 90)

Abbr.	Name	Unit	Source
B	ratio of permeability through stratum corneum versus viable epidermis	-	(eq. 196)

→ Absorbed dose per event for inorganic contaminants

For uptake of inorganic contaminants, B and τ_{event} are assumed to be 0 as the viable epidermis hardly forms a barrier for these compounds. K_p values can not be calculated and are thus required chemical input data. Values can be found in the literature or on the US-EPA website (http://epa.gov/oswer/riskassessment/ragse/index.htm#background).

(eq. 205)

$$ADE_{dermal\_bathing} = K_p \times C_{dw} \times t_{bathing} \times CF_2$$

(eq. 206)

$$ADE_{dermal\_showering} = K_p \times (1 - k_{wa}) \times C_{dw} \times t_{sh} \times CF_2$$

Where

Abbr.	Name	Unit	Source
$ADE_{dermal\_bathing}$	Absorbed dose via skin contact through bathing	mg/m^2.event	(eq. 205)
$ADE_{dermal\_showering}$	Absorbed dose via skin contact through showering	mg/m^2.event	(eq. 206)
K_p	dermal permeability coefficient	cm/h	user input (chem. prop.)
C_{dw}	concentration in drinking-water	mg/m^3	(eq. 26)
$t_{bathing}$	time in bath	h	Table 33
t_{sh}	time under the shower	h	Table 33
CF_2	unit conversion factor	m/cm	Table 33
k_{wa}	degree of volatilization	-	(eq. 90)

→ Absorbed dose during bathing and showering

(eq. 207)

$$AD^{daily}_{dermal\_bathing} = \frac{ADE_{dermal\_bathing} \times EV_{bathing} \times SA_{total}}{BW}$$

(eq. 208)

$$AD^{daily}_{dermal\_showering} = \frac{ADE_{dermal\_showering} \times EV_{showering} \times SA_{total}}{BW}$$

(eq. 209)

$$AD_{dermal\_bathing}^{yearly} = \frac{AD_{dermal\_bathing}^{daily} \times EF_{bathing}}{365}$$

(eq. 210)

$$AD_{dermal\_showering}^{yearly} = \frac{AD_{dermal\_showering}^{daily} \times EF_{showeirng}}{365}$$

(eq. 211)

$$AD_{dermal\_water}^{yearly} = AD_{dermal\_bathing}^{yearly} + AD_{dermal\_showering}^{yearly}$$

Where

Abbr.	Name	Unit	Source
$AD_{dermal\_bathing}^{daily}$	Daily uptake via dermal contact with water during bathing	mg/kg.d	(eq. 207)
$AD_{dermal\_showering}^{daily}$	daily uptake via dermal contact with water during showering	mg/kg.d	(eq. 208)
$AD_{dermal\_bathing}^{yearly}$	yearly average uptake via dermal contact with water during bathing	mg/kg.d	(eq. 209)
$AD_{dermal\_showering}^{yearly}$	yearly average uptake via dermal contact with water during showering	mg/kg.d	(eq. 210)
$AD_{dermal\_water}^{yearly}$	yearly average uptake via dermal contact with water	mg/kg.d	(eq. 211)
$ADE_{dermal\_bathing}$	uptake via dermal contact with water during a bathing event	mg/m².event	(eq. 201) or (eq. 203) or (eq. 205)
$ADE_{dermal\_showeirng}$	uptake via dermal contact with water during a showering event	mg/m².event	(eq. 202) or (eq. 204) or (eq. 206)
SA_{total}	total body surface area	m²	Table 32
$EV_{bathing}$	number of baths per day	1/d	Table 51
$EV_{showering}$	number of showers per day	1/d	Table 51
$EF_{bathing}$	exposure frequency for bathing	d/y	(eq. 212)
$EF_{showering}$	exposure frequency for showering	d/y	(eq. 212)
BW	body weight	kg	Table 28

(eq. 212)

$$EF_{bathing/showering} = EF_{week;bathing/showering} \times EF_{year}$$

Where

Abbr.	Name	Unit	Source
$EF_{bathing/showering}$	Exposure frequency for bathing or showering	d/y	(eq. 212)
$EF_{week;bathing/showering}$	Frequency on a weekly basis	d/w	Table 51
EF_{year}	Frequency on a yearly basis	w/y	Table 35 or Table 36 or Table 37 or Table 38 or Table 39 or Table 40 or Table 41 or Table 42

Table 32: Total body surface area (m²)

	SA_{total}
1 - < 3 yr	0.560
3 - < 6 yr	0.737
6 - < 10 yr	0.994
10 - < 15 yr	1.394
15 - < 21 yr	1.736
21 - < 31 yr	1.829
31 - < 41 yr	1.849
41 - < 51 yr	1.846
51 - < 61 yr	1.880
60 - … yr	1.853

9.3.3. TOTAL DERMAL DOSE

The total dermal absorbed dose is then given by the sum of the doses from dermal contact with soil, dust and water.

(eq. 213)

$$AD_{dermal}^{daily} = AD_{dermal\_soil/dust}^{daily} + \max\left(AD_{dermal\_bathing}^{daily}; AD_{dermal\_showering}^{daily}\right)$$

(eq. 214)

$$AD_{dermal}^{yearly} = AD_{dermal\_soil/dust}^{yearly} + AD_{dermal\_water}^{yearly}$$

Where

Abbr.	Name	Unit	Source
AD_{dermal}^{daily}	Daily uptake via dermal contact	mg/kg.d	(eq. 213)
$AD_{dermal_{soil}/dust}^{daily}$	Daily uptake via dermal contact with soil and dust	mg/kg.d	(eq. 188)
$AD_{dermal\_bathing}^{daily}$	Daily uptake via dermal contact with water during bathing	mg/kg.d	(eq. 207)
$AD_{dermal\_showering}^{daily}$	daily uptake via dermal contact with water during showering	mg/kg.d	(eq. 208)
AD_{dermal}^{yearly}	Yearly average uptake via dermal contact	mg/kg.d	(eq. 214)
$AD_{dermal_{soil}/dust}^{yearly}$	Yearly average uptake via dermal contact with dust and soil	mg/kg.d	(eq. 191)
$AD_{dermal\_water}^{yearly}$	yearly average uptake via dermal contact with water	mg/kg.d	(eq. 211)

9.4. INHALATION EXPOSURE

The fate and transfer module calculates gas-phase ambient air concentrations for a child and an adult. The child concentrations are used for the ages till 10 years. The adult concentrations are used from the age of 10 years and older. Exposure is calculated from the sum of gas-phase and particle concentrations.

Inhalation risk assessment is based on concentrations, following recommendations in US-EPA (2009b) and Ginsberg et al. (2010). Concentrations are time-averaged and weighted according to an inhalation weighting factor. The default inhalation rate for adults corresponds with the inhalation rate used for derivation of toxicological reference values for inhalation (20 m³/d, 70 kg). Inhalation weighting factors are then calculated from an age-based inhalation ratio times an activity-based inhalation ratio. These factors express the ratio between the body-weight normalized inhalation rate for a certain scenario and age compared to the default adult body-weight normalized inhalation rate. In residential areas, only an age-based inhalation ratio applies. This is in line with the proposal of Ginsberg et al. (2010) who argues that the intraspecies uncertainty factor in the derivation of toxicological reference values does not adequately account for the difference in inhalation and deposition rate between children and adults. The ratio is derived from age-dependent inhalation rates published in Brochu et al. (2011), divided by body weight. Body-weight based inhalation rates in children are higher than in adults. We do not distinguish between indoor and outdoor inhalation rates in residential area (although differences exist due to different activity levels, e.g. sleeping). The age-based inhalation ratios are lower than if the inhalation rates in US-EPA (2009a) would be used.

An additional activity-based weighting factor is applied for scenarios with higher activity patterns, resulting in higher inhalation rates, than in the residential scenario (industry, recreation). For short-term recreational scenarios and adults, short-term inhalation rates are based on US-EPA (2009a), the value for day recreation indoor and outdoor corresponds with 2/3 moderate activity and 1/3 high intensity activity (P95 values). For children in day recreation outdoor, the value corresponds to the P95 of moderate activity. For children in day recreation indoor, the value corresponds with 2/3 moderate activity and 1/3 high intense activity. From this the ratio with the residential inhalation rate is calculated.

(eq. 215)

$$C_{inhalation\_out}^{daily} = \frac{C_{ao} \times WF_{age} \times WF_{act} \times t_{out}}{24}$$

(eq. 216)

$$C_{inhalation\_in}^{daily} = \frac{C_{ia,t} \times (t_{in} + t_{sleep}) \times WF_{age} \times WF_{act}}{24}$$

(eq. 217)

$$C_{inhalation\_shower}^{daily} = \frac{(C_{sh,a} \times t_{sh} + C_{br,a} \times t_{br}) \times EV_{showering} \times WF_{age} \times WF_{act}}{24}$$

(eq. 218)

$$C_{inhalation}^{daily} = C_{inhalation\_out}^{daily} + C_{inhalation\_in}^{daily} + C_{inhalation\_shower}^{daily}$$

Where

Abbr.	Name	Unit	Source
$C_{inhalation\_out}^{daily}$	daily inhalation rate weighted concentration in outdoor air	mg/m³	(eq. 215)
$C_{inhalation\_in}^{daily}$	daily inhalation rate weighted concentration in indoor air	mg/m³	(eq. 216)
$C_{inhalation\_shower}^{daily}$	daily inhalation rate weighted air concentration during showering	mg/m³	(eq. 217)
$C_{inhalation}^{daily}$	total daily inhalation rate weighted air concentration	mg/m³	(eq. 218)
C_{ao}	total concentration in ambient air	mg/m³	(eq. 46)
$C_{ia,t}$	total concentration in indoor air	mg/m³	(eq. 88)
$C_{sh,a}$	concentration in shower stall air	mg/m³	(eq. 89)
$C_{br,a}$	concentration in bathroom air	mg/m³	(eq. 94)
WF_{age}	age-dependent inhalation rate based weighting factor	-	Table 52
WF_{act}	activity-dependent inhalation rate based weighting factor	-	Table 52
$EV_{showering}$	number of showers per day	1/d	Table 51
t_{in}	time indoor	h/d	Table 35 or Table 36 or Table 37 or Table 38 or Table 39 or Table 40 or Table 41 or Table 42
t_{out}	time outdoor	h/d	Table 35 or Table 36 or Table 37 or Table 38 or Table 39 or Table 40 or Table 41 or Table 42
t_{sleep}	time sleeping	h/d	Table 35 or Table 36 or Table 37 or Table 38 or Table 39 or Table 40 or Table 41 or Table 42
t_{sh}	time under the shower	h/shower	Table 33
t_{br}	time in the bathroom after showering	h/shower	Table 33

(eq. 219)

$$C_{inhalation\_out}^{yearly} = \frac{C_{inhalation\_out}^{daily} \times EF}{365}$$

(eq. 220)

$$C_{inhalation\_in}^{yearly} = \frac{C_{inhalation\_in}^{daily} \times EF}{365}$$

(eq. 221)

$$C_{inhalation\_shower}^{yearly} = \frac{C_{inhalation\_shower}^{daily} \times EF_{showering}}{365}$$

