SPSD II

CHAIN MODEL FOR THE IMPACT ANALYSIS OF CONTAMINANTS IN PRIMARY FOOD PRODUCTS

P. SEUNTJENS, W. STEURBAUT, J. VANGRONSVELD

PART 1

SUSTAINABLE PRODUCTION AND CONSUMPTION PATTERNS

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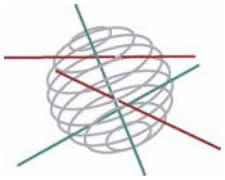
SCIENTIFIC SUPPORT PLAN FOR A SUSTAINABLE DEVELOPMENT POLICY
(SPSD II)



Part 1:
Sustainable production and consumption patterns

FINAL REPORT

CHAIN MODEL FOR THE IMPACT ANALYSIS OF CONTAMINANTS IN PRIMARY FOOD PRODUCTS

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TABLE OF CONTENTS

LIST OF TABLES

LIST OF FIGURES

1 PROJECT TITLE

The title of the project is “Chain model for the impact analysis of contaminants in primary food products”.

2 INTRODUCTION

2.1 Context and summary

Food safety is one of the major issues on the Agenda of the European Commission and the Belgian government. Incidents like the dioxin- and BSE-crisis lead to important economic losses and to concern about the protection of public health through the food chain. At the European level, the White Paper on Food Safety (EC, 2000) was published, including the organisation of a European Food Authority which defines priorities for research and regulation. At the Belgian level, the Federal Agency of Food Safety was established. Following these initiatives, regulatory initiatives for setting limits on contaminants in human and animal food products are accelerated (EC, 2001a; EC, 2001b; EC, 2002). The Belgian Food Safety Agency is well aware that risk assessment strategies and models are essential for the construction of a food safety policy.

Existing instruments such as LCA and HACCP are primarily concerned with environmental impact, quality control and risk-assessment in the production and distribution part of the food chain, i.e., after the products have left the farm (post-farm gate). Quality control and risk evaluation of the food chain starting from the farm to the primary food products (pre-farm gate) is gaining importance. This is clearly acknowledged by the food processing industries and the retailers (see e.g., EUREPGAP, GFSI initiatives).

An integrated instrument that calculates transfer of contaminants from the inlet of the farm to primary food products (crops, cereals, meat, eggs, milk), and that assesses impacts of contaminated primary food products on public health is urgently needed. Currently, no generic modeling tools are available that predict the impact of contaminants in the environment to the primary food chain.

In this project, an integrated model tool called XtraFOOD (Xenobiotics transfer in the primary FOOD chain) was developed that calculates transfer of contaminants in the primary food chain. The transfer model was coupled to historical food consumption data to estimate human exposure to contaminated food products. The model is illustrated for various contaminants. This report summarizes the research activities and the results of the project.

2.2 Objectives

The main objectives of the research project were:

- to develop a generic model for the calculation of contaminant transfer in the agro-ecosystem to primary food products
- to develop a methodology for the impact analysis of contaminated primary food products
- to couple the transfer and the impact analysis modules in an integrated model environment
- to demonstrate the integrated model for three typical food contaminants (cadmium, dioxins, pesticides)
- to evaluate the model against experimental data

2.3 Expected outcome

The expected outcome of the project was an integrated model for contaminant transfer and impact in the production chain of primary food products.

Specific model outputs are:

- a quantitative estimation of the impact of diffuse, local or incidental contamination in the environment on the quality of primary food products, and on human health (and related costs)
- a quantitative estimation of impacts of changes in farming practices on the quality of primary food products, and on human health (and related costs)
- indication of locations where safe food may no longer be guaranteed due to (historical)

environmental contamination
- a definition of critical points in the primary food chain based on a sensitivity analysis of the integrated model

The added value of the research project is the coupling between various numerical model approaches of contaminant transfer, human exposure and human health impact (i.e., transfer in the agro-ecosystem to primary food products, redistribution, impact on human health and related costs). To estimate impacts of changing boundary conditions (i.e. farming practices, local emissions, …) a dynamic model (time-varying) formulation will be adopted. Uncertainty and variation in the model variables will be incorporated in the model calculations.

The model is illustrated by three selected demonstration cases. In the demonstration phase, calculations are compared to measured concentrations in food products. Doing so, confidence in the model results is built.

