

# Comparison of Risk Assessment Parameters for Homegrown Produce in Various Models

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## **I. Introduction**

This document provides a guide of the parameters used in assessing chemical exposure through homegrown produce. Exposure assessments are an effective way to estimate the risk associated with exposure to harmful chemicals. They act as a more efficient substitute compared to directly sampling chemical concentrations. Because harmful chemicals can enter a human body via many different pathways, such as air, water, skin contact, or ingestion through food, it is important to quantify each exposure pathway separately. In addition to the various pathways, exposure assessments also take into account the amount of contaminant to which a person is exposed, the frequency of exposure, age and other population characteristics, and the sources of the contaminant (CLEA Report p. 10). Exposure assessments have a high degree of uncertainty because many factors are involved. Therefore, parameters should be as accurate as possible to be applicable at many different sites. Standardized parameters for the exposure pathway of homegrown food consumption are not yet established in US Environmental Protection Agency (EPA) models.

This document draws comparisons between the Contaminated Land Exposure Assessment (CLEA) model from the United Kingdom's Environment Agency, the S-Risk model from Belgium, the CSOIL model from the Netherlands, ... The parameters used to model exposure through food consumption vary slightly from country to country, but they fundamentally rely on the same science. Vegetable consumption is modelled in all countries included in this document, but only Belgium's S-Risk model includes consumption of meat, milk and eggs; only the CLEA model includes consumption of fruit.

## **II. Vegetable Consumption**

Many people grow a portion of their produce in gardens at home. If these plants are grown in contaminated soil, the plant can take up some of the contaminant and enter the human body when eaten. This pathway of contamination can be important when calculating a person's total exposure to a harmful chemical; it can push an exposure rate over the threshold value that is considered unsafe according to environmental regulations. In the Netherlands CSOIL model, it is common that the combined exposure from ingestion of soil particles, inhalation of contaminants in indoor air, and the consumption of contaminated vegetables typically contribute around 90% of all exposure for a person. All other exposure pathways are typically less than 10% of the total exposure (CSOIL). However, not all countries include vegetable consumption. See Appendix 1 for the exposure pathways included in European exposure models.

Contaminants that enter plants are typically water-soluble. Therefore, they enter the roots as part of the soil pore water. From there, the contaminants are distributed throughout the plant by the xylem and phloem. Aboveground plant parts can further be contaminated by soil splash,

which is small soil particles landing on leaves or stems as plants are watered, or through the air. The models use fresh weight (fw) of the vegetable because it is the typical measure of how much of the vegetable is eaten, but there is a conversion factor for each produce group to dry weight (dw) because soil concentrations are typically given in dry weight. Fresh weight of vegetables generally does not take into account changes in water content as vegetables are cooked.

The amount of contaminant to which a person is exposed can be modelled using the following equation, as found in CLEA:

$$IR = C_s \times CF \times CR \times BW \times HF \quad (1)$$

Where	IR is the intake rate of the contaminant [mg/d]
	$C_s$ is the soil concentration of the contaminant [mg/g dw]
	CF is the soil-to-plant concentration factor for the produce group [mg/g fw per mg/g dw]
	CR is the rate of food consumption per unit body weight for the produce group [g fw/kg bw/d]
	BW is the body weight [kg]
	HF is the homegrown fraction for the produce group [unitless]

The units for each variable differ between models. Each variable is associated with a set of parameters that will be further explained below. The exposure through homegrown produce can be calculated using soil properties measured at a site, combined with parameters that have a standard value based on population averages or chemical properties.

#### A. Concentration Factor

The concentration factor (CF), also called the bio-concentration factor, is the most difficult value to model because there are many complicated interactions between soil, plant, and water that must be explained empirically (source). It is described by the following equation:

$$CF = \frac{C_{plant}}{C_s} \quad (1)$$

Where  $C_{plant}$  is the chemical concentration in edible plant tissues, mg g<sup>-1</sup> fw plant, and  $C_s$  is the total soil concentration in mg g<sup>-1</sup> dw soil. The concentration factor can be input by the user of the model, but each model has a series of equations that calculate a concentration factor based on soil, chemical, and plant properties.

Each model distinguishes between root vegetables, tubers (potatoes), and aboveground green/foiar vegetables. Each model includes different vegetables within each category (Appendix 2). The approach for calculating the concentration factor also differs for organic contaminants, inorganic contaminants, and metals.

All concentration factors use a parameter that describes the fraction of dry mass in a plant. A large percentage of plant material is water, and consumption of vegetables is measured in fresh weight, which includes the water content. Soil contaminant concentration, however, is measured in dry weight. The fraction of dry mass (dm) is needed to convert between soil concentration and fresh weight of vegetables. The values of dm used in each model are found in Appendix #.