(eq. 222)

$$C_{inhalation}^{yearly} = C_{inhalation\_out}^{yearly} + C_{inhalation\_in}^{yearly} + C_{inhalation\_shower}^{yearly}$$

Where

Abbr.	Name	Unit	Source
$C_{inhalation\_out}^{yearly}$	yearly averaged inhalation rate weighted air concentration in outdoor environment	mg/m³	(eq. 219)
$C_{inhalation\_in}^{yearly}$	yearly averaged inhalation rate weighted air concentration in indoor environment	mg/m³	(eq. 220)
$C_{inhalation\_shower}^{yearly}$	yearly averaged inhalation rate weighted air concentration during showeirng	mg/m³	(eq. 221)
$C_{inhalation}^{yearly}$	total yearly averaged inhalation rate weighted air concentration	mg/m³	(eq. 222)
$C_{inhalation\_out}^{daily}$	daily inhalation rate weighted air concentration in outdoor environment	mg/m³	(eq. 215)
$C_{inhalation\_in}^{daily}$	daily inhalation rate weighted air concentration in indoor environment	mg/m³	(eq. 216)
$C_{inhalation\_shower}^{daily}$	daily inhalation rate weighted air concentration during showering	mg/m³	(eq. 217)
$C_{inhalation}^{daily}$	total daily inhalation rate weighted air concentration	mg/m³	(eq. 218)
EF	exposure frequency	d/y	(eq. 164)
$EF_{showering}$	exposure frequency for showering	d/y	(eq. 212)

Table 33: Parameter values for exposure calculations

Abbr.	Name	Unit	value
CF	Conversion factor from mg/d to kg/d	kg/mg	1E-6 (fixed value)
CF_2	conversion factor from cm to m	m/cm	1E-2 (fixed value)
EV_{out}	number of “soil” events	events/d	1 if $t_{out} > 0$, else = 0 (fixed value)
EV_{in}	number of “dust” events	events/d	1 if in $t_{in} > 0$, else =0 (fixed value)
l_{sc}	apparent thickness of the stratum corneum	cm	1E-3 (fixed value)
t_{sh}	time under the shower	h	0.25
t_{br}	time in the bathroom after showering	h	0.25
$t_{bathing}$	time in the bath	h	0.33

Table 34: Chemical properties for exposure calculations

Abbr.	Name	Unit	Value	Range
RBA_{soil}	relative bioavailability of contaminants in soil	-	1 (default)	0 - 1
RBA_{dust}	relative bioavailability of contaminants in settled dust	-	1 (default)	0 – 1
$RBA_{drinking\_Water}$	relative bioavailability of contaminants in drinking-water	-	1 (default)	
ABS_{dermal}	dermal absorption factor for soil and dust	-	user input (chem. prop.) [default of 0.25 for blank chemical]	0 – 1
$K_{p,organic}$	dermal permeability coefficient for organic chemicals in water	cm/h	if not filled in, then calculated, (eq. 192)	
$K_{p,inorganic}$	dermal permeability coefficient for inorganic chemicals in water	cm/h	0 (default)	

9.5. BACKGROUND EXPOSURE W

Bbackground exposure is not taken into account in the Walloon Region. The following sections are kept for information only.

9.5.1. INTRODUCTION

As is explained in the risk characterization chapter (CHAPTER 10), we distinguish between threshold effects and non-threshold effects. In the first case, total exposure is calculated, including exposure resulting from the contaminated site and general population exposure (so-called background exposure) from air, food and drinking-water. In the latter case an excess risk approach in followed. The excess risk is defined as the increased risk due to the contaminated site and thus, background exposure is not accounted for.

Background exposure is only calculated for the yearly averaged exposures, not for the daily averaged exposure.

9.5.2. ORAL BACKGROUND EXPOSURE FROM FOOD AND DRINKING-WATER

Background exposure from food is scenario-dependent as the general population's dietary exposure is corrected for the fraction that is coming from the contaminated site. For example, in the default residential scenario with garden, a fraction of vegetables is from local origin. The general population's dietary intake is reduced by the average intake from vegetables times the local fraction (on a vegetable category basis). Background exposure from drinking-water is corrected if there is local consumption of groundwater. If local consumption applies, the user is thus requested to specify normal background concentrations in the predefined food groups. A background concentration in drinking-water is always requested.

(eq. 223)

$$ED_{food}^{background} = ED_{food}^{population} - \left[\sum\left(C_{veg\_category}^{background} \times Q_{veg\_category} \times f_{veg\_category}^{garden}\right) + \sum\left(C_{animal\_product}^{background} \times Q_{animal\_product} \times f_{animal\_product}^{local}\right)\right]$$

(eq. 224)

$$ED_{drinking\_water}^{background} = \frac{C_{drinking\_water}^{background} \times RBA_{drinking\_water} \times Q_{drinking\_water}}{BW \times 1000} \times \left(1 - \frac{f_g \times EF \times RF_{drinking\_water}}{365}\right)$$

(eq. 225)

$$ED_{oral}^{background} = ED_{food}^{background} + ED_{drinking\_water}^{background}$$

Where

Abbr.	***Name***	***Unit***	***Source***
$ED_{food}^{background}$	*yearly average background intake from food*	*mg/kg.d*	*(eq. 223)*
$ED_{drinking\_water}^{background}$	*yearly average intake from drinking-water*	*mg/kg.d*	*(eq. 224)*
$ED_{food}^{populatior}$	*yearly average intake of the general population from food*	*mg/kg.d*	*user input (chem. prop.)*
$ED_{oral}^{background}$	*yearly average oral background intake*	*mg/kg.d*	*(eq. 225)*
$f_{vegetable\_category}^{garden}$	*fraction of locally grown vegetables by category*	*-*	*Table 45*
$f_{animal\_product}^{local}$	*fraction of animal product from local production*	*-*	*Table 45*
$C^{background}$	*average background concentration in vegetable category, animal product or drinking-water*	*mg/kg fw (vegetable, animal product) mg/m³ (drinking-water)*	*user input (chem. prop.)*
Q_i	*consumption of vegetable category, animal product or drinking-water*	*kg/d (vegetable, animal product) l/d (drinking-water)*	*Table 29, Table 30, Table 31*
$RBA_{drinking\_water}$	*relative bioavailability in drinking-water*	*-*	*user input (chem. prop.)*
f_g	*fraction of groundwater used as drinking-water*	*-*	*Table 45*
EF	*exposure frequency*	*d/y*	*(eq. 164)*
$RF_{drinking\_water}$	*factor for local fraction of drinking-water*	*-*	*Table 45*
BW	*body weight*	*kg*	*Table 28*

In general, dietary intake for the general population is known for adults only or for a limited set of ages. Based on calculations for trace metals, it is possible to convert a dietary intake value for adults to a value for the different child age classes. The intake of adults (expressed in mg/kg.d) can be multiplied with the below given values to have the population intake for children (in mg/kg.d):

Age	*1-<3 yr*	*3 - <6 yr*	*6 - <10 yr*	*10 - <15 yr*	*15 - <21 yr*	*21 - <31 yr*	*31 - <41 yr*
Ratio	*1.72*	*1.85*	*1.56*	*1.21*	*1.06*	*0.99*	*1.00*

9.5.3. INHALATION BACKGROUND EXPOSURE

The model's fate and transfer module predicts concentrations in outdoor and indoor air due to the contamination. Inhalation background exposure results from general environmental levels; this background concentration is considered scenario-independent. The model allows to distinguish between background concentrations in outdoor and indoor air. The average inhalation background exposure is then calculated from these concentrations and the outdoor/indoor time pattern of the residential scenario.

(eq. 226)

$$C_{inhalation}^{background} = \frac{\left(C_{ao}^{background} \times t_{out}^{RES} + C_{ai}^{background} \times t_{in}^{RES}\right) \times \frac{\left(24 - t_{sleep}^{RES}\right)}{\left(t_{out}^{RES} + t_{in}^{RES}\right)} + C_{ai}^{background} \times t_{sleep}^{RES}}{24} \times WF_{inh}^{RES}$$

(eq. 227)

$$WF_{inh}^{RES} = WF_{age} \times WF_{act}$$

Where

Abbr.	***Name***	***Unit***	***Source***
$C_{inhalation}^{background}$	*yearly average inhalation rate weighted background air concentration*	*mg/m³*	*(eq. 226)*

Abbr.	*Name*	*Unit*	*Source*
$C_{ao}^{background}$	*background concentration in outdoor air*	*mg/m³*	*user input (chem. Prop.)*
$C_{ai}^{background}$	*background concentration in indoor air*	*mg/m³*	*user input (chem. Prop.)*
t_{out}^{RES}	*time spent outdoor in scenario RES*	*h/d*	*Table 36*
t_{in}^{RES}	*time spent indoor in scenario RES*	*h/d*	*Table 36*
t_{sleep}^{RES}	*time sleeping in scenario RES*	*h/d*	*Table 36*
WF_{inh}^{RES}	*inhalation rate based weighting factor in scenario RES*	-	*(eq. 227)*
WF_{age}	*age-dependent inhalation rate based weighting factor*	-	*Table 52 (scenario RES)*
WF_{act}	*activity-dependent inhalation rate based weighting factor*	-	*Table 52 (scenario RES)*

9.6. DESCRIPTION OF SCENARIOS

Scenarios are characterized by their exposure pathways (Table 27), which are further differentiated on the basis of the exposure parameters. Values for the scenario dependent exposure parameters are provided in this chapter.

9.6.1. TIME PATTERNS

Time-use patterns for the residential scenarios are based on a combination of average and high-end estimates. Time patterns for the garden are taken from participants of time-enquiries (i.e. persons reported to have been doing that activity), whereas overall time-use are the average values for non-working individuals. Total time at the location is less than 24 h/d. For children aged 3 years and more, time spent at school was taken into account. For 3 - < 6 years, it was assumed that the children only go to school for half a day.

Time-use for light industry covers mainly indoor industrial and commercial activities. Time-use for heavy industry assumes that majority of the time is spent outside.

For recreation, the data represent average values for people participating in recreation. We consider outside recreation and indoor sporting and time spent in a holiday resort (with major time spent inside because of indoor air exposure considerations, as soil and dust intake is independent from time in continuous recreational exposure).

More detailed information can be found in Cornelis et al. (2008) and in Cornelis (2012). The latter document explains some modifications to the time spent on-site for residential and recreational scenarios.