3 GENERAL OVERVIEW OF THE SCIENTIFIC METHODOLOGY

The development of XtraFOOD consisted of the following tasks:

Task A: development of a model for contaminant transfer in the agro-ecosystem
- Subtask A.1: transfer in soil/plant/atmosphere continuum
- Subtask A.2: transfer to primary food products

Task B: development of an impact analysis model
- Subtask B.1: exposure modeling and health risk analysis
- Subtask B.2: external cost modeling

Task C: computer programming of the integrated model XtraFOOD: linking the modules on transfer and impact; linking models to databases including testing of the code
- Subtask C.1: linking soil/plant/atmosphere modules
- Subtask C.2: linking plant/cattle modules
- Subtask C.3: linking transfer/impact modules
- Subtask C.4: linking calculation models to databases

Task D: demonstration and evaluation of XtraFOOD
- Subtask D.1: development of databases
- Subtask D.2: heavy metals
- Subtask D.3: pesticides
- Subtask D.4: dioxins

The role of the respective network partners in the project is specified in Table 1.

Table 1: General overview of the research activities

Task	Description	Project Partner
A	transfer in soil-plant-atmosphere continuum transfer to primary food products: - atmosphere – crop modeling - soil - crop modeling - pesticide residue modeling	VITO VITO UH[1] UG
B	human exposure and risk analysis	VITO
C	programming XtraFOOD	VITO
D	demonstration and evaluation of XtraFood	VITO-UH-UG

[1] UH, University of Hasselt, formerly known as LUC (Limburg University Centre)

Figure 1 illustrates the adopted scientific methodology. In task A, the agro-ecosystem model was built, including transfers to crops and animals. In task B, the food consumption data were compiled, food consumption scenarios were chosen and criteria for risk assessment were established. In task C, the agro-ecosystem model was coupled to the food consumption data within a database-oriented software application (SQL). Calculations with XtraFOOD were performed in task D for the demonstration cases.