### Root Vegetables – Organic Contaminants

Root vegetables are the simplest vegetable category to model because the only way roots take up contaminants is through the soil. Soil splash and interactions with the atmosphere are not considered for root vegetables in any of the models. Roots are typically thick enough that the water inside them is not in equilibrium with the soil chemistry. The way that chemicals partition between soil and roots are described by the root-water partition coefficient, calculated using the following equation:

$$K_{rw} = \frac{W}{\rho_p} + \frac{L_{plant}}{\rho_p} a K_{ow}^b \quad (\#)$$

The variables are described in Table #. Only the CLEA model uses a plant root density ( $\rho_p$ ), and the default value is 1. The equations and parameters used to calculate to concentration factor for root vegetables are found in Table #. In Belgium’s S-Risk model, surface area is parameterized as 1m<sup>2</sup> for each plant.

Table #. Root-water partition coefficient and associated parameters.

Variable					Value		
S-Risk	CSOIL	CLEA	Description	Units	CLEA	CSOIL	S-Risk
K_RW	K_rootwater	K_rw	equilibrium partition coefficient between root and water	cm <sup>3</sup> /g fw	Eq #	Eq #	Eq #
W	Fwater_root	W	root water content	g/g	0.89	0.833	1-dm (Apppendix #)
		rho_p	plant root density	g/cm <sup>3</sup>	1	-	-
L_plant	Flipid_root	L	root lipid content on a mass basis	g/g	0.025	0.005	0.025*
a_1		a	density correction factor between water and octanol	unitless	1.22	-	1.22
K_ow	K_ow	K_ow	octanol-water partition coefficient	unitless	chemical properties	chemical properties	chemical properties

b_1	b_root	b	Briggs correction coefficient for roots	unitless	0.77	0.8	0.77
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\*for potatoes,  $L_{\text{plant}} = 0.0015$  and for corn,  $L_{\text{plant}} = 0.054$  in S-Risk.

Table #. Concentration factor for root vegetables.

	Equation	Variable		Definition	CLEA		S-Risk	
		CLEA	S-Risk		Value	Units	Value	Units
CLEA and S-Risk		CF	CF	soil-to-plant concentration factor for root vegetables	Equation	mg/g fw plant / mg/g dw soil	Equation	mg/kg fw plant / mg/kg dw soil
		K <sub>d</sub>	K <sub>d</sub>	soil-water distribution coefficient		cm <sup>3</sup> /g dw		L/kg
		K <sub>rw</sub>	K <sub>RW</sub>	equilibrium partition coefficient between root and water	Equation #	cm <sup>3</sup> /g fw	Equation #	L/kg fw
		Q	Q <sub>transp</sub> *1000	transpiration rate of the plant	1000	cm <sup>3</sup> /d	Vegetable-dependent (Appendix)	m <sup>3</sup> /m <sup>2</sup> /d
		rho <sub>p</sub>	rho <sub>r</sub>	plant root density	1	g fw/cm	Vegetable-dependent (Appendix)	kg/m <sup>3</sup>
		V	V <sub>r</sub>	root volume	1000	cm <sup>3</sup>	Vegetable-dependent (Appendix)	m <sup>3</sup> /m <sup>2</sup>
		k <sub>g</sub>	a <sub>growth</sub>	plant growth rate	0.1	1/d	Vegetable-dependent (Appendix)	1/d
		k <sub>m</sub>	a <sub>metabolism</sub>	plant metabolization rate	0	1/d	0	1/d

						Value	Units
CSOIL			BCFrootTM	soil-to-plant concentration factor for root vegetables		Equation	g/m <sup>3</sup> / mg/m <sup>3</sup>
			K <sub>rootwater</sub>	equilibrium partition coefficient between root and water		Equation #	unitless
			RHO <sub>root</sub>	density of root tissue		1000	kg/m <sup>3</sup>
			RHO <sub>water</sub>	density of water		1000	kg/m <sup>3</sup>

### Green Vegetables – Organic Contaminants

The modelling of green/fo liar vegetables, which are any vegetable that grows aboveground, varies from model to model. Unlike root vegetables, there are multiple transfer pathways that can be considered because the plant interacts with both soil and air. Uptake from the roots and subsequent transfer to other plant parts is described in all models. However, the uptake of pollution from air is considered as part of the plant exposure pathway in S-Risk and CSOIL but is not considered in CLEA. Ingestion of small soil particles stuck to the surface of plants, called soil loading, is only described in the CLEA model (see Section E). Soil splash and subsequent transfer of contaminants from small soil particles to leaves, however, is only accounted for in S-Risk. The exposure pathways specific to green vegetables are described in Table #.

Table #. Exposure pathways included for green vegetables.

Pathway	CLEA	S-Risk	CSOIL
soil-to-root uptake	X	X	X
translocation from roots to aboveground plant parts	X	X	X
Atmospheric deposition		X	X
Soil splash (leaves in direct contact with soil particles)		X	X
Soil loading (direct ingestion of soil particles)	X		

Due to the complicated nature of contaminant uptake in green vegetables, the equations used in each model vary. In CLEA, the equation describing the soil-to-plant concentration factor is based only on the octanol-water partition coefficient ( $K_{ow}$ ) and soil properties. The equation shares similarities with the other models, including a term called the transpiration stream concentration factor. This term, according to CLEA, only yields accurate calculations for  $\log K_{ow}$  values from 0 to 4. In S-Risk, the value is set at a constant 0.038 when  $\log K_{ow}$  is greater than 4.5.