Table 35: Time-use for landuse type agricultural residential area with vegetable garden (AGR)

Age	Sleeping (t_{sleep})	Awake Inside (t_{in})	Outside (t_{out})	Total* on site	EF_{week}	EF_{year}
	h/day	h/day	h/day	h/day	d/week	weeks/year
1 - < 3 year	12	11.5	0.5	24	7	52
3 - < 6 year	11	9.7	1.38	22.08	7	52
6 - < 10 year	10	8.7	1.57	20.27	7	52
10 - < 15 year	9	10.6	1.12	20.72	7	52
15 - < 21 year	8	8.5	0.8	17.3	7	52
21 - < 31 year	8	9.0	1.0	18	7	52
31 - < 41 year	8	11.5	1.3	20.8	7	52
41 - < 51 year	8	11.5	1.5	21	7	52
51 - < 61 year	8	11.5	1.8	21.3	7	52
≥ 61 years	8	11.5	1.7	21.2	7	52

* sum of hours ‘sleeping’. ‘awake’ and ‘outside’

Table 36: Time-use for landuse type residential with vegetable garden (RES-veg)

Age	**Sleeping (t_{sleep})**	**Awake Inside (t_{in})**	**Outside (t_{out})**	**Total* on site**	**EF_{week}**	**EF_{year}**
	h/day	h/day	h/day	h/day	d/week	weeks/year
1 - < 3 year	12	11.5	0.5	24	7	52
3 - < 6 year	11	9.7	1.38	22.08	7	52
6 - < 10 year	10	8.7	1.57	20.27	7	52
10 - < 15 year	9	10.6	1.12	20.72	7	52
15 - < 21 year	8	8.5	0.8	17.3	7	52
21 - < 31 year	8	9.0	1.0	18	7	52
31 - < 41 year	8	11.5	1.3	20.8	7	52
41 - < 51 year	8	11.5	1.5	21	7	52
51 - < 61 year	8	11.5	1.8	21.3	7	52
≥ 61 years	8	11.5	1.7	21.2	7	52

* sum of hours 'sleeping'. 'awake' and 'outside'

Table 37: Time-use for landuse type residential with garden (RES)

Age	**Sleeping (t_{sleep})**	**Awake inside (t_{in})**	**Outside (t_{out})**	**Total* on site**	**EF_{week}**	**EF_{year}**
	h/day	h/day	h/day	h/day	d/week	weeks/year
1 - < 3 year	12	11.5	0.5	24	7	52
3 - < 6 year	11	9.7	1.38	22.08	7	52
6 - < 10 year	10	8.7	1.57	20.27	7	52
10 - < 15 year	9	10.6	1.12	20.72	7	52
15 - < 21 year	8	8.5	0.4	16.9	7	52
21 - < 31 year	8	9.0	0.4	17.4	7	52
31 - < 41 year	8	11.5	0.7	20.2	7	52
41 - < 51 year	8	11.5	1.0	20.5	7	52
51 - < 61 year	8	11.5	1.3	20.8	7	52
≥ 61 years	8	11.5	1.0	20.5	7	52

* sum of hours 'sleeping'. 'awake' and 'outside'

Table 38: Time-use for landuse type residential without garden (RES-ng)

Age	**Sleeping (t_{sleep})**	**Awake inside (t_{in})**	**Outside (t_{out})**	**Total* on site**	**EF_{week}**	**EF_{year}**
	h/day	h/day	h/day	h/day	d/week	weeks/year
1 - < 3 year	12	11.5	0.5	24	7	52
3 - < 6 year	11	9.7	1.38	22.08	7	52
6 - < 10 year	10	8.7	1.57	20.27	7	52
10 - < 15 year	9	10.6	1.12	20.72	7	52
15 - < 21 year	8	8.5	0.3	16.8	7	52
21 - < 31 year	8	9.0	0.3	17.3	7	52
31 - < 41 year	8	11.5	0.4	19.9	7	52
41 - < 51 year	8	11.5	1.0	20.5	7	52
51 - < 61 year	8	11.5	1.0	20.5	7	52
≥ 61 years	8	11.5	1.0	20.5	7	52

* sum of hours 'sleeping'. 'awake' and 'outside'

Table 39: Time-use for landuse type day recreation for children and adults in indoor sport scenario (REC-dayin)

Age	Sleeping (t_{sleep})	Awake inside (t_{in})	Outside (t_{out})	Total* on site	EF_{week}	EF_{year}
	h/day	h/day	h/day	h/day	d/week	weeks/year
1 - < 3 year	0	2.1	0	2.1	2	44
3 - < 6 year	0	2.1	0	2.1	2	44
6 - < 10 year	0	1.9	0	1.9	3	44
10 - < 15 year	0	1.9	0	1.9	3	44
15 - < 21 year	0	1.9	0	1.9	3	44
21 - < 31 year	0	2.1	0	2.1	2	44
31 - < 41 year	0	2.1	0	2.1	2	44
41 - < 51 year	0	2.5	0	2.5	2	44
51 - < 61 year	0	2.5	0	2.5	2	44
≥ 61 years	0	3.1	0	3.1	2	44

* sum of hours ‘sleeping’. ‘awake’ and ‘outside’

Table 40: Time-use for landuse type day recreation for children and adults (REC-dayout)

Age	Sleeping (t_{sleep})	Awake Inside (t_{in})	Outside (t_{out})	Total* on site	EF_{week}	EF_{year}
	h/day	h/day	h/day	h/day	d/week	weeks/year
1 - < 3 year	0	0	8	8	5	8
3 - < 6 year	0	0	8	8	5	8
6 - < 10 year	0	0	8	8	5	8
10 - < 15 year	0	0	8	8	5	8
15 - < 21 year	0	0	8	8	5	8
21 - < 31 year	0	0	2.1	2.1	2	44
31 - < 41 year	0	0	2.1	2.1	2	44
41 - < 51 year	0	0	2.5	2.5	2	44
51 - < 61 year	0	0	3.1	3.1	2	44
≥ 61 years	0	0	3.1	3.1	2	44

* sum of hours ‘sleeping’. ‘awake’ and ‘outside’

Table 41: Time-use for landuse type light industry (IND-l)

Age	Sleeping (t_{sleep})	Awake inside (t_{in})	Outside (t_{out})	Total* on site	EF_{week}	EF_{year}
	h/day	h/day	h/day	h/day	d/week	weeks/year
1 - < 3 year	0	0	0	0	5	47
3 - < 6 year	0	0	0	0	5	47
6 - < 10 year	0	0	0	0	5	47
10 - < 15 year	0	0	0	0	5	47
15 - < 21 year	0	7	1	8	5	47
21 - < 31 year	0	7	1	8	5	47
31 - < 41 year	0	7	1	8	5	47
41 - < 51 year	0	7	1	8	5	47
51 - < 61 year	0	7	1	8	5	47
≥ 61 years	0	7	1	8	5	47

* sum of hours ‘sleeping’. ‘awake’ and ‘outside’

Table 42: Time-use for landuse type heavy industry with outside activity (IND-h)

Age	Sleeping (t_{sleep})	Awake inside (t_{in})	Outside (t_{out})	Total* on site	EF_{week}	EF_{year}
	h/day	h/day	h/day	h/day	d/week	weeks/year
1 - < 3 year	0	0	0	0	5	47
3 - < 6 year	0	0	0	0	5	47
6 - < 10 year	0	0	0	0	5	47
10 - < 15 year	0	0	0	0	5	47
15 - < 21 year	0	1	7	8	5	47
21 - < 31 year	0	1	7	8	5	47
31 - < 41 year	0	1	7	8	5	47
41 - < 51 year	0	1	7	8	5	47
51 - < 61 year	0	1	7	8	5	47
≥ 61 years	0	1	7	8	5	47

* sum of hours ‘sleeping’. ‘awake’ and ‘outside’

9.6.2. SOIL AND DUST INGESTION

Table 43: Daily soil and dust ingestion rates and fraction of soil contributing to soil and dust ingestion

Age	AGR / RES-veg / RES		RES-ng		IND-l		IND-h	
	$IR_{soil/dust\_daily}$ (mg/d)	F_{oral_soil} (-)	$IR_{soil/dust\_daily}$ (mg/d)	F_{oral_soil} (-)	$IR_{soil/dust\_daily}$ (mg/d)	F_{oral_soil} (-)	$IR_{soil/dust\_daily}$ (mg/d)	F_{oral_soil} (-)
1 - < 3 year	152	0.45	125	0.32	0.0	0.0	0.0	0.0
3 - < 6 year	122	0.45	100	0.32	0.0	0.0	0.0	0.0
6 - < 10 year	93	0.45	73	0.25	0.0	0.0	0.0	0.0
10 - < 15 year	89	0.45	68	0.23	0.0	0.0	0.0	0.0
15 - < 21 year	85	0.45	63	0.20	26	0.20	38.5	0.8
21 - < 31 year	77	0.45	53	0.20	26	0.20	38.5	0.8
31 - < 41 year	77	0.45	53	0.20	26	0.20	38.5	0.8
41 - < 51 year	77	0.45	53	0.20	26	0.20	38.5	0.8
51 - < 61 year	77	0.45	53	0.20	26	0.20	38.5	0.8
≥ 61 years	77	0.45	53	0.20	26	0.20	38.5	0.8

Table 44: Hourly soil and dust ingestion values for recreation

Age	REC-dayin / REC-dayout	
	IR_{soil_hourly} (mg/h)	IR_{dust_hourly} (mg/h)
1 - < 3 year	26	4
3 - < 6 year	20	3
6 - < 10 year	13	2
10 - < 15 year	11	2
15 - < 21 year	9	2
21 - < 31 year	5	1.8
31 - < 41 year	5	1.8
41 - < 51 year	5	1.8
51 - < 61 year	5	1.8
≥ 61 years	5	1.8

9.6.3. FRACTIONS OF LOCAL FOOD AND DRINKING-WATER

Table 45: Fraction of intake from food and drinking-water coming from local sources

food category	AGR	RES-veg	RES	RES-ng	REC-dayout	REC-dayin	IND-l	IND-h
Potatoes	0.5	0.39	0	0	0	0	0	0
Root and tuberous plants	1	0.36	0	0	0	0	0	0
Bulbous plants	1	0.52	0	0	0	0	0	0
Fruit vegetables	1	0.39	0	0	0	0	0	0
Cabbage	1	0.21	0	0	0	0	0	0
Leafy vegetables	1	0.36	0	0	0	0	0	0
Leguminous plant	1	0.42	0	0	0	0	0	0
Stem plants	1	0.10	0	0	0	0	0	0
beef	1	0	0	0	0	0	0	0
organ meat	1	0	0	0	0	0	0	0
milk	1	0	0	0	0	0	0	0
butter	1	0	0	0	0	0	0	0
eggs	1	0.6	0.1	0	0	0	0	0
groundwater	0	0	0	0	0	0	0	0
$RF_{drinking\_water}$	1	1	1	1	0	0	0.5	0.5

9.6.4. OTHER SCENARIO DEPENDENT PROPERTIES

Table 46: Other scenario dependent properties

Scenario	$F_{soil/settled\text{-}dust}$ (fraction soil in indoor settled dust)	Z_{0r} (roughness length, m)
AGR	0.5	0.1
RES-veg	0.5	0.6
RES	0.5	0.6
RES-ng	0.25	1.1
REC-dayout	0.25	0.1

Scenario	$F_{soil/settled-dust}$ (fraction soil in indoor settled dust)	Z_{0r} (roughness length, m)
REC-dayin	0.25	0.1
IND-l	0.25	0.6
IND-h	0.25	0.6