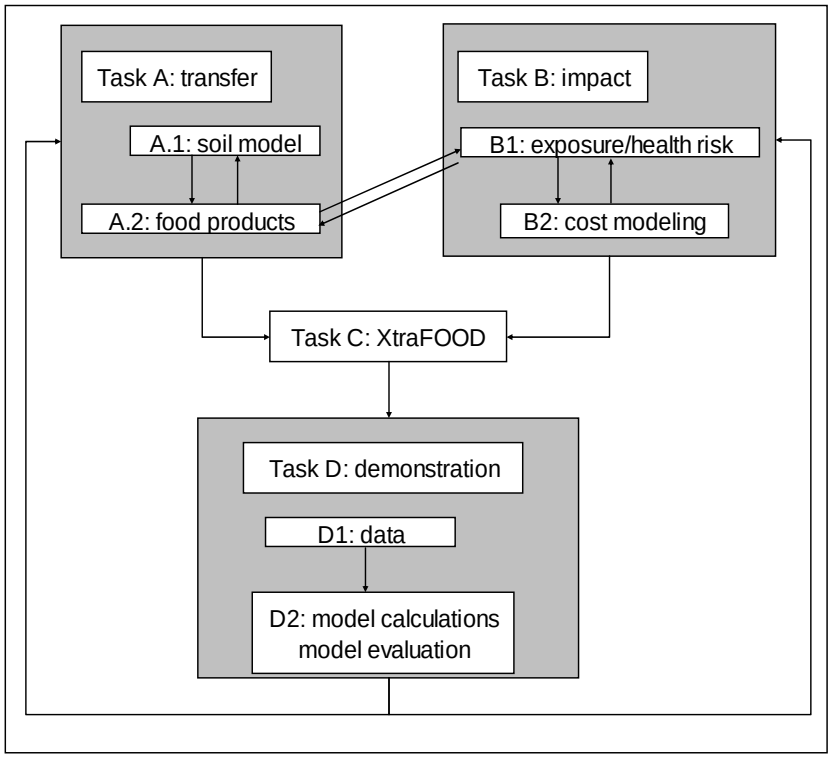


Figure 1: Overview of the scientific methodology

4 TRANSFER AND EXPOSURE MODEL FOR FOOD CONTAMINANTS

4.1 Model components

4.1.1 Transfer part

Figure 2 shows the various possible transfers of contaminants in a model agro-ecosystem. Contaminants are transferred either directly or indirectly to the food products. Chemicals can enter the agro-ecosystem via the soil through irrigation, (wet and dry) atmospheric deposition or the application of fertilisers. Contaminants can be deposited either directly on the soil or on the aboveground parts of the crop. The application of plant protection products is a direct input term for pesticides to soil or crops. Contaminants can also enter the farm through the import of animal manure or through feed supplies. Contaminants can leave the agro-ecosystem via the soil through volatilisation to the atmosphere, run-off to surface water or leaching to groundwater, or they can be degraded in the soil. Contaminants can leave the agro-ecosystem by exporting animal manure as waste, and by exporting cattle and/or crops as food products. Internal flows are plant uptake (soil->plant) and cattle intake (soil->plant->cattle or soil->cattle). Indirect transfer of contaminants to food products thus partly occurs via the soil system. Crops are closely connected to the soil by their root system, extracting water and nutrients (or contaminants). Cattle ingests plants growing in the soil and soil particles. Modeling the transfer of contaminants in soils of agro-ecosystems therefore is indispensable for the impact analysis. Examples of contaminant transfer modeling in agro-ecosystems can be found in Welsch-Pausch and McLachlan (1998), McLachlan (1997), Harrad and Smith (1997), Fiedler et al. (2000), Keller (2000) and Molenaar (1998).

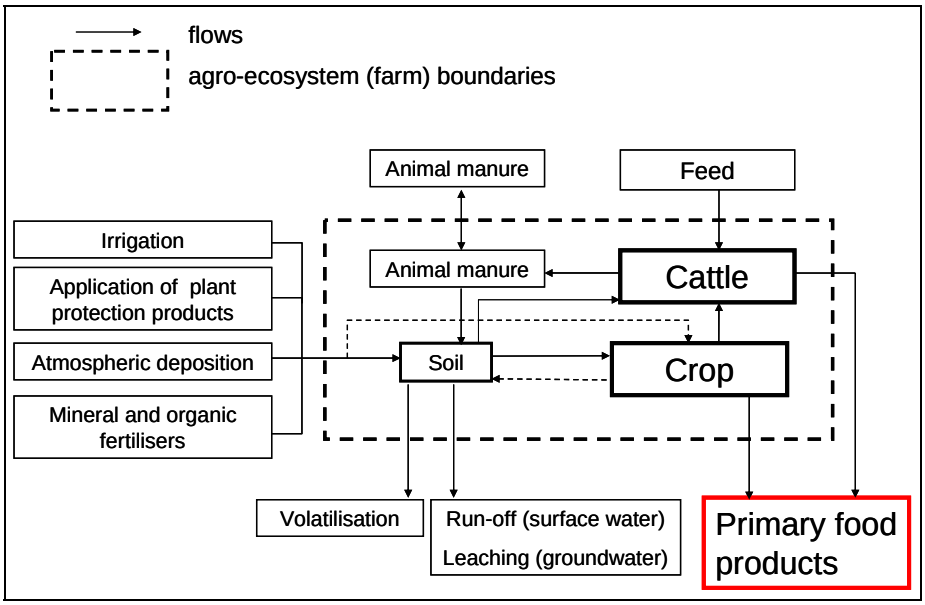


Figure 2: Overview of contaminant flows in the agro-ecosystem to the food chain

4.1.2 Exposure part

The lower part of Figure 3 illustrates the link between contamination level of farm-related foods (crops and animal parts) and human exposure to chemicals via the food intake pathway. A crucial factor here is the assessment of food intake by humans. Detailed food records are necessary in order to match the detail level of contaminant concentrations in crop or animal product calculated in the biological transfer part. For example, vegetables consumption should be reported at vegetable species

level since also transfer (and thus concentration) is calculated at the species level. Contaminant concentrations can be reduced by food preparation such as frying, boiling, peeling and washing (De Temmerman, 1999; Alberti-Fidanza *et al.,*2002; Hori *et al.,*2005). Contaminant fluxes from primary food products to processed food need also to be accounted for weight changes by shrinkage/expansion. Another aspect here is the splitting composed foods into different primary food products.

From a toxicological point of view, cumulative lifetime exposure should be evaluated for (chronic) risk of some chemicals. Hereto, food records for different age/gender categories are needed. An important aspect in risk assessment is the risk for highly-exposed subpopulations. Statistical distribution of food intake in these food records (average, median, 5th, 25th, 75th and 95th percentile consumptions) allow the risk assessment of specific subpopulations.
If we want to estimate the health risks and get insight in the importance of the food exposure pathway associated with the exposure from a certain contaminant, it is necessary to address also exposure from other relevant pathways such as inhalation exposure, oral exposure like from dust, dermal exposure.