S-Risk and CSOIL include terms that describe chemical elimination. As the plant grows and metabolizes, chemical concentration decreases. Volatilization and photodegradation can also eliminate some of the chemicals in the plant. The root-to-plant concentration factor calculations also use the plant conductivity, which in S-Risk is found using a chemical property called the **unitless Henry's Law Constant ( $H'$ )**, as well as the surface area and volume of the aboveground plant parts, the transpiration rate, and the density of plant tissue. The values used for each of these parameters are found in Table #.

Table #. Parameters used to find the concentration factor for aboveground plant parts via the roots.

Parameter	Description	CSOIL	S-Risk	Units	
a_growth, k_growth	chemical elimination due to plant growth	0.035	veggie type	1/d	
a_metabolism, k_metabolism	chemical elimination due to plant metabolism	0	0	1/d	
a_photodegradation, k_photo	chemical elimination due to plant photodegradation	0	0	1/d	
a_volatilization		-	calculated using A, g, V, octanol-air partition coefficient	1/d	
g	plant conductivity	80	(log K <sub>ow</sub> - log H')	g	m/d
			≤5	47.5	
			>5 - ≤7.5	173	
			>7.5 - ≤10	346	
			>10	432	
A, AREA_plant	surface area of the aboveground plant parts	5 m <sup>2</sup>	veggie type (m <sup>2</sup> /m <sup>2</sup> )		
V, V_leaf	volume of the aboveground plant parts	0.002 m <sup>3</sup>	veggie type (m <sup>3</sup> /m <sup>2</sup> )		
Q_transp	transpiration rate	0.001 m <sup>3</sup> /d	veggie type (m <sup>3</sup> /m <sup>2</sup> /d)		
rho, RHO_plant	density of plant tissue	800	veggie type	kg/m <sup>3</sup>	

Several parameters are also used that are not common between models. To find both the concentration due to translocation from roots and from atmospheric deposition, S-Risk uses a growth period of the plant. For atmospheric deposition, S-Risk calculations use plant yield, particle deposition rate, annual rainfall and amount of rainfall retained, a washout factor, and a plant weathering constant. Soil splash calculations use a ratio of particles on leaves relative to the total weight of the plant (Table #).

In CSOIL, a soil-plant partition coefficient is calculated using the same formula as Eq. #, but the fraction of water, fraction of lipids, and correction for differences between lipid and octanol have different values than for roots. For atmospheric deposition, a deposition constant, surface area of aerosol particles, and the Junge constant are used (Table #).

Table #. Parameters unique to the S-Risk and CSOIL models for green vegetable concentration factors.

Model	Parameter	Description	Use	Value	Units
CSOIL	Flipid_plant	volume fraction lipid in plant tissue	root-to-plant translocation	0.01	
	b	correction for lipid/octanol differences	root-to-plant translocation	0.95	
	Dpconst	deposition constant	atmospheric deposition	0.01	kg dw soil/kg dw plant
	CONjunge	Junge constant	atmospheric deposition	0.4	unitless
	SURF_aer	surface area of aerosol particles	atmospheric deposition	0.00025	unitless
S-Risk	t	growth period of the plant	root-to-plant translocation, atmospheric deposition		d
	Y_v	plant yield	atmospheric deposition	veggie type	kg fw/m <sup>2</sup>
	V_d	dry particle deposition rate	atmospheric deposition	865	m/d
	R_n	annual rainfall	atmospheric deposition	0.0022	m/d
	R_w	fraction of rainfall that is retained	atmospheric deposition	1	unitless
	W_c	volumetric washout factor for particle	atmospheric deposition	5.00x10 <sup>5</sup>	unitless
	k_w	plant weathering constant	atmospheric deposition	0.049	1/d
	F_eff	fraction of soil particles taken up by the plant	soil splash	1	unitless
R	ratio of the particles on the leaves relative to the total weight of the plant	soil splash	0.005	g/g fw	

### *Potatoes and Other Tubers – Organic Contaminants*

Potatoes are part of a vegetable group called tubers. These vegetables are different from root vegetables because they are storage systems for the stem of the plant. Therefore, the concentration factor must be calculated differently from root vegetables. Potatoes are also notably a large part of European diets (see Section B). They contain very high levels of carbohydrates, which affects chemical equilibrium.

In CSOIL, the categories of “potato” and “other vegetables” are only used for metal contaminants. Empirical bio-concentration factors from available studies are used for metals, so there are no equations or parameters associated with finding the concentration in potatoes.