9.6.5. DERMAL EXPOSURE FACTORS AND TIME PATTERNS FOR SHOWERING AND BATHING

Table 47: Soil adherence (AF_{soil_skin}) values in mg/m²

Age	AGR RES-vg	RES	RES-ng	REC-dayout	REC-dayin	IND-l	IND-h
1 - < 3 year	2000	2000	600	4000	4000	0	0
3 - < 6 year	2000	2000	600	4000	4000	0	0
6 - < 10 year	2000	2000	600	4000	4000	0	0
10 - < 15 year	2000	2000	600	4000	4000	0	0
15 - < 21 year	1000	700	100	1000	1000	100	100
21 - < 31 year	1000	700	100	1000	1000	100	100
31 - < 41 year	1000	700	100	1000	1000	100	100
41 - < 51 year	1000	700	100	1000	1000	100	100
51 - < 61 year	1000	700	100	1000	1000	100	100
≥ 61 years	1000	700	100	1000	1000	100	100

Table 48: Dust adherence (AF_{dust_skin}) values in mg/m²

Age	AGR RES-vg	RES	RES-ng	REC-dayout	REC-dayin	IND-l	IND-h
1 - < 3 year	100	100	100	100	100	0	0
3 - < 6 year	100	100	100	100	100	0	0
6 - < 10 year	100	100	100	100	100	0	0
10 - < 15 year	100	100	100	100	100	0	0
15 - < 21 year	100	100	100	100	100	100	100
21 - < 31 year	100	100	100	100	100	100	100
31 - < 41 year	100	100	100	100	100	100	100
41 - < 51 year	100	100	100	100	100	100	100
51 - < 61 year	100	100	100	100	100	100	100
≥ 61 years	100	100	100	100	100	100	100

Table 49: Skin surface areas for soil contact (m²)

Age	AGR RES-vg	RES	RES-ng	REC-dayout	REC-dayin	IND-l	IND-h
1 - < 3 year	0.143	0.143	0.143	0.180	0.180	0.060	0.060
3 - < 6 year	0.211	0.211	0.211	0.266	0.266	0.080	0.080
6 - < 10 year	0.281	0.281	0.281	0.360	0.360	0.100	0.100
10 - < 15 year	0.425	0.425	0.425	0.544	0.544	0.133	0.133
15 - < 21 year	0.511	0.511	0.511	0.642	0.642	0.147	0.147
21 - < 31 year	0.566	0.566	0.566	0.703	0.703	0.152	0.152
31 - < 41 year	0.566	0.566	0.566	0.703	0.703	0.152	0.152
41 - < 51 year	0.566	0.566	0.566	0.703	0.703	0.152	0.152
51 - < 61 year	0.566	0.566	0.566	0.703	0.703	0.152	0.152
≥ 61 years	0.566	0.566	0.566	0.703	0.703	0.152	0.152

Table 50: Skin surface areas for dust contact (m²)

Age	AGR RES-vg	RES	RES-ng	REC-dayout	REC-dayin	IND-l	IND-h
1 - < 3 year	0.143	0.143	0.143	0.180	0.180	0.060	0.060
3 - < 6 year	0.211	0.211	0.211	0.266	0.266	0.080	0.080
6 - < 10 year	0.281	0.281	0.281	0.360	0.360	0.100	0.100
10 - < 15 year	0.425	0.425	0.425	0.544	0.544	0.133	0.133
15 - < 21 year	0.511	0.511	0.511	0.642	0.642	0.147	0.147
21 - < 31 year	0.566	0.566	0.566	0.703	0.703	0.152	0.152
31 - < 41 year	0.566	0.566	0.566	0.703	0.703	0.152	0.152
41 - < 51 year	0.566	0.566	0.566	0.703	0.703	0.152	0.152
51 - < 61 year	0.566	0.566	0.566	0.703	0.703	0.152	0.152
≥ 61 years	0.566	0.566	0.566	0.703	0.703	0.152	0.152

Table 51: Showering and bathing frequency by land use

Age	AGR / RES-veg / RES / RES-ng				REC-dayout				REC-dayin				IND-l / IND-h			
	showering		bathing		showering		bathing		showering		bathing		showering		bathing	
	d/week	EV (1/d)	d/week	EV (1/d)	d/week	EV (1/d)	d/week	EV (1/d)	d/week	EV (1/d)	d/week	EV (1/d)	d/week	EV (1/d)	d/week	EV (1/d)
1 - < 3 year	0	0	5	1	0	0	0	0	0	0	0	0	0	0	0	0
3 - < 6 year	0	0	3	1	0	0	0	0	0	0	0	0	0	0	0	0
6 - < 10 year	3	1	1	1	1	0	0	0	3	0	0	0	0	0	0	0
10 - < 15 year	3	1	1	1	1	0	0	0	3	0	0	0	0	0	0	0
15 - < 21 year	3	1	1	1	1	0	0	0	3	0	0	0	5	0	0	0
21 - < 31 year	3	1	1	1	1	0	0	0	2	0	0	0	5	0	0	0
31 - < 41 year	3	1	1	1	1	0	0	0	2	0	0	0	5	0	0	0
41 - < 51 year	3	1	1	1	1	0	0	0	2	0	0	0	5	0	0	0
51 - < 61 year	3	1	1	1	1	0	0	0	2	0	0	0	5	0	0	0
≥ 61 years	3	1	1	1	1	0	0	0	2	0	0	0	5	0	0	0

9.6.6. INHALATION WEIGHTING FACTORS

Table 52: Weighting factors for differences in inhalation rate due to age (WF_{age}) and activity (WF_{act})

Age	WF_{age}	$WF_{activity}$			
		AGR/RES-vg/RES/RES-ng/ /shower	REC-dayout*	REC dayin**	IND-l / IND-h
1 - < 3 yr	1.9	1	2.7	3.6	1.5
3 – < 6 yr	1.8	1	2.7	3.6	1.5
6 – < 10 yr	1.6	1	2.7	3.6	1.5
10 - < 15 yr	1.3	1	2.7	3.6	1.5
15 - < 21 yr	1.2	1	2.7	3.6	1.5
adults	1	1	3.6	3.6	1.5

*: assuming playing activities during summer holidays during the day until 21 years of age and sporting for adults;

**: assuming sporting for all ages

CHAPTER 10 RISK CHARACTERIZATION

10.1. INTRODUCTION

Risk characterization is only implemented for the yearly average exposure. Daily average doses are reported, but are not compared with toxicological reference values.

The health effects of chemical substances are generally subdivided into two classes: threshold and non-threshold effects. Genotoxic mutagens are generally considered as non-threshold chemicals. In case of threshold effects, the toxicological reference value is expressed as a TDI (Tolerable Daily Intake) or RfD (Reference Dose). In case of non-threshold effects, the toxicological reference value is expressed as a slope factor (SF), which expresses the excess cancer risk per unit of dose.
In the Flanders version of S-Risk a pseudo-threshold is used for non-threshold chemicals in some cases. In that case, we use the term pseudo-TDI. **This is not used in the Walloon version** ***W***.
Risk characterization for inhalation is based on time and inhalation rate weighted concentrations. The reference values for the inhalation routes are expressed as a TCA (Tolerable Concentration in Air) for threshold effects and as a UR (unit risk) for non-threshold effects.

Effects can be local, where the health effect is seen at the place of contact (e.g. skin, lungs) or systemic, where the health effect is seen at a place in the body distinct from the place of entry (e.g. liver, kidney, …). If the toxicological reference value for an exposure route is based on a local effect, the risk is not summed over exposure routes. If the toxicological reference value is based on systemic effects, then a consistent set of toxicological reference values is required for each route and the risk is summed over routes. Substances can show both threshold and non-threshold effects and a combination of local and systemic effects.
Depending upon the mode of action, susceptibility to the effect of a substance can be different depending on the age window. For example, children are more sensitive to lead exposure than adults due to their developing brain. As well, averaging time can depend from substance to substance.

To account for this, a default and flexible approach for risk characterization is provided in the model. This is illustrated in Figure 7.

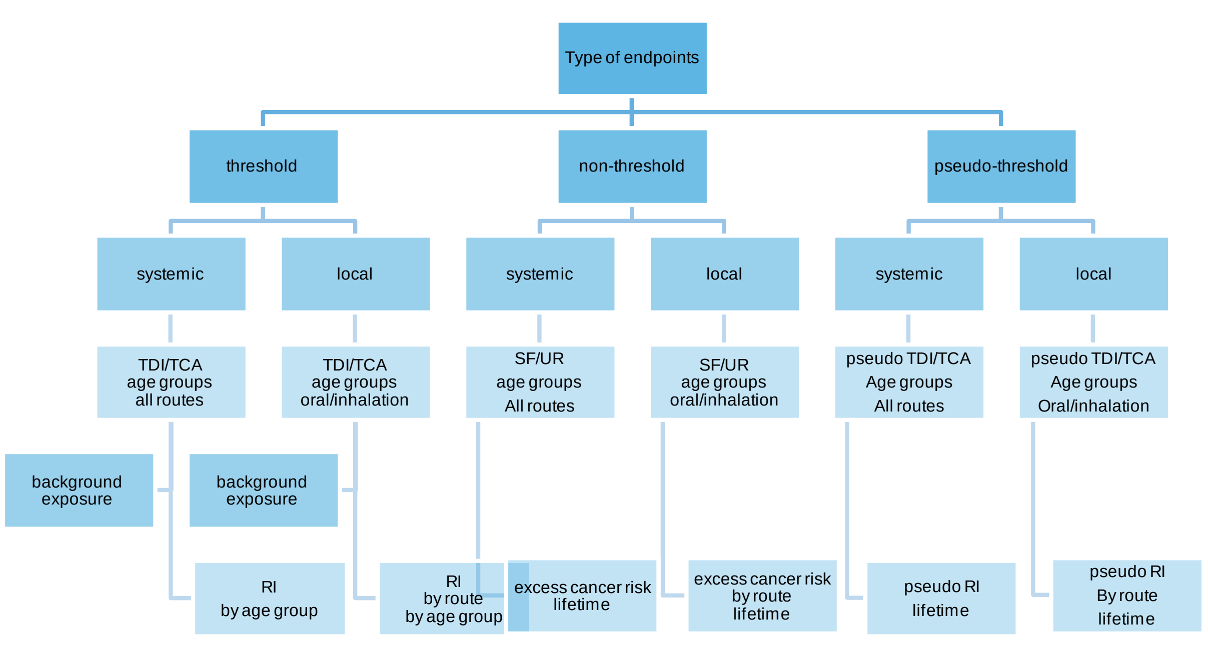

Figure 7: Flow scheme for risk characterization

The user should first indicate whether the chemical shows effects with a threshold and/or without a threshold.

For each of the activated categories, the user should then assign the toxicological reference values to systemic or local effects. In Wallonia, if a pollutant is not listed in S-Risk WAL, the expert has to introduce the toxicological reference values contained in the non-normalised pollutants database. That database is available on http://dps.environnement.wallonie.be/. ***W***
If local effects apply, a value can be filled in for the oral and the inhalation route. Although local effects can occur via the dermal route, this is not included in the risk characterization. For local effects, the unit of exposure should be dose/area of skin. The exposure calculation for dermal contact with soil/dust is suited to provide this information, however the exposure calculation for dermal contact with water directly calculates the absorbed dose from a concentration in water and does not provide the amount of chemical on the skin. Therefore we did not include risk characterization for local skin effects.
If systemic effects apply, it is possible that the user has one toxicological reference value for a certain route or has reference values for each route. If there is only one reference value, then extrapolation to the other routes should be done according to general accepted rules based on route-specific absorption values. For systemic effects, a value needs to be filled in for the oral, the inhalation and the dermal route. The toxicological reference value for the dermal route refers to an absorbed dose.