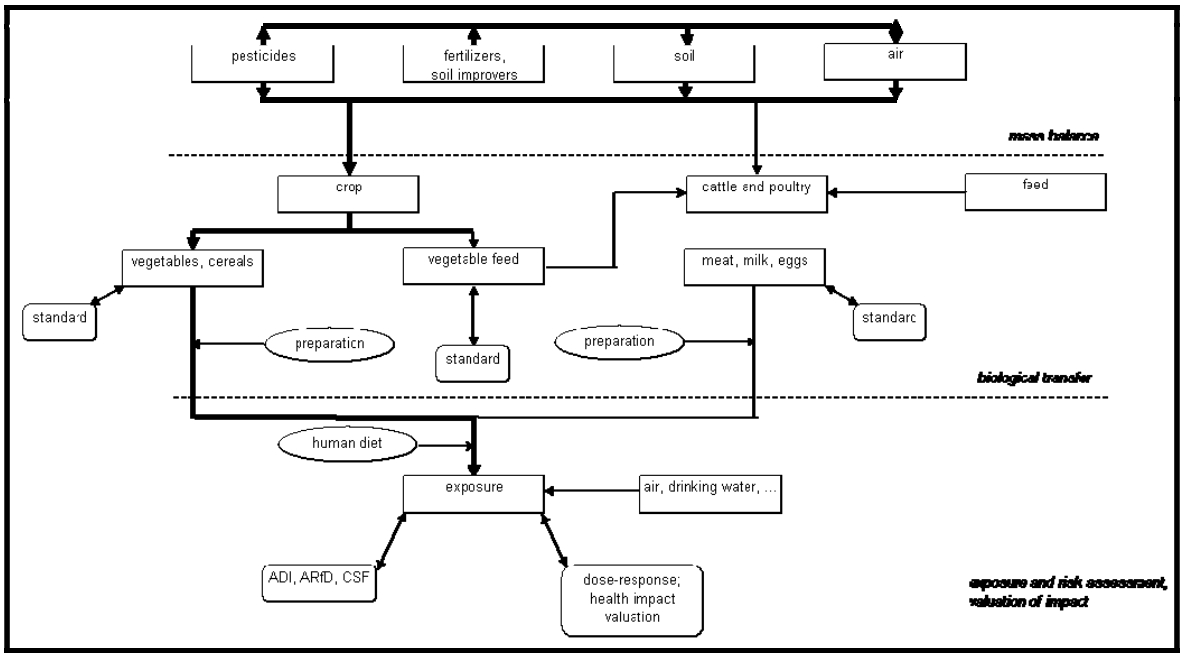


Figure 3: Human exposure routes of contaminated food products

4.2 Transfer in soil

4.2.1 Literature review and selection of mass-balance model

Existing models of contaminant transfer in soils were reviewed and evaluated for use in the food chain model. A wealth of models exist for describing contaminant behaviour and transport in soils. They vary in complexity in describing the various transfer processes from purely mechanistic white-box to empirical black-box (transfer function) models. At the highest level of complexity, purely mechanistic models may be suitable for modeling and explaining various micro-scale processes (e.g., geochemical models describing chemical reactions at the molecular level, root models describing microscopic uptake processes), but are not widely used to large-scale problems or exposure modeling. At the next level of complexity, process-based models include mathematical descriptions of processes with lumped variables, which can be measured relatively easily in the lab or the field. Examples of these are models describing water flow and solute transport in the soil-plant-atmosphere continuum (e.g., HYDRUS (Simunek et al., 1999); Macro (Jarvis, 2001); SWAP (Kroes et al., 1999); PEARL (Leistra

et al., 2001); WAVE (Vanclooster et al., 1996)). They have been mainly implemented in calculating contaminant or pesticide leaching to groundwater, or in nutrient management of agro-ecosystems.

At a third lower level of complexity, transfer of contaminants is modeled using simple black box models with transfer factors or transfer functions representing the soil system. This type of models is frequently used in dynamic exposure assessment of contaminants (Vissenberg and van Grinsven, 1995; CalTOX, 1993; Mackay, 2001). They are suitable for persistent, non- or semi-volatile, and less mobile contaminants accumulating in the food chain.