In CLEA and S-Risk, potato concentrations are calculated using a potato-water partition coefficient, described by the following equation:

$$K_{PW} = K_{RW} + f_{ch} \times K_{ch} \quad (\#)$$

Where

Variable	Description	Value		Units	
		CLEA	S-Risk	CLEA	S-Risk
K_PW	potato-water partition coefficient	Eq. #		cm <sup>3</sup> /g fw	L/kg fw
K_RW	root-water partition coefficient	Eq. #		cm <sup>3</sup> /g fw	L/kg fw
K_ch	carbohydrate-water partition coefficient	Table #		cm <sup>3</sup> /g fw	L/kg fw
W	root water content	0.79	0.8	g/g	unitless
L	root lipid content on a mass basis	0.001	0.0015	g/g	unitless
f_ch	fraction of carbohydrates in the potato	0.209	0.19	unitless	kg/kg
rho_p	plant root density	1	-	g/cm <sup>3</sup>	-

Table #. Values of K<sub>ch</sub>, based on the octanol-water partition coefficient. Values are the same for CLEA and S-Risk.

Log K <sub>ow</sub>	K <sub>ch</sub>
<0	0.1
≥0 - <1	0.2
≥1 - <2	0.5
≥2 - <3	1
≥3 - <4	2
≥4	3

The equations used, as well as associated parameters, are listed below.

CLEA:

$$CF_{tubers} = \frac{23 \left( \frac{3600 D_{water} (W^{7/3} / \rho_p)}{K_{sw}} \right) / R^2}{23 \left( \frac{3600 D_{water} (W^{7/3} / \rho_p)}{K_{pw} R^2} \right) + k_g} \quad (\#)$$

$$S\text{-Risk: } CF_p = \frac{\frac{23 \times D_w \times W^{7/3}}{1000 \times r_p^2}}{\frac{23 \times D_w \times W^{7/3}}{K_{PW} \times r_p^2} + a_{growth} + a_{metabolism}} \quad (\#)$$

Where

Variable		Definition	CLEA		S-Risk	
CLEA	S-Risk		Value	Units	Value	Units
CF_tubers	CF_p	Concentration factor for tubers/potatoes	Eq #	mg/g fw plant / mg/g dw soil	Eq #	mg/kg fw plant / mg/kg dw soil
D_water	D_w	effective diffusion coefficient for the potato	chemical properties	m <sup>2</sup> /s	chemical properties	m <sup>2</sup> /d
W	W	root water content	0.79	g/g	0.8	unitless
rho_p	-	plant root density	1	g/cm <sup>3</sup>	-	-
K_pw	K_PW	potato-water partition coefficient	Eq. #	cm <sup>3</sup> /g fw	Eq. #	L/kg fw
R	r_p	radius of potato	0.04	m	0.04	m
k_g	a_growth	plant growth rate	0.1	1/d	0.139	1/d
-	a <sub>metabolism</sub>	chemical elimination via plant metabolism	-	-	0	1/d

### *Inorganic Contaminants*

The concentration of inorganic contaminants follows similar, but more simplified, modelling compared to organic contaminants. All models assume that the concentration in the roots is directly proportional to the soil concentration because inorganic contaminants are typically dissolved in water, which is taken up by the plant (CSOIL). CSOIL estimates the root concentration of inorganic contaminants as the pore water concentration times the water content of the plant (1-dm). S-Risk multiplies the total soil concentration, water content, and a user-defined bioconcentration factor to find the concentration in the plant roots. The CLEA model uses the total soil concentration and an availability correction  $\delta$  that is element-specific (Table #). Contaminants that are chemically similar to elements utilized in metabolic processes have a higher rate of uptake. For CSOIL and S-Risk, this value is not included but is essentially equal to one.

Table #. Availability correction  $\delta$  from CLEA.

Category	$\delta$
Very low uptake potential elements (for example, lanthanides and higher actinides)	0.5
Essential to metabolic plant processes or chemically similar to such elements (for example, most common heavy metals including arsenic, cadmium, lead, mercury, and nickel)	5
Unusually high uptake potential elements (for example, selenium)	50

Once the root concentration is determined, calculation of root-to-plant translocation and atmospheric deposition proceeds following the equations for organic chemicals. In the S-Risk model, soil splash is not considered for inorganic contaminants. Similarly, the CSOIL model simplifies the calculations for inorganic contaminants by using the root concentration rather than root-to-plant translocation. Some inorganic contaminants, such as lead and cadmium, are exceptions to the typical modelling technique because they are very well-studied (CSOIL). Therefore, CLEA and CSOIL recommend special attention and review of the literature when modelling them.

#### B. Consumption of Vegetables

The consumption of vegetables is determined by national dietary surveys, and it varies slightly by country. Some models have broad vegetable categories, while others include consumption rates for each vegetable. Root vegetables are a category found in every model due to the relative simplicity of modelling their concentration factor. Tubers are also a category in each model because potatoes are a tuber, and they make up a very large portion of many people's diets.