With regard to risk calculations and required toxicological reference values, we recommend to fill in the data according to the default option (Figure 8), the default option is the approach used in the Vlier-Humaan model. In the default option, which should be used in the absence of data that indicate the need for a different approach, two age groups are distinguished for threshold effects: 1 - < 6 yr and 15 yr and older. The TDI or TCA value for these groups can be the same or different and the risk value is given for both groups. A time period of 6 years is close to the minimal time period for chronic exposure as defined by US-EPA (10 % of a lifespan) and thus the age group for children < 6 years is assessed separately in the default option. In case of non-threshold effects, the default option is one slope factor / unit risk and the risk is expressed as a lifetime average. If a more specific approach is needed, the user can specify toxicological reference values by age groups. For threshold effects, age groups can overlap. For non-threshold effects, age groups should be consecutive and as a total cover the whole lifetime.

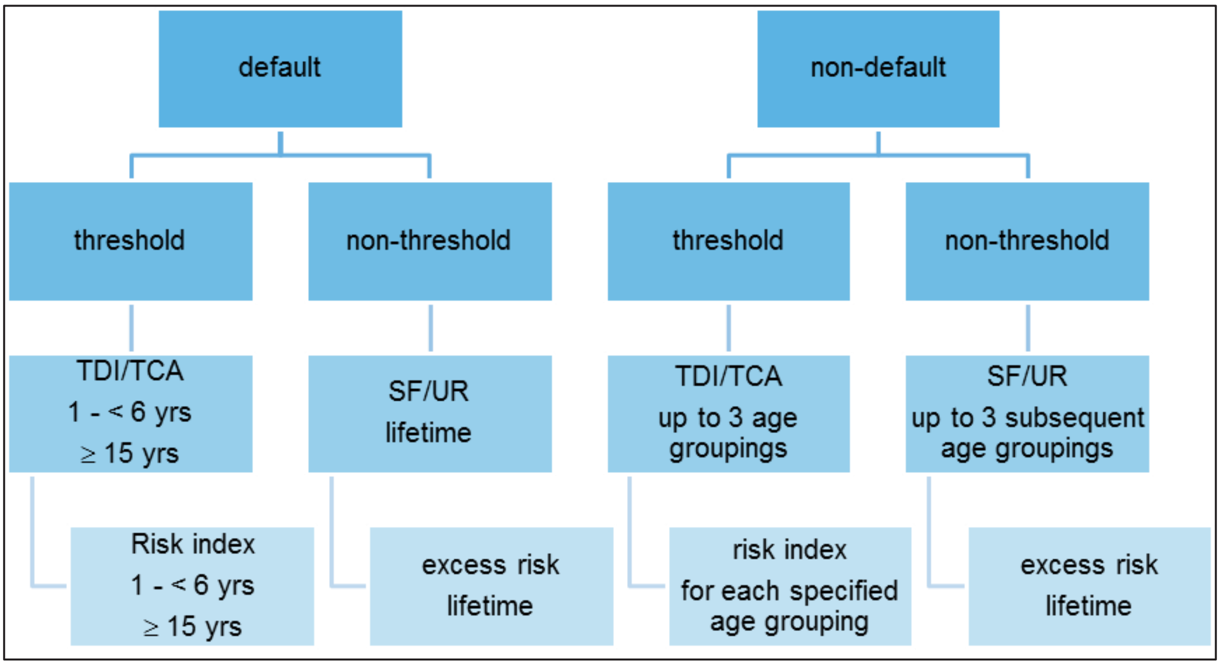

Figure 8: Specification of TDI / TCA values and slope factors by age

In the case of threshold effects, the age groups for which the TDI / TCA is specified are also the age groups for which the risk index is calculated. Under the default option, the risk index for children and adults is reported. In the case of non-threshold effects, the reported excess risk is always a lifetime risk, even if slope factors / unit risks differ by age.

To allow comparison with legal concentration limits, concentration reference values can be filled in for air (outdoor) and drinking-water (W).

The toxicological dataset is given in Table 53.

Table 53: Toxicological properties

Abbr.	Name	Unit
TDI_{oral_syst}	oral Tolerable Daily Intake for systemic effects	mg/kg.d
TCA_{inhal_syst}	Tolerable Concentration in air for systemic effects	mg/m^3
TDU_{dermal_syst}	dermal Tolerable Daily Uptake for systemic effects	mg/kg.d
TDI_{oral_local}	oral Tolerable Daily Intake for local effects	mg/kg.d
TCA_{inhal_local}	Tolerable Concentration in air for local effects	mg/m^3
TDU_{dermal_local}	dermal Tolerable Daily Uptake for local effects	mg/kg.d
SF_{oral_syst}	oral Slope Factor for systemic effects	$(mg/kg.d)^{-1}$
UR_{inhal_syst}	inhalation Unit Risk for systemic effects	$(mg/m^3)^{-1}$
SF_{dermal_syst}	dermal Slope Factor for systemic effects (absorbed dose)	$(mg/kg.d)^{-1}$
SF_{oral_local}	oral Slope Factor for local effects	$(mg/kg.d)^{-1}$

Abbr.	Name	Unit
UR_{inhal_local}	inhalation Unit Risk for local effects	$(mg/m^3)^{-1}$
SF_{dermal_local}	dermal Slope Factor for local effects (absorbed dose)	$(mg/kg.d)^{-1}$
TC_{air}	Tolerable Concentration in outdoor air	mg/m^3
TC_{dw}	Tolerable Concentration in drinking-water	mg/m^3

Inhalation risks for systemic and local effects both use the age and activity weighted air concentrations. This may be too conservative in case of local effects from reactive gases, where current information does not point to significant differences between child and adult dosimetry (Ginsberg, et al., 2010). In case of sufficient information for local effects from reactive gases, the age-dependent part of the inhalation weighting factor could be eliminated, but the activity dependent part should be maintained. However, reactive gases are generally not encountered at contaminated sites.

10.2. DEFAULT APPROACH

An age-averaged dose is calculated for each exposure route (oral, inhalation, dermal). For threshold effects, two doses are calculated (children 1 - < 6 yr, adults older than 15 yr). For non-threshold effects (slope factor or pseudo-threshold), a lifelong dose is calculated. We describe the default approach here, but this approach is not programmed explicitly. It results automatically from the input data (age categories). It is a special case of the general approach outlined further on.

10.2.1. THRESHOLD EFFECTS

In case of threshold effects, in Flanders, the risk characterization is based on the sum of exposure coming from the contaminated site and from background exposure. In Wallonia, the risk characterization is only based on the exposure coming from the contaminated site (**W**). The dose from the contaminated site is given for evaluation purposes in view of contaminated site management.

(eq. 228)

$$D^{child}_{site,oral/dermal} = \frac{\sum_{i=1-2} D^{yearly,i}_{oral/dermal} \times Yr_i}{\sum_{i=1-2} Yr_i}$$

(eq. 229)

$$C^{child}_{site,inhalation} = \frac{\sum_{i=1-2} C^{yearly,i}_{inhalation} \times Yr_i}{\sum_{i=1-2} Yr_i}$$

(eq. 230)

$$D^{adult}_{site,oral/dermal} = \frac{\sum_{i=5-10} D^{yearly,i}_{oral/dermal} \times Yr_i}{\sum_{i=5-10} Yr_i}$$

(eq. 231)

$$C^{adult}_{site,inhalation} = \frac{\sum_{i=5-10} C^{yearly,i}_{inhalation} \times Yr_i}{\sum_{i=5-10} Yr_i}$$

(eq. 232)

$$RI_{oral/dermal}^{child} = \frac{D_{site,oral/dermal}^{child}}{TDI/U_{oral/dermal}^{child}}$$

(eq. 233)

$$RI_{inhalation}^{child} = \frac{C_{site,inhalation}^{child}}{TCA^{child}}$$

(eq. 234)

$$RI_{oral/dermal}^{adult} = \frac{D_{site,oral/dermal}^{adult}}{TDI/U_{oral/dermal}^{adult}}$$

(eq. 235)

$$RI_{inhalation}^{adult} = \frac{C_{site,inhalation}^{adult}}{TCA^{adult}}$$

For local effects, only the risk indices by route are reported and the route and age with the highest RI value is critical. For systemic effects, an overall RI (summed over routes) is calculated and the age with highest RI value is critical.

(eq. 236)

$$RI^{child} = \sum RI_{route}^{child}$$

(eq. 237)

$$RI^{adult} = \sum RI_{route}^{adult}$$

Where

Abbr.	Name	Unit	Source
$D_{site,oral/dermal}^{child}$	average yearly intake/uptake from the location for a child by the oral or dermal route	mg/kg.d	(eq. 228)
$D_{site,oral/dermal}^{adult}$	average yearly intake/uptake from the location for an adult by the oral or dermal route	mg/kg.d	(eq. 230)
$D_{oral/dermal}^{yearly,i}$	average yearly intake/uptake from the location by the oral or dermal route and age category i	mg/kg.d	ED or AD from CHAPTER 9

Abbr.	Name	Unit	Source
$C_{site,inhalation}^{child}$	average yearly air exposure concentration from the location for a child	mg/m³	(eq. 229)
$C_{site,inhalation}^{adult}$	average yearly air exposure concentration from the location for an adult	mg/m³	(eq. 231)
$C_{inhalation}^{yearly,i}$	average yearly air exposure concentration from the location for age category i	mg/m³	(eq. 222)
Yr_i	number of years in age category i	-	Table 55
$RI_{oral/dermal}^{child}$	risk index for a child by the oral or dermal route	-	(eq. 232)
$RI_{oral/dermal}^{adult}$	risk index for an adult by the oral or dermal route	-	(eq. 234)
$RI_{inhalation}^{child}$	risk index for a child by inhalation	-	(eq. 233)
$RI_{inhalation}^{adult}$	risk index for an adult by inhalation	-	(eq. 235)
RI^{child}	risk index for a child for systemic effects	-	(eq. 236)
RI^{adult}	risk index for an adult for systemic effects	-	(eq. 237)
$TDI/U_{oral/dermal}^{child}$	Tolerable Daily Intake/Uptake for a child by the oral or dermal route	mg/kg.d	Table 53
$TDI/U_{oral/dermal}^{adult}$	Tolerable Daily Intake/Uptake for an adult by the oral or dermal route	mg/kg.d	Table 53
TCA^{child}	Tolerable Concentration in air for a child	mg/m³	Table 53
TCA^{adult}	Tolerable Concentration in air for an adult	mg/m³	Table 53

10.2.2. NON-THRESHOLD EFFECTS

In case of non-threshold effects, an excess risk is considered and only the dose resulting from the contaminated site is accounted for in the risk characterization.

(eq. 238)

$$D_{site,oral/dermal} = \frac{\sum_{i=1-10} D_{oral/dermal}^{yearly,i} \times Yr_i}{\sum_{i=1-10} Yr_i}$$

(eq. 239)

$$C_{site,inhalaton} = \frac{\sum_{i=1-10} C_{inhalaton}^{yearly,i} \times Yr_i}{\sum_{i=1-10} Yr_i}$$

(eq. 240)

$$EXCR_{oral/dermal} = D_{site,oral/dermal} \times SF_{oral/dermal}$$

(eq. 241)

$$ExCR_{inhalation} = C_{site,inhalation} \times UR$$

For local effects, only the excess cancer risks by route are reported and the route with the highest ExCR value is critical. For systemic effects, an overall ExCR (summed over routes) is calculated.