For the purpose of XtraFOOD, a simple first-order model, based on the model description of Vissenberg and van Grinsven (1995), was selected to calculate soil contaminant concentrations. The mathematical description of the soil model is given in Annex.

4.3 Transfer from the environment to primary food products

4.3.1 Atmosphere-plant transfer

4.3.1.1 Literature review and selection of the atmosphere–plant transfer model

The direct transfer of contaminants from air-to-plant(-to-animal) has been the subject of numerous modelling efforts. Uptake of airborne contaminants by plant foliage can occur by both dry gaseous deposition and particle-bound deposition (wet and dry). Figure 4 gives a schematic overview of different air-to-plant transfer modelling approaches.

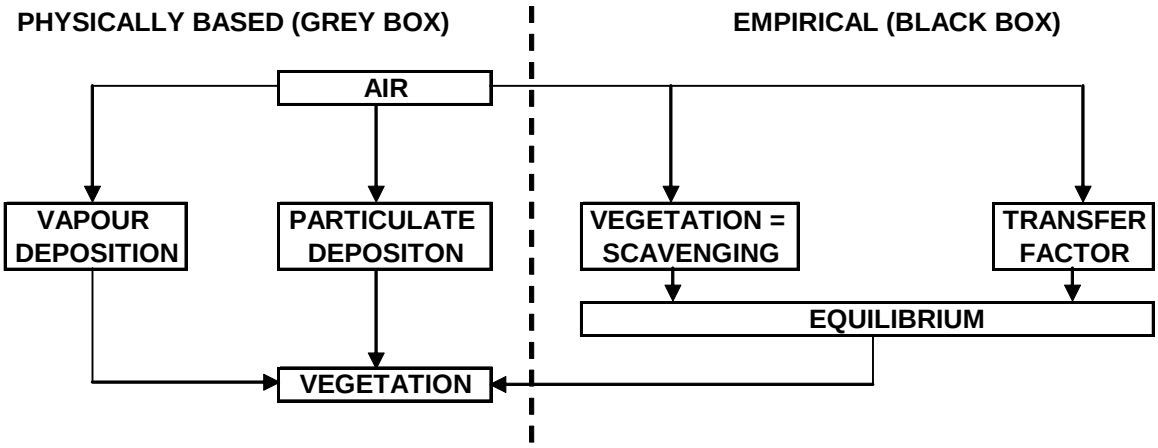


Figure 4: Schematic overview of different air-to-plant transfer modelling approaches.

McLachlan et al. (1999) developed a kinetic physically-based model for hydrophobic chemicals. The model assumes that the uptake of organic contaminants is related to the octanol-air partition coefficient (K_{OA}).

The atmosphere – crop model in XtraFOOD includes dry gaseous (kinetic) deposition of chemicals present in the gas phase, dry and wet (kinetic) particle deposition according to the McLachlan framework. The model accounts for three types of data availability:

- only data on total concentrations in air are available: then the model calculates partitioning of chemicals between gas and particle phase, and subsequently crop concentrations due to deposition of both phases;
- data on gas phase and particulate phase concentrations in air are available; the model directly calculates concentrations in crops due to deposition of both phases;

- data on dry and wet deposition are available; the model calculates crop concentrations due to wet and dry deposition.

The mathematical description of the atmosphere-crop model is given in Annex. In XtraFOOD, the vapour deposition term is included as a source term in the plant model itself (PlantX, see further).

For heavy metals, particle deposition is assumed to be the only relevant air-plant transfer route, such that only the particle deposition term is included.

4.3.1.2 Validation of model calculations

Data from McLachlan (1996) were used to validate the air-plant pathway. Coupled data were available on congener concentrations of PCDD/PCDFs in air (both gaseous and particle concentrations), soil, pasture, and milk. Pasture concentrations were predicted with XtraFOOD using air concentrations and chemical properties of the various congeners. The results are displayed in Figure 5 (symbols are individual congeners). The results show that concentrations in pasture are overpredicted by the model by a factor 3 in case a pasture growing period of 105 days is assumed. Overprediction is reduced to a factor 2 when a pasture growing period of 30 days is taken. Since predictions were made using default chemical and plant parameters and only varying the growing period, the results were satisfying.