Table #. Consumption of vegetables by age group and produce type.

		Consumption (g fw/kg bw/d)					
	Age	Green Vegetables	Root Vegetables	Tubers	Herbaceous fruit	Shrub fruit	Tree fruit
CLEA	0-1	7.12	10.69	16.03	1.83	2.23	3.82
	1-4	6.85	3.3	5.46	3.96	0.54	11.96
	4-16	3.74	1.77	3.38	1.85	0.16	4.26
	16-75	2.94	1.4	1.79	1.61	0.22	2.97

Note that the consumption is measured in g fw of vegetable per kg body weight per day.

		Consumption (g fw/d)

	Age	Potatoes	Root and tuberos vegetables	bulbous vegetables	fruit vegetables	cabbages	leafy vegetables	leguminous vegetables
	S-Risk	1-2	36.3	9.81	5.84	8.89	7.24	7.82
3-5		85.35	15.54	9.25	14.09	11.47	12.39	8.66
6-9		100.81	16.71	10.94	21.62	11.29	16.46	9.94
10-14		120.69	18.24	13.1	31.3	11.06	21.8	11.59
15-20		140.21	23.81	16.72	49.77	13.54	27.11	13.8
21-30		129.9	26.94	19.14	79.15	18.5	32.7	15.62
31-40		124.54	26.94	19.14	79.15	18.5	32.7	15.62
41-50		129.29	26.94	19.14	79.15	18.5	32.7	15.62
51-60		134.31	26.94	19.14	79.15	18.5	32.7	15.62
≥61		137.19	26.94	19.14	79.15	18.5	32.7	15.62

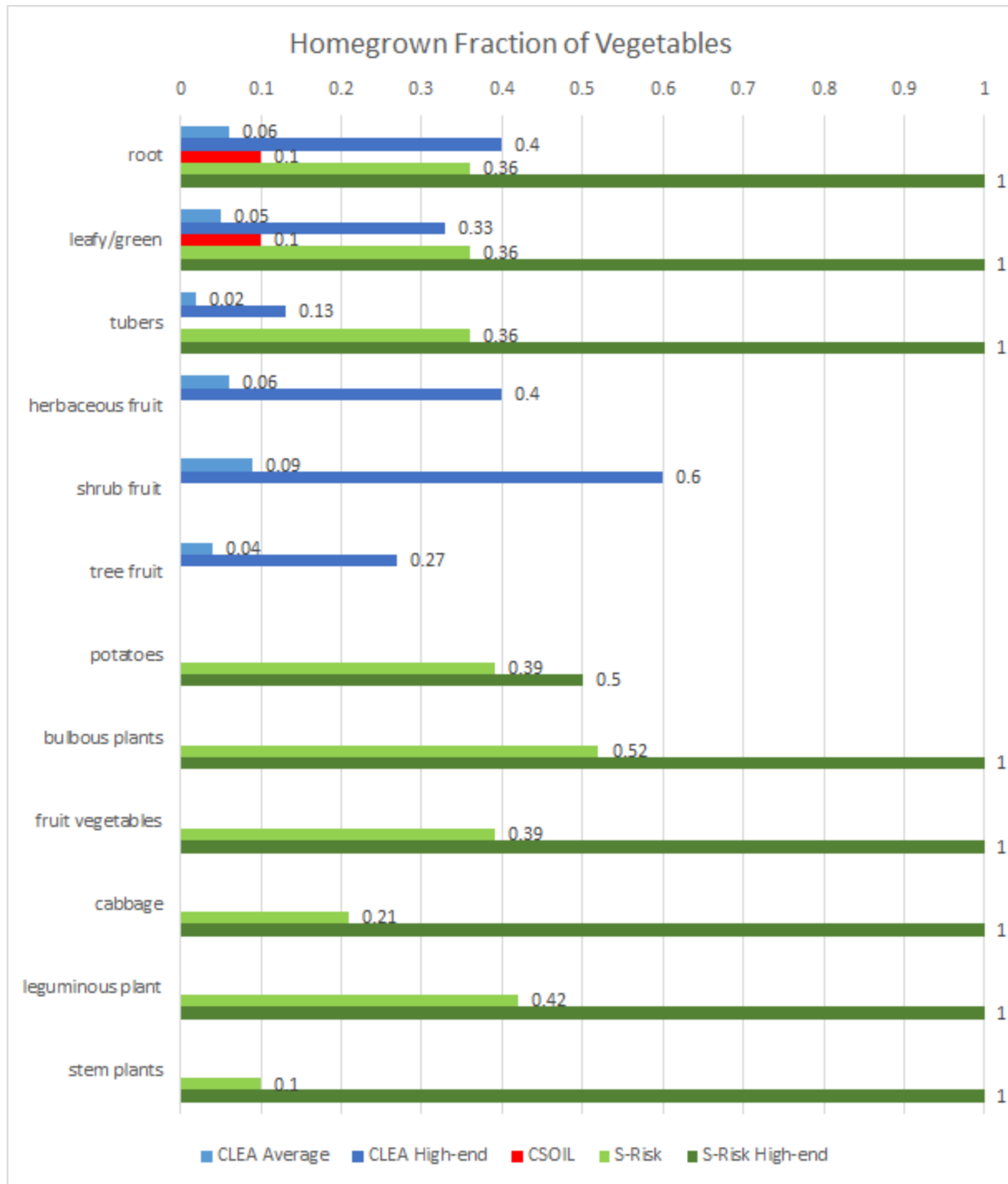
		Consumption (g fw/d)			
CSOIL	Age	Rooty Vegetables	Leafy Vegetables	Potatoes*	Other Vegetables*
	1-6	48	55	39	64
	7-70	100	111	74	137