(eq. 242)

$$ExCR = \sum ExCR_{route}$$

Where

Abbr.	Name	Unit	Source
$D_{site,oral/dermal}$	yearly average lifelong intake/uptake from the location by the oral or dermal route	mg/kg.d	(eq. 238)
$D_{oral/dermal}^{yearly,i}$	yearly average intake/uptake from the location by the oral or dermal route and age category i	mg/kg.d	ED or AD from CHAPTER 9
$C_{site,inhalation}$	yearly average exposure air concentration from the location	mg/m³	(eq. 239)
$C_{inhalation}^{yearly,i}$	yearly average exposure air concentration from the location for age category i	mg/m³	(eq. 222)
Yr_i	number of years in age category i	-	Table 55
$ExCR_{oral/dermal}$	excess lifelong cancer risk by the oral or dermal route	-	(eq. 240)
$ExCR_{inhalation}$	excess lifelong cancer risk by inhalation	-	(eq. 241)
ExCR	overall excess lifelong cancer risk for systemic effects	-	(eq. 242)
$SF_{oral/dermal}$	slope factor for non-threshold effects by the oral or dermal route	$(mg/kg.d)^{-1}$	Table 53
UR	unit risk for inhalation	$(mg/m^3)^{-1}$	Table 53

10.3. USER-SPECIFIC APPROACH

A user-specific approach can be followed for threshold effects or non-threshold effects. If a user-specific approach is chosen, the user is required to specify how ages should be grouped into age groups and to provide the adequate toxicological criterion for each age group.

10.3.1. THRESHOLD EFFECTS

Age groups are not necessarily consecutive and can overlap. At least one age group should cover adult age categories (≥ 15 yrs) to enable calculations for the industrial scenarios, where the default assumes the absence of children.

(eq. 243)

$$D_{site,oral/dermal}^{age\ group} = \frac{\sum_{i=x-y} D_{oral/dermal}^{yearly,i} \times Yr_i}{\sum_{i=x-y} Yr_i}$$

(eq. 244)

$$C_{site,inhalation}^{age\ group} = \frac{\sum_{i=x-y} C_{inhalation}^{yearly,i} \times Yr_i}{\sum_{i=x-y} Yr_i}$$

(eq. 245)

$$RI_{oral/dermal}^{age\ group} = \frac{D_{site,oral/dermal}^{age\ group}}{TDI/U_{oral/dermal}^{age\ group}}$$

(eq. 246)

$$RI_{inhalation}^{age\ group} = \frac{C_{site,inhalation}^{age\ group}}{TCA^{age\ group}}$$

For local effects, only the risk indices by route are reported and the route with the highest RI value is critical. For systemic effects, an overall RI (summed over routes) is calculated.

(eq. 247)

$$RI^{age\ group} = \sum RI_{route}^{age\ group}$$

Where

Abbr.	Name	Unit	Source
$D_{site,oral/dermal}^{age\ group}$	yearly average intake/uptake from the location by the oral or dermal route for the specified exposure duration / averaging time	mg/kg.d	(eq. 243)
$D_{oral/dermal}^{yearly,i}$	yearly average intake/uptake from the location by the oral or dermal route and age category i	mg/kg.d	ED or AD from CHAPTER 9
$C_{site,inhalation}^{age\ group}$	yearly average exposure air concentration for the specified exposure duration / averaging time from the location	mg/m³	(eq. 244)
$C_{inhalation}^{yearly,i}$	yearly average exposure air concentration for age category i	mg/m³	(eq. 222)
Yr_i	number of years in age category i	yr	Table 55
$RI_{oral/dermal}^{age\ group}$	risk index by the oral or dermal route for the specified exposure period	-	(eq. 245)
$RI_{inhalation}^{age\ group}$	risk index by inhalation for the specified exposure period		(eq. 246)
$RI^{age\ group}$	risk index for systemic effects for the specified exposure period	-	(eq. 247)
$TDI/U_{oral/dermal}^{age\ group}$	Tolerable Daily Intake/Uptake by the oral or dermal route for the age group	mg/kg.d	Table 53
$TCA^{age\ group}$	Tolerable Concentration in air	mg/m³	Table 53

10.3.2. NON-THRESHOLD EFFECTS

(eq. 248)

$$D_{site,oral/dermal}^{age\ group} = \frac{\sum_{i=x-y} D_{oral/dermal}^{yearly,i} \times Yr_i}{\sum_{i=x-y} Yr_i}$$

(eq. 249)

$$C_{site,inhalaton}^{age\ group} = \frac{\sum_{i=x-y} C_{inhalation}^{yearly,i} \times Yr_i}{\sum_{i=x-y} Yr_i}$$

(eq. 250)

$$ExCR_{oral/dermal} = \frac{\sum_{\text{age groups}} \left(D_{oral/dermal}^{yearly,age\ group} \times SF_{oral/dermal}^{age\ group} \times \sum Yr_i\right)}{\sum_{i=1-10} Yr_i}$$

(eq. 251)

$$ExCR_{inhalation} = \frac{\sum_{\text{age groups}} \left(C_{site,inhalation}^{age\ group} \times UR^{age\ group} \times \sum Yr_i\right)}{\sum_{i=1-10} Yr_i}$$

For local effects, only the excess cancer risks by route are reported and the route with the highest ExCR value is critical. For systemic effects, an overall ExCR (summed over routes) is calculated.

(eq. 252)

$$ExCR = \sum ExCR_{route}$$

Where

Abbr.	Name	Unit	Source
$D_{site,oral/dermal}^{age\ group}$	yearly average intake/uptake from the location by the oral or dermal route for the specifiekd exposure duration	mg/kg.d	(eq. 248)
$D_{oral/dermal}^{yearly,i}$	yearly average intake/uptake from the location by the oral or dermal route and age category i	mg/kg.d	ED or AD from CHAPTER 9
$C_{site,inhalation}^{age\ group}$	yearly average exposure air concentration from the location for the specified exposure duration / averaging time	mg/m³	(eq. 249)
$C_{inhalation}^{yearly,i}$	yearly average exposure air concentration for age category i	mg/m³	(eq. 222)
Yr_i	number of years in age category I	-	Table 55
$ExCR_{oral/dermal}$	excess cancer risk by the oral or dermal route for lifetime exposure	-	(eq. 250)
$ExCR_{inhalation}$	excess lifelong cancer risk by inhalation	-	(eq. 251)
ExCR	overall excess cancer risk for systemic effects for lifetime exposure	-	(eq. 252)
$SF_{oral/dermal}^{age\ group}$	slope factor for non-threshold effects by the oral or dermal route for the selected age group	$(mg/kg.d)^{-1}$	Table 53
$UR^{age\ group}$	unit risk for non-threshold effects for the selected age group	$(mg/m^3)^{-1}$	Table 53

10.4. COMPARISON WITH CONCENTRATION LIMITS

Concentration limits are used to compare available concentrations in the environmental compartments. Whereas the term Tolerable Concentration (in air) refers to a reference concentration derived on toxicological data, the term concentration limits is used to refer to regulatory limits that are not necessarily based on toxicological considerations (alone).

The concentration index CI is calculated as the ratio between concentration and concentration limit LIM.

(eq. 253)

$$CI = \frac{\mathrm{C_i}}{\mathrm{LIM_i}}$$

Where

Abbr.	Name	Unit	Source
CI	concentration index	-	(eq. 253)
C_i	concentration in compartment i	mg/kg mg/m^3	from fate and transfer chapters
LIM_i	Concentration Limit in compartment i	mg/kg mg/m^3	Table 54

Comparison with concentration limits is scenario dependent and occurs if limit values (TCs) are filled in. Specifications are given in Table 54.

Table 54: Concentration limits comparison and scenario specifications (***W***).

Compartment	Scenario	
C_{dw} (concentration in drinking-water)	if exposure pathway inhalation indoor air is active	
C_{ao} (concentration in ambient air)	if exposure pathway inhalation indoor air is active	(highest value – height dependent)

10.5. RISK CUT-OFFS

For threshold effects, there is a conclusion of risk once the RI is > 1. For non-threshold effects, where a slope factor is used, there is a conclusion of risk once the excess (lifetime) cancer risk is > 1.10^{-5}. There is also a conclusion of risk if one of the CI is > 1.

RI and CI values are reported for all of the criteria filled in the chemical properties database, unless they are not applicable for the land use (e.g. vegetable concentrations if no vegetable garden).

In calculating general remediation values or site-specific remediation goals, soil concentrations are calculated for each criterion, setting the RI and CI at 1 or the excess (lifetime) cancer risk at 1.10^{-5}.

Table 55: Age categories and number of years

Age category	Number	Number of years
1 - < 3 year	1	2
3 - < 6 year	2	3
6 - < 10 year	3	4
10 - < 15 year	4	5
15 - < 21 year	5	6
21 - < 31 year	6	10
31 - < 41 year	7	10
41 - < 51 year	8	10
51 - < 61 year	9	10
≥ 61 year	10	10

REFERENCES

Allen, R., Pereira, L., Raes, D., & Smith, M. (1998). Crop evapotranspiration - guidelines for computing crop water requirements.

Andelman, J. B. (1985). Inhalation exposure in the home to volatile organic compounds of drinking water. *Science of The Total Environment, 47*, 443-460.

Baes, C. F., Sharp, R. D., Sjoreen, A. L., & Shor, R. W. (1984). A review and analysis of parameters for assessing transport of environmentally released radionuclides through the agriculture.

Bakker, J., Lijzen, J. P. A., & van Wijnen, H. J. (2008a). Site-specific human risk assessment of soil contamination with volatile compounds. (Report 711701049/2008).

Bakker, J., Lijzen, J. P. A., & van Wijnen, H. J. (2008b). Site-specific human risk assessment of soil contamination with volatile compounds.

Bintein, S., & Devillers, J. (1994). QSAR for organic chemical sorption in soils and sediments. *Chemophere, 28*(6), 1171-1188.

Birak, P., Yurk, J., Adeshina, F., Lorber, M., Pollard, K., Choudhury, H., & Kroner, S. (2001). Travis and Arms revisited: a second look at a widely used biocontration algorithm. *Toxicology and Industrial Health, 17*(5-10), 163-175.

Briggs, G. G., Bromilow, R. H., & Evans, A. A. (1982). Relationships between lipophilicity and root uptake and translocation of non-ionised chemicals by barley. *Pesticide Science, 13*(5), 495-504.

Brochu, P., Brodeur, J., & Krishnan, K. (2011). Derivation of physiological inhalation rates in children, adults, and elderly based on nighttime and daytime respiratory parameters. *Inhalation Toxicology, 23*(2), 74-94.

Chiou, H., Chiou, S., Hsu, Y., Chou, Y., Tseng, C., Wei, M., & Chen, C. (2001). Incidence of transitional cell carcinoma and arsenic in drinking water: A follow-up study of 8,102 residents in an arseniasis-endemic area in northeastern Taiwan. *American Journal of Epidemiology, 153*(5), 411-418.