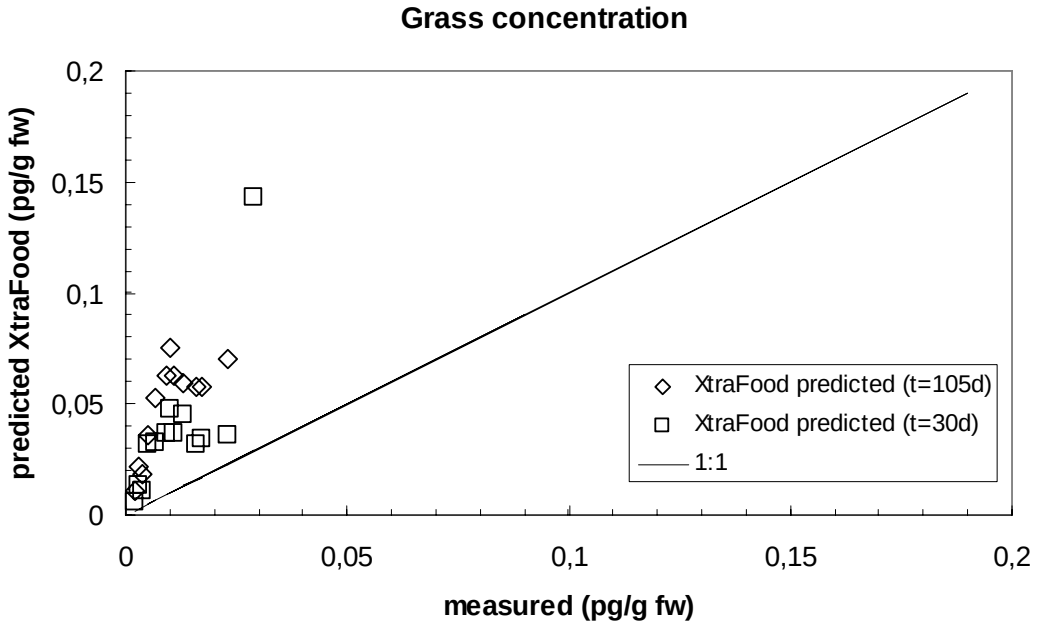


Figure 5: Measured grass PCDD/PCDF congener concentrations versus concentrations predicted by XtraFood

4.3.2 Soil – crop transfer

4.3.2.1 Literature review and selection of the soil-crop model

Organic chemicals

The fate of organic pollutants in soil is complex and determines the bio-concentration of organic pollutants in plants. Also plant-specific mechanisms can alter plant-concentrations of organic chemicals. The harm caused by the organic chemicals to organisms depends on their toxicity and their fate in the environment. Their fate is determined by their molecular, chemical and physical characteristics and by the soil properties and conditions. Chemical and physical properties of compounds are function of the type of their chemical bounds, nature of their functional chemical

groups, molecular weight, spatial structure of their molecules.

A variety of models is available for predicting the uptake, translocations, elimination and bioaccumulation of organic chemicals in plants. Recently, Collins and Fryer (2003) performed a model intercomparison for the uptake for organic chemicals by plants. They concluded that dynamic models perform better for acute exposure. Regression based and equilibrium models perform well in estimating chronic exposure.

An equilibrium approach is mostly used to estimate chemical uptake from soil into root vegetables. The performance of this type of model is good for soil uptake (Collins and Fryer 2003). In recent years some dynamic models have become available to model root uptake for e.g. neutral lipophilic organics or neutral and ionisable organic compounds (Trapp 2000, 2002).

Each method or model has its own range of applicability and its own restrictions. Regressions used in the assessment of indirect human exposure have a common regression range from log K_{ow} 3.0-4.6. Most models are compartment models, which do not consider a spatial distribution of the chemical, and were originally developed for non-dissociating, lipophilic persistent chemicals with measurable vapor pressure. Taking this into account, most models are only applicable for a minority of chemical classes. Less acurate results will be obtained with dissociating compounds, ions, polar and very non-polar compounds. Also effects of mixtures cannot be investigated, except for hydrocarbons. Using the example of plant uptake, it is shown that in certain cases uptake is underestimated by the model due to processes not considered.

The selected model in XtraFOOD for uptake of organic chemicals from soil is the PlantX model (Trapp and Matthies, 1995) (see Annex for detailed model formulation). The model has been validated for non-ionic organic chemicals and has been extensively applied in risk assessment modeling (TGD, EUSES).