\*The potatoes and other vegetables categories are only used for metal contaminants.

### C. Homegrown Fraction

Many people grow a portion of their total produce consumption; however, few people achieve full subsistence farming. Not every scenario laid out in each model includes homegrown produce, but several do. The CLEA model includes an exposure scenario called

In CLEA, a high-end value is given for the fraction of homegrown produce. Studies of the U.K. population indicated that only 15% of the population grows any homegrown produce at all. Of that 15%, many people grow a significant portion of what they eat, and the higher values for the homegrown fraction reflect this.



#### D. Bodyweight

The average body weight is one of the parameters needed to calculate the risk of consuming contaminated food. An average weight is obtained from national health surveys and is therefore specific to each individual country. CSOIL and Sweden use more generic values drawn from multinational health surveys. They separate age groups into children and adults,

while S-Risk and CLEA have more specific body weights based on smaller age groups. Table (#) shows the average body weight by age for each model. These values are the default weight used in calculations.

The body weight values are comparable across each model, with the largest variation in ages 7-20. These ages are classified as part of the adult age group for CSOIL and Sweden, but they are distinct age classes in CLEA and S-Risk.

Table (#).

Age	Body Weight (kg)			
	CLEA*	S-Risk	CSOIL	Sweden
0	5.6	12.3	15	15
1	9.8	12.3	15	15
2	12.7	12.3	15	15
3	15.1	17.6	15	15
4	16.9	17.6	15	15
5	19.7	17.6	15	15
6	22.1	26.8	15	15
7	25.3	26.8	70	70
8	27.5	26.8	70	70
9	31.4	26.8	70	70
10	35.7	44.4	70	70
11	41.3	44.4	70	70
12	47.2	44.4	70	70
13	51.2	44.4	70	70
14	56.7	44.4	70	70
15	59	62.5	70	70
16	70	62.5	70	70
17-20	70	62.5	70	70
21-30	70	68.5	70	70
31-40	70	70.5	70	70
41-50	70	71	70	70
51-60	70	74	70	70

61-64	70	72.5	70	70
65-70	70.9	72.5	70	70**
71-75	70.9	72.5	-	70**

\*CLEA uses female weight as the default, but also includes an average male weight for each age class. These values can be found on page 67 of the CLEA Report.

\*\*Ages 66-80 are considered as exposure years only for scenarios involving sensitive land in Sweden's model.

#### E. Soil Loading

When plants are harvested, a small amount of soil particles remain on the outside of the plant. Even after produce has been washed, small traces of dirt remain. The CLEA model accounts for this small amount of soil that is indirectly ingested, called soil loading. The intake rate is calculated similarly to Eq. #, replacing the concentration factor with values of soil loading, a preparation factor, and a dry weight conversion factor. The preparation factor accounts for washing and peeling vegetables, which removes much of the dirt. The values based on category are listed below in Table #.

Table #. Soil loading, preparation factor, and dry weight conversion factor as found in CLEA.

Produce category	Soil loading (SL)	Preparation factor (PF)	Dry weight conversion factor (DW) <sup>1</sup>
	g g <sup>-1</sup> dw	dimensionless	g dw g <sup>-1</sup> fw
Green vegetables	0.001	0.2	0.096
Root vegetables	0.001	1.0	0.103
Tuber vegetables	0.001	1.0	0.210
Herbaceous fruit	0.001	0.6	0.058
Shrub fruit	0.001	0.6	0.166
Tree fruit	0.001	0.6	0.157

### III. Meat, Milk, and Egg Consumption

Only belgium

### IV. Fruit Consumption

Fruit consumption is only considered in the CLEA model. The concentration of contaminant in tree fruit is different from green vegetables because trees grow for many years and have highly developed root systems. Therefore, equilibrium partitioning is based on the

partitioning between wood and water. This value is calculated using the octanol-water partition coefficient, using this equation:

$$\log K_{wood} = -0.27 + 0.632 \log K_{ow} \quad (\#)$$

The concentration in the stem is calculated via the following equation:

$$C_{stem} = \frac{\left(\frac{C_s}{K_{sw}}\right) 0.756 e^{\frac{-(\log K_{ow} - 2.50)^2}{2.58}} \left(\frac{Q}{M}\right)}{\frac{Q}{K_{wood} M} + k_e + k_g} \quad (\#)$$