Cornelis, C. (2012a). Evaluatie van de wegingsfactoren voor inhalatie - nota MRG/N97F2/2013-002. 4 p.

Cornelis, C. (2012b). Nota uitdamping binnenlucht juni 2012.

Cornelis, C. (2013). Overwegingen rond het ventilatievoud.

Cornelis, C., & Bierkens, J. (2012). Modifications to the S-Risk prototype v2010.

Cornelis, C., Bierkens, J., Standaert, A., & Willems, H. (2011). Test report of the S-Risk prototype.

Cornelis, C., Provoost, J., Seuntjens, P., & De Raeymaecker, B. (2008). Herziening Vlier-Humaan - ontwerp eindrapport.

Cornelis, C., & Swartjes, F. (2007). Ontwikkeling van een geharmoniseerde methodiek voor de beoordeling van gezondheidsrisico's door bodemverontreiniging in de Kempenregio - eindrapport.

Demarest, S., & Drieskens, S. (2004). Health Interview Survey Belgium, 1997-2001-2004.

Devriese, S., Huybrechts, I., Moreau, M., & Van Oyen, H. (2006). De Belgische Voedselconsumptiepeiling 1 - 2004.

DLV. (2007). Melkveevoeding.

DLV. (2008). Voeding van runderen van het Belgisch witblauwe ras.

Douben, P., Alcock, R., & Jones, K. (1997). Congener specific transfer of PCDD/Fs from air to cow's milk: an evaluation of current modelling approaches. *Environmental Pollution, 95*(3), 333-344.

EC. (1993). CORINE landcover technical guide.

ECB. (2003). Technical Guidance Document on Risk Assessment - Part III.

ECETOC. (1992). Hazard assessment of chemical contaminants in soil.

Ginsberg, G., Foos, B., Dzubow, R. B., & Firestone, M. (2010). Options for incorporating children's inhaled dose into human health risk assessment. *Inhal Toxicol, 22*(8), 627-647.

GSI. (2007). Software guidance manual RBCA toolkit for chemical releases - version 2.

Jury, W. A., Farmer, W. J., & Spencer, W. F. (1984). Behavior assessment model for trace organics in soil: II. Chemical classification and parameter sensitivity. *Journal of Environmental Quality, 13*(4), 567-572.

Kizinievic, V., & Kizinievic, O. (2009). Influence of structural parameters on the frost resistance of clay masonry units. *Materials Science, 15*(1), 59-63.

Komp, P., & McLachlan, M. S. (1997a). Influence of temperature on the plant/air partitioning of semivolatile organic compounds. *Environmental Science & Technology, 31*(3), 886-890.

Komp, P., & McLachlan, M. S. (1997b). Interspecies variability of the plant/air partitioning of polychlorinated biphenyls. *Environmental Science & Technology, 31*(10), 2944-2948.

Lorber, M., Cleverly, D., Schaum, J., Philips, L., Schweer, G., & Leighton, T. (1994). Development and validation of an air-to-beef food chain model for dioxin-like compounds. *Science of The Total Environment, 156*(1), 39-65.

Meneses, M., Schuhmacher, M., & Domingo, J. L. (2002). A design of two simple models to predict PCDD/F concentrations in vegetation and soils. *Chemosphere, 46*, 1393-1402.

Mensink, C., Colles, A., Janssen, L., & Cornelis, J. (2003). Integrated air quality modelling for the assessment of air quality in streeds against the council directive. *Atmospheric Environment, 37*(37), 5177-5184.

Naik, T., Kraus, R., Chun, Y., & Botha, F. (2005). Cast-concrete products made with FBC ash and wet-collected coal-ash. *Journal of Materials in Civil Engineering, 17*, 659-663.

OVAM. (2005). Bepaling van risico's door uitloging en beschrijving evolutie van de bodemkwaliteit - deel 2: handleiding uitloging.

Pröhl, G. (2009). Interception of dry and wet deposited radionuclides by vegetation. *Journal of Environmental Radioactivity, 100*, 675-682.

Riederer, M. (1995). Partitioning and transport of organic chemicals between the atmospheric environment and leaves. In S. Trapp & C. McFarlane (Eds.), *Plant contamination - modeling and simulation of organic chemical processes*): Lewis Publishers.

Roelants, M., & Hauspie, R. (2004). Groeicurven Vlaanderen 2004.

Römkens, P. F. A. M., Zeilmaker, M. J., Rietra, R. P. J. J., Kan, C. A., van Eickeren, J. C. H., Van Raamsdonk, L. W. D., & Lijzen, J. P. A. (2007). Blootstelling en opname van cadmium door runderen in de Kempen: Een modelstudie.

Sabljic, A., & Gusten, H. (1995). QSARs for soil sorption. In J. L. M. Hermens (Ed.), *Overview of structure-activity relationships for environmental endpoints. Report prepared within the framework of the project "QSAR for prediction of fate and effects of chemicals in the environment", an international project of the environmental technologies RTD* *programme (DG XII/D-1) of the European Commission under contract number EV5V-CT92-0211.*).

Samsoe-Petersen, L., Larsen, E., Larsen, P., & Bruun, P. (2002). Uptake of trace elements and PAHs by fruit and vegetables from contaminated soils. *Environmental Science & Technology, 36*(14), 3057-3063.

Seuntjens, P., Steurbaut, W., & Vangronsveld, J. (2006a). Chain model for the impact analysis of contaminants in primary food products.

Seuntjens, P., Steurbaut, W., & Vangronsveld, J. (2006b). Chain model for the impact analysis of contaminants in primary food products. *Scientific Support Plan for a Sustainable Development Policy (SPSDII) - Part 1: Sustainable production and consumption patterns*.

Smolders, E., Jansson, G., Van Laer, L., Ruttens, A., Vangronsveld, J., Römkens, P. F. A. M., De Temmerman, L., Waegeneers, N., & Bries, J. (2007). Teeltadvies voor de landbouw in kader van het Interregg project BeNeKempen.

Swartjes, F. A., Dirven-Van Breemen, E. M., Otte, P., Van Beelen, P., Rikken, M. G. J., Tuinstra, J., Spijker, J., & Lijzen, J. P. A. (2007). Towards a protocol for the assessment of site-specific human health risks for consumption of vegetables from contaminated sites.

Thompson, N. (1983). Diffusion and uptae of chemical vapour volatilising from a sprayed target area. *Pesticide Science, 14*(1), 33-39.

Trapp, S. (2002). Dynamic root uptake model for neutral lipophilic organics. *Environmental Toxicology and Chemistry, 21*(1), 203-206.

Trapp, S., Cammarano, A., Capri, E., Reichenberg, F., & Mayer, P. (2007). Diffusion of PAH in potato and carrot slices and application for a potato model. *Environmental Science & Technology, 41*(9), 3103-3108.

Trapp, S., & Matthies, M. (1995). Generic one-compartment model for uptake of organic chemicals by foliar vegetation. *Environmental Science & Technology, 29*(9), 2333-2338.

Travis, C., & Arms, A. (1988). Bioconcentration of organics in beef, milk and vegetation. *Environmental Science & Technology, 22*, 271-274.

US-EPA. (1996a). Soil screening guidance: Technical background document.

US-EPA. (1996b). Soil Screening Guidance: Technical background document. (EPA/540/R95/128).

US-EPA. (1997). Exposure factors handbook.

US-EPA. (2004a). Risk Assessment Guidance for Superfund Volume I: Human Health Evaluation Manual (Part E, Supplemental Guidance for Dermal Risk Assessment).

US-EPA. (2004b). User's guide for evaluating subsurface vapor intrusion into buildings.

US-EPA. (2009a). Metabolically derived human ventilation rates: a revised approach based upon oxygen consumption rates.

US-EPA. (2009b). Risk assessment guidance for Superfund - Volume I: human health evaluation manual (Part F: supplemental guidance for inhalation risk assessment) - final. (EPA-540-R-070-002).

Van Holderbeke, M., Cornelis, C., Bierkens, J., & Torfs, R. (2008). Review of the soil ingestion pathway in human exposure assessment - final report.

Study in support of the BeNeKempen project - subproject on harmonization of the human health risk assessment methodology.

Van Raamsdonk, L. W. D., Kan, C. A., Meijer, G. A. L., & Kemme, P. A. (2007). Kerngetallen van enkele landbouwhuisdieren en hun consumptiepatronen.

Voedingscentrum. (2002). Zo eten jonge peuters in Nederland 2002 - resultaten van het Voedingsstoffen Inname Onderzoek 2002.

Vonk, M. W. (1985). Permeation of organic chemicals through piping materials (in Dutch).

Waegeneers, N., De Steur, H., De Temmerman, L., Van Steenwinkel, S., & Viaene, J. (2009). Transfer of soil contaminants to home-produced eggs from Belgium: levels, contamination sources and health risks. *Science of The Total Environment, 407*(15), 4438-4446.

Wolff, C. J. M., & van der Heijde, H. B. (1982). A model to assess the rate of evaporation of chemical compounds from surface waters. *Chemophere, 11*(2), 103-117.

WTCB. (2006). TV 228: Natuursteen.

ANNEX I – AIR PERMEABILITY OF BASEMENT WALLS

Bakker et al. (2008b) did not provide open porosity values for basement walls. In case basement walls are from poured concrete, with the same quality as basement floors, air permeability and porosity of basement floors can be taken. When other materials are used, different values are required.

We looked for values for open porosity for different building materials. The values are given in Table 56.

Table 56: Literature values for open porosity ofbuilding materials

Material	Value	Source
limestone	0.01 – 0.19	website WTCB
Portland cement	0.075 – 0.094	website WTCB
ceramic masonry units	0.20 – 0.26	Kizinievic et al. (2009)
hollow cement blocks with fly ash	0.08 – 0.13	Naik et al. (2005)
solid cement blocks with fly ash	0.159 – 0.184	Naik et al. (2005)

The values for open porosity of the cement blocks with fly ash were calculated from measured water absorption. Water absorption, measured under vacuum (e.g. NBN EN 1936:1999) can be used to calculate open porosity when the apparent volumetric mass (kg/m^3) is known:

open porosity (%) = apparent vol. mass (kg/m^3) * water absorption under vac.(kg/100 kg) / 1000.

It can also be calculated directly from the water absorption test (WTCB, 2006).

ANNEX II – INVENTORY OF INDOOR AIR EXCHANGE RATES

In order to arrive at representative indoor air exchange rates in Flanders, we searched for information on the actual situation. The inventory revealed that the information is limited. The "Energy Prestation Regulation" gives rules for the ventilation of residential and non-residential buildings. The text hereafter shortly discusses the applicable regulation and the available numbers, it is the translation of a note of 17/10/2012 that was used to take final decisions on the default values for ventilation rates in application I. It can be used to estimate values for site-specific assessments.

VENTILATION IN RESIDENTIAL BUILDINGS

Ventilation in residential buildings in Flanders should meet the requirements of the Energy Prestation Regulation (Energieprestatieregelgeving) Appendix IX. The requirements for ventilation are mainly based on the Belgian Standard NBN D50-001 (edition October 1991). The general rule is a ventilation of 3.6 m^3/m^2.hr.

Specific conditions are given in Table 57.