Heavy metals
The transfer of heavy metals to plants and crops is modeled using bioconcentration factors (BCF), i.e., measured concentrations in paired soil and crop samples. The BCF of metals is variable and influenced by plant and soil factors. Plant species, cultivar and plant organ are important plant dependent factors. Soil type, pH, organic matter content and total metal concentration are important soil related factors.

For the calculation of the models several studies were used:
1. (Z1) Cadmibel-study (1985-1989).
2. (Z2) 'Saneringsonderzoek van met zware metalen gecontamineerde tuinen in Noord-Limburg' (study ordered by OVAM, 1996).
3. (Z3) Own data (LUC) collected in the 90^{ties} in the province of Limburg.
4. (Z4) 'Afweging van de risico's tot transfer van metalen in de voedselketen: studie van de overdracht via landbouwgewassen geteeld in de onmiddelijke omgeving van vroegere zinkfabrieken (study ordered by OVAM, 2001)
5. (L1) A study of polluted kitchen gardens in Flanders (the owner of the study asked not to give more specifications)
6. (L2) Reports of IWONL projects with convention numbers. D1/4-4701/4620 A (1985), D1/4-4736/5031 A (1987), D1/4-5378/5297 A (1989), D1/4-4228/5428 A (1991) by 'Laboratorium voor Analytische Agrochemie (Rijksuniversiteit Gent)', Prof. Dr. Ir. A Cottenie and Prof. Dr. Ir. M. Verloo.

Due to the limited number of Flemish data on heavier soil types also a French study (source n° 7) was used providing data from soils polluted by non ferro activities in the North of France. These data can be added to the Flemish data because of similarities in soil type and climate.

7 (L3) Etude d'un secteur pollué par les métaux. 1ère partie. Volume III: Qualité des productions végétale. Programme de recherches concertées. Environnement et Acivités humaines. Rapport de la

deuxième phase: 1996-1997 (Ministère de l' Enseignement Supérieur et de la Recherche + Region Nord Pas de Calais + FEDER).

In 2006, the dataset was further updated based on the recent report 'Teeltadvies voor de landbouw in kader van het Interreg project BeNeKempen : Tussentijds verslag: opmaak van een teeltadvies op korte termijn op basis van verschillende datasets , Maart 2006.' (Gunilla Jansson (KULeuven) , Ann Ruttens (Universiteit Hasselt), Paul Römkens (Alterra, Nederland) en Erik Smolders (KULeuven)).

8 Dataset of the Wageningen University and Alterra
9 Dataset of CODA (Min. of agriculture)
10 Dataset of the Belgische Bodemkundige dienst

In this approach models were developed for assessment of the BCF taking into account the plant species (crops, feed), metal concentration in the soil and soil pH. Because not all variables can be included in the model, some variation in the model will be present. Because several datasets were used in the model calculations, the variation in the model reflects the variation caused by other factors not included in the model.

The resulting regression models for bioconcentration factors are given below, using crop specific parameters given in Table 2.

$$\log BCF = a + b \times soil\ pH + c \times \log soil\ Cd$$

Table 2: crop specific parameters for BCF (bioconcentration factor) models

crop	model parameters		
	a	b	c
potatoes	-0,5	-0,05	-0,73
endives	1,99	-0,32	-0,42
cumcumber	-0,86		-0,26
leek	1,18	-0,25	-0,42
french beans	0,43	-0,34	0,24
scorzonera	1,4	-0,32	-0,58
celery	1,07	-0,13	-0,43
lettuce	1,06	-0,14	-0,4
spinach	0,53	-0,06	-0,37
tomatoes	-0,16	-0,06	-0,66
carrots	0,43	-0,12	-0,51

For crops that were not included in the above mentioned datasets, bioconcentration models based on studied performed under similar climatic conditions were used. For example, the BCFs for wheat and barley used in Xtrafood originate from a soil Cd/grain Cd survey in the U.K. (Adams *et al.,* 2004). However, BCFs for some crops were still lacking. We assigned BCFs to these crops based on known BCFs of plants with similar plant physiological properties. Crops that were not included in Table 2 and for which no BCF models were found in a literature survey were assigned BCFs of plant with similar plant physiological properties, or proportionality factors were used according to the methodology applied in the derivation of soil cleanup guidelines for Flanders (Bierkens et al., 2006).