The concentration factor for the fruit is then calculated using the stem concentration, via the following equation:

$$CF_{tree\ fruit} = \frac{\left(M_f Q_{fruit} DM_{fruit}\right) \left(\frac{C_{stem}}{K_{wood}}\right)}{M_f C_s} \quad (\#)$$

Where

Variable	Description	Value	Units
$K_{wood}$	Wood-water partition coefficient	Eq. #	$\frac{mg/dw\ wood}{mg/cm^3\ water}$
$K_{ow}$	Octanol-water partition coefficient	Chemical parameter	unitless
$C_{stem}$	Chemical concentration in the woody stem	Eq. #	mg/g dw
$C_s$	Chemical concentration in the soil	User input	mg/g dw
$K_{sw}$	Total soil-water partition coefficient	Calculated from soil properties (Appendix 3)	cm <sup>3</sup> /g
Q	Transpiration stream flow rate	25,000,000	cm <sup>3</sup> /yr
M	Mass of the woody stem	50,000	g dw
$k_e$	Rate of chemical metabolism	0	1/yr
$k_g$	Rate of dilution due to wood growth	0.01	1/yr
$CF_{tree\ fruit}$	Concentration factor for tree fruit	Eq. #	$\frac{mg/g\ fw\ plant}{mg/g\ dw\ soil}$
$M_f$	Mass of the fruit	1	g fw
$Q_{fruit}$	Water flow rate per unit mass of fruit	20	cm <sup>3</sup> /g fw



$DM_{\text{fruit}}$	Fraction of dry matter for fruit	0.16	unitless
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Contaminant ingestion from fruit also includes soil loading, which is the ingestion of small soil particles found on the fruit (see Section II, E).

## **V. Conclusion**

Further study - more countries, outdoor soil dermal contact



Appendix 2. Detailed vegetable categories for each model.

Model	Produce Group	Crops
CLEA	Green vegetables	beans, brussels sprouts, cabbage and kale, cauliflower, lettuce, spinach, peas, stem vegetables (broccoli, celery, asparagus), okra, globe artichokes, Chinese leaves, endives, chicory, chard, dandelion, watercress, fresh herbs
	Root vegetables	beetroot, carrot, casava, garlic, ginger, jerusalem artichoke, leeks, onions, parsnips, radish, rhubarb, salsify, swede, sweet potato, turnips and yam
	Tubers	potatoes
	Herbaceous fruit	eggplant, zucchini, cucumber, marrow, pumpkin, strawberry, tomato
	Shrub fruit	bilberries, blackberries, cranberries, goosberries, loganberries, mulberries, ground cherries, raspberries, blackcurrants, redcurrants, whitcurrants
	Tree fruit	apples, apricots, cherries, peaches, pears, plums
S-Risk	Aboveground non-foliar	bulbous vegetables: onion, leek
		fruit vegetables: tomatoes, cucumber, paprika
		cabbages: cabbage, cauliflower, sprouts
		leguminous vegetables: beans, peas
		corn*
	Root vegetables	carrot, raddish, scorzonera
	Tubers	potatoes
Foliar/leafy vegetables	lettuce, Lamb's lettuce, endive, spinach, chicory, celery, grass*	
CSOIL	Aboveground vegetables	
	Underground vegetables	
	Potatoes**	
	Other vegetables**	

\*Grass and corn are included in S-Risk for modeling animal contaminant concentrations.

\*\*Potatoes and all other vegetables are used as vegetable categories only for metal contaminants in CSOIL.

Appendix 3. Equation for total soil-water partition coefficient  $K_{sw}$  (CLEA Report, p. 86)

$$K_{sw} = \frac{\theta_w + (K_d \rho_s) + (K_{aw} \theta_a)}{\rho_s}$$

Where:  $K_{sw}$  is the total soil- water partition coefficient,  $\text{cm}^3 \text{g}^{-1}$   
 $K_d$  is the sorbed soil-water partition coefficient,  $\text{cm}^3 \text{g}^{-1}$   
 $\theta_w$  is the water-filled soil porosity,  $\text{cm}^3 \text{cm}^{-3}$   
 $\theta_a$  is the air-filled soil porosity,  $\text{cm}^3 \text{cm}^{-3}$   
 $\rho_s$  is the dry soil bulk density,  $\text{g cm}^{-3}$   
 $K_{aw}$  is the air-water partition coefficient at ambient temperature,  $\text{cm}^3 \text{cm}^{-3}$

Appendix 4. Vegetable type-specific parameters for Belgium's S-Risk model.