Table 57: Minimum required design flow rates by indoor space for input, throughput and removal (Flemish Energy Prestation Regulation)

Indoor space	Floor area	Air supply	Air throughput : capacity (or free section)	Air removal towards the outside
bedroom, bureau, room for playing or hobbies (or equivalent)	less than 7 m^2	25 m^3/h	25 m^3/h (of 70 cm^2)	
	between 7 and 20 m^2	3.6 $m^3/h.m^2$		
	more than 20 m^2	72 m^3/h		
living room, drawing room, dining room (or equivalent)	less than 21 m^2	75 m^3/h	25 m^3/h (of 70 cm^2)	
	between 21 and 42 m^2	3.6 $m^3/h.m^2$		
	More than 42 m^2	150 m^3/h		
Toilet			25 m^3/h (of 70 cm^2)	25 m^3/h
kitchen (closed), bath room, washing room (or equivalent)	less than 14 m^2		kitchen: 50 m^3/h (or 140 cm^2) Rest: 25 m^3/h (or 70 cm^2)	50 m^3/h
	between 14 and 21 m^2			3.6 $m^3/h.m^2$
	more than 21 m^2			75 m^3/h
Open kitchen				75 m^3/h

If we take as an example the default dimensions of a residential building, used in S-Risk (surface area 50 m^2, height 3 m), ventilation would be 3.6 x 50 = 180 m^3/h. This is an approximation as the ventilation requirements differ by room type. If we convert this to air changes, we arrive at 150 / (50 x 3) = 1 h^{-1}, which is double the value that we initially took as average based on Bakker et al. (2008).

Brits et al. (2005) mention values on season averaged ventilation in Flemish residences enrolled in the SENVIVV study. The SENVIVV study investigated 200 Flemish residences, built between 1987 and 1993. Ventilation rates and air changes were derived from the air tightness of buildings (n50) according to the following equation.

$$n\left({}^{1}/_{h}\right)=\frac{n_{50}\left({}^{1}/_{h}\right)}{f}$$

The factor f varies as a function of building type and depends on exposure to the wind. The value for f used in this study equaled 20. The calculated values are applicable to natural ventilation conditions (without opening of doors and windows). The Q-Intair study (De Brouwere et al., 2009) refers as well to the SENVIVV study. The requirements for a passive building is n50 = 0.6 h^{-1}.

Table 58: Average natural ventilation in residences (Brits et al., 2005, De Brouwere et al. 2009, based on SENVIVV, 1998), 50 residences

Building type	n_{50} (h^{-1})	Air changes (h^{-1})
all buildings	7.8	0.4 (0.1 – 6.0)
apartments	4.1	0.2
house in a row	5.3	0.25
semi-detached or detached houses	8.3	0.4
detached houses	9.5	0.5

The Q-Intair study (De Brouwer et al., 2009) concluded that there were insufficient adequate data on ventilation of residences (combining air tightness and ventilation). Therefore simulations were run under varying conditions, assuming an air tightness of 12 m^3/m^2.h (3 m^3/m^2.h for ventilation system D – low energy) and that the requirements of NBN D50-001 were met. Various ventilation systems (A, B, C, D) were simulated. The average air changes are given in

Table 59: Calculated air changes for residences (De Brouwere et al., 2009)

Scenario*	Air changes (h^{-1})	Air tightness (h^{-1})	Ventilation (h^{-1})
A – default	1.03		
C – default	1.01		
D – default	1.29	0.368	0.921
D – low energy	0.60	0.142	0.461
D - occupied	0.83		

Ventilation systems: A (natural ventilation), C (free inflow, mechanical outflow), D (mechanical in and outflow)

According to De Brouwer et al. (2009), the SENVIVV study made a theoretical calculation of the air changes of 200 residences, assuming application of the ventilation standard. This lead to an air change of 0.3 h^{-1} for large residences and 0.95 h^{-1} for small residences. If one adds an average air tightness of 0.3 h^{-1} (SENVIVV average n50 of 7.8 h^{-1} divided by 25 – De Brouwere et al. (2009) and the default of the Energy Prestation Regulation use a value of 25 for f), one arrives at an overall air change of 0.6 – 1.2 h^{-1}. The Q-Intair report states that 1 h^{-1} could be used as an average value for residences in case of simplified calculations.

De Brouwere and Van de Velde (2010) measured the air tightness in 51 newly built residences (2006-2009). They also added results of 133 residences with data from blower door companies (in the latter case one can expect a higher than average air tightness of the building). The authors state that the n50 was not correctly calculated in the SENVIVV study, as the SENVIVV study used the outer volume (protected volume) of the building while one should use the inner volume. They propose a corrected average of 11.3 h^{-1} instead of 7.8 h^{-1}. The average air change would then be 0.6 h^{-1} instead of 0.8 h^{-1} (theoretical calculation when meeting the NBN).

Table 60: Air tightness and air changes in newly built residences (2006-2009), based on data in De Brouwere and Van de Velde (2010)

	n_{50} (h^{-1})	Air change (h^{-1})*
own measurements	6 (1 – 19.2)	0.3 (0.05 – 1.0)
blower door companies - LEW	1.3 (0.2 – 3.2)	0.07 (0.01 – 0.16)
blower door companies - non-LEW	3.7 (2.0 – 16.2)	0.19 (0.1 – 0.8)

LEW: low energy residence
*: own calculation assuming natural ventilation, factor f = 20

The authors also measured ventilation supply and removal rates in 27 residences, 19 of which with ventilation type C and 8 with ventilation type D. Measurements were done under maximum ventilation (nominal position), which is generally higher than the typical use condition. For the residences with ventilation type C, about half of the living rooms met the ventilation requirements, whereas the other residences were equally distributed between over and under dimension. The residences with ventilation type D typically showed lower flow rates than required in the living room.

VENTILATION IN NON-RESIDENTIAL BUILDINGS

Ventilation in non-residential Flemish buildings should meet the Energy Prestation Regulation. This regulation gives minimum requirements as a function of room type. For S-Risk, we look at the requirements for rooms intended for human occupation (non-smokers). The minimum requirement equals 22 m^3/h (lower limit IDA-3 of NBN-13779:2004, IDA-3 corresponds with “acceptable air quality”). In case of smoking in the room, ventilation requirements are higher. In addition to the general requirement, the regulation also specifies the required surface area per person as a function of room type.

Table 61: Floor surface area per person to enable the quantification of the occupation, required for the calculation of the minimum design flow rate in rooms meant for human occupation (appendix X of the Energy Prestation Regulation)

	Floor area per person (m^2/pers)
Catering	
restaurants, cafeteria, snakc bar, canteen, bars, cocktail bars	1.5
kitchens, kitchenettes	10
Hotels, motels, holiday resorts	
bed rooms in hotel, motel, holiday resort	10
dormitories in holiday resorts	5
lobby, entrance	2
meeting rooms, polyvalent rooms	2
Office buildings	
office	15
reception, reception rooms, meeting rooms	3.5
main entrance	10
Public buildings	
departure halls, waiting rooms	1
library	10

	Floor area per person (m^2/pers)
public meeting rooms	
churches and other religious buildings, office buildings, lawcourts, museums and galeries	2.5
Shops	
shops (except shopping centres)	7
shopping centre	2.5
hairdresser’s, beauty salon	4
shops for voor furniture, carpets, textile, ...	20
super market, department store, pet shop	10
laundrette	5
Sports and leisure	
sports hall, stadium, gymnasium	3.5
dressing rooms	2
spectator rooms, stands	1
disco, dance hall	1
sportclub: aerobic rooms, fitness rooms, bowling club	10
Working rooms	
picture studio, dark room, ...	10
pharmacy (preparation of medication)	10
counter in banks, I strong room for public	20
copy room I printer room	10
computer room (without printers)	25
educational establishments	
class rooms	4
polyvalent rooms	1
Health care	
infirmary	10
treatment and examination rooms	5
operating room, delivery room, recovery room, intensive care, physiotherapy	5
Penitentiary	
cells, dagverblijf	4
guard posts	7
registraion room, waiting room	2
other rooms	
other rooms	15

According to the Belgian legislation for worker protection, rooms should be at least 2.5 m high. Every worker should have a real space of 10 m^3 and a free floor area of 2 m^2 (if we divide 10 m^3 by 2.5 m, we arrive at a total area of 4 m^2). Supply of fresh air and removal of polluted air should be ensured at a rate of 30 m^3/hr and per worker present.

If we take 10 m^3 for workers and a flow rate of 30 m^3/hr per person, this gives us an air change of 3 h^{-1}. When we regroup numbers towards land use types IV and V en take into account the main rooms (where most of the time is spent), we obtain the air changes of Table 62. With regard to the Flemish regulation, we assumed 22 m^3/h per person and a room height of 2.5 m. The air changes were then calculated using floor surface area (ventilation (m^3/h) / floor surface (m^2) / height (m)).

Table 62: Calculated air changes for non-residential buildings and for worker places

	Air change (h^{-1})
Land use type IV	
bed rooms in hotel, motel, holiday resort	0,88
dormitories in holiday resorts	1,76
sports hall, stadium, gymnasium	2,51
sportclub : aerobic rooms, fitness rooms, bowling club	0,88
Land use type V	
offices	0,59
shopping centres	3,52
shops	1,26
work place (worker regulation)	3
other spaces	0,59

We can add a value of 0.3 h^{-1} to these values to account for air tightness.

REFERENCES

Energieprestatiebesluit van de Vlaamse Regering van 19 november 2010 en bijlage IX (ventilatievoorzieningen in woongebouwen) en bijlage X (ventilatie in niet-residentiële gebouwen)

NBN D50-001 (1991) – Ventilatievoorzieningen in woongebouwen
NBN 13779:2004 – Ventilatie voor niet-residentiële gebouwen - Prestatie-eisen voor ventilatie- en luchtbehandelingssystemen.

Brits E., Goelen, E., Koppen, G., Spruyt, M., Torfs, R. (2005). The influence of contaminants in ambient air on the indoor air quality – Part I: Exposure of children – report of work package 1. VITO, Mol, België.

De Brouwere, K., Caillou, S., Torfs, R., Van den Bossche, P. (2009). Q-INTAIR: modellering van binnenluchtkwaliteit op basis van bouwmaterialenemissies, gebouwluchtdichtheid en ventilatie van woningen.

WTCB. 1998. SENVIVV - Studie van de Energieaspecten van Nieuwbouwwoningen in Vlaanderen: Isolatie, Ventilatie, Verwarming (Vliet Vlaams Impulsprogramma Energietechnologie - Project 930.256 - 1.1.1995-31.12.1997 Eindverslag) - Studiedag 13 maart 1998 te Gent. Bruxelles, CSTC-WTCB, 1998.

De Brouwere, T. en Van de Velde, S. (2010). Meting van luchtdichtheid en binnenluchtkwaliteit in nieuwbouwwoningen (bouwjaar 2006-2009). Masterthesis, Universiteit Gent, Vakgroep Architectuur en Stedenbouw.

Arbeidsreglementering: http://www.werk.belgie.be/defaultTab.aspx?id=607

ANNEX III – DEFAULT VALUES FOR THE CALCULATION OF SOIL REMEDIATION VALUES

Annex III is available as a separate document.