plant	type	Q_transp (m <sup>3</sup> /m <sup>2</sup> /d)	a_growth (1/d)	L_plant (kg/kg)	f_CH (kg/kg)	t (days)	rho / rho_r (kg/m <sup>3</sup> )	V/V_r (m <sup>3</sup> /m <sup>2</sup> )	A (m <sup>2</sup> /m <sup>2</sup> )	Y_v (kg fw/m <sup>2</sup> )	dm (%)
Potato	tuber	n/a	0.139	0.0015	0.19	128	1020	0.0038	n/a	3.897	20
Carrot	root	0.000778	0.1	0.025	n/a	120	1020	0.0051	n/a	5.2	11
Raddish	root	0.001292	0.1	0.025	n/a	29	820	0.0024	n/a	2	5
Scorzoner	root	0.000271	0.1	0.025	n/a	120	1020	0.0025	n/a	2.5	9
Onion	aboveground non-foliar	0.001008	0.035	0.025	n/a	55	800	0.0043	5	3.4	11
Leek	aboveground non-foliar	0.001563	0.035	0.025	n/a	179	800	0.0046	5	3	13
Tomatoes	aboveground non-foliar	0.000658	0.035	0.025	n/a	150	800	0.0496	5	39.7	5
Cucumber	aboveground non-foliar	0.000658	0.035	0.025	n/a	150	800	0.0423	5	33.8	4
Paprika	aboveground non-foliar	0.000658	0.035	0.025	n/a	150	800	0.0203	5	16.2	9
Cabbage	aboveground non-foliar	0.000658	0.035	0.025	n/a	91	800	0.0069	5	5.5	8
Cauliflower	aboveground non-foliar	0.001	0.035	0.025	n/a	91	800	0.003	5	2.4	8.1
Sprout	aboveground non-foliar	0.000512	0.035	0.025	n/a	117	800	0.0023	5	1.8	17
Lettuce	foliar	0.001225	0.035	0.025	n/a	69	610	0.0072	5	4.4	4
Lamb's lettuce	foliar	0.000442	0.035	0.025	n/a	69	650	0.0015	5	1	4
Endive	foliar	0.000925	0.035	0.025	n/a	69	735	0.0068	5	5	6.2
Spinach	foliar	0.001225	0.035	0.025	n/a	69	630	0.0032	5	2	8

Chicory	foliar	0.000563	0.035	0.025	n/a	73	700	0.0021	5	1.5	6
Celery	foliar	0.000392	0.035	0.025	n/a	120	800	0.0079	5	6.3	8
Beans	aboveground non-foliar	0.000392	0.035	0.025	n/a	77	800	0.0031	5	2.5	11
Peas	aboveground non-foliar	0.000533	0.035	0.025	n/a	95	800	0.001	5	0.8	18
Grass	foliar	0.001563	0.035	0.025	n/a	30	820	0.002	5	5.93	35
Corn	aboveground non-foliar	0.0012	0.035	0.054	n/a	183	800	0.0057	5	4.53	25

Appendix 5. Dry weight conversion factor (dm).

CLEA		Belgium Flanders			CSOIL	
Plant Type	dm (% weight)	Plant	Type	dm (%)	Plant Type	dm (fraction)
Green vegetables	9.6	Potato	tuber	20	leafy vegetables	0.098
Beans	13.1	Carrot	root	11	root vegetables	0.167
Cabbage and kale	10.5	Raddish	root	5		
Cauliflower	7.6	Scorzoner	root	9		
Lettuce	4	Onion	aboveground non-foliar	11		
Spinach	6.3	Leek	aboveground non-foliar	13		
Peas	17.8	Tomatoes	aboveground non-foliar	5		
Fresh herbs	11.3	Cucumber	aboveground non-foliar	4		
Other fresh green vegetables (including okra and endives)	8	Paprika	aboveground non-foliar	9		
Stem vegetables (including broccoli, celery, and asparagus)	7.9	Cabbage	aboveground non-foliar	8		
		Cauliflower	aboveground non-foliar	8.1		
Root Vegetables	10.3	Sprout	aboveground non-foliar	17		
Carrot	9.7	Lettuce	foliar	4		
Fresh turnips and swede	9.4	Lamb's lettuce	foliar	4		
Fresh onions and leeks	9.7	Endive	foliar	6.2		
Fresh rhubarb	8.7	Spinach	foliar	8		
Other (including beetroot, parsnip, radish, Jerusalem artichoke)	13.8	Chicory	foliar	6		
		Celery	foliar	8		
Tuber vegetables	21	Beans	aboveground non-foliar	11		
Potato	21	Peas	aboveground non-foliar	18		
		Grass	foliar	35		
Herbaceous fruit	5.8	Corn	aboveground	25		

			non-foliar			
Cucumber	4					
Marrow, courgettes, aubergine, and pumpkin	5.8					
Tomato	5.3					
Other fruit (strawberries)	8					
Shrub fruit	16.6					
Other soft fruit (including blackcurrant, gooseberry, raspberry)	16.6					
Tree fruit	15.7					
Fresh apples	16					
Fresh pears	16					
Fresh stone fruit (including apricots, cherries, peaches, and plums)	15					