4.3.3 Transfer to animal products

4.3.3.1 Literature review and selection of the cattle model

"Cattle models" include models that calculate contaminant transfer to various animal products, i.e. milk, meat, eggs, organs (liver, kidneys, …). In general, two types of models can describe transfer in cattle: steady state and biokinetic (transient) models (Sweetman et al., 1999). Most exposure models assume steady-state, i.e. the transfer within the animal is fast as compared to transfers in the environment. Feeding studies have shown that the half-life of many persistent organic compounds in milk is about 40-60 days (Olling et al., 1991). Experiments with nonlactating cows show half-lifes of 100-200 days (Richter and McLachlan, 2001). Under normal agricultural conditions of a constant feed for several weeks to months, the steady-state assumption may be valid. In case of incidents with a short release of a large amount of contaminant, kinetic models with a time scale of about 1 day will be necessary to adequately predict the concentration in the animal tissues. Other factors determining whether an animal is in steady-state, are farming practice and lactation state of the cow.

Steady-state models
In case steady-state is valid, transfer can be calculated using transfer factors assuming equilibrium between contaminant sources (soil, water, grass, silage, supplement) and animal products. The most commonly used steady-state models for the prediction of concentrations in animal products are bioconcentration factors and biotransfer factors (Stevens, 1991;1992; McLachlan, 1992; Sweetman et al., 1999). The bioconcentration factor (BCF) is defined as the ratio between the contaminant concentration in the animal tissue of interest and the concentration in the contaminant source (grass, silage, supplement …). The biotransfer factor (BTF) is defined as the ratio between the contaminant concentration in the animal tissue of interest and the contaminant intake flux. Both factors are related through:

$$BTF = \frac{BCF}{q}$$

where q is the feed intake rate (kg d^{-1}).

A specific transfer factor is the carry-over rate (COR). The dimensionless COR is defined as the ratio between the contaminant flux in the animal product and the contaminant flux in the feed. The assumed advantage of a COR over a BCF or BTF is that it takes into account both feed intake and product output and therefore is less prone to variation and uncertainty. Thomas et al. (1999) found a relative standard deviation in COR values of 17-35% between five cows in a controlled feeding experiment. The same authors (Thomas et al., 1998) showed however that variation in BCFs and CORs in a farm survey study in NW-England was similar. BCFs, and to a lesser extent BTFs, are believed to be more variable because variations in input (grass intake) and/or output fluxes (milk production) are not accounted for.

In literature, various relationships between transfer factors and properties of the chemicals were established. A notable example is the work of Travis and Arms (1988), relating the BCF of organic compounds to the n-octanol/water partition coefficient K_{ow} (implemented in EUSES, 1997):

$$\log BCF_{meat} = -7.6 + \log K_{ow}$$

$$\log BCF_{milk} = -8.1 + \log K_{ow}$$

The relationship is valid for compounds with log K_{ow} values between 3 and 6.5. Eq. 9 suggests that transfer to milk is directly related to lipophilicity of the compound. Based on a fugacity-based three-compartiment model for lactating cows, McLachlan (1994) derived relationships between the maximum fraction absorbed E_M (for labile contaminants) and K_{ow}, and between the fraction absorbed E_o (for persistent contaminants showing no transformation or metabolisation) and K_{ow}:

$$\frac{1}{E_M} = 1.2 + 2.875e-8 \cdot K_{ow}$$

$$\frac{1}{E_o} = 1.283 + 2.875e-8 \cdot K_{ow}$$

The parameters of Eq. 10 were obtained by fitting the model to data of a mass-balance study of a lactating 4-year-old Simmenthal cow. For persistent compounds, the fraction absorbed E_o is equivalent to the carry-over rate. Eq. 9 implies that the carry-over rate of persistent organic contaminants is independent of K_{ow} over a broad range. For very hydrophobic compounds such as PCDD and TCDD-congeners (log K_{ow} 6-8) the COR decreases with K_{ow}. This means that the approach of Travis and Arms (1988) is not valid for very hydrophobic compounds. An overview of BCFs, BTFs and CORs for organic contaminants is given in the Annex, together with a detailed discussion of biotransfer of heavy metals.

A steady state model predicting transfer from feed or soil to animal products was selected for use in XtraFood. For the transfer of heavy metals to milk, muscle, liver and kidney, a biotransfer factor is used that relates the metal intake flux to animal product concentration (see Annex for formulation). The selection of the appropriate biotransfer factor is made based on an extensive literature search.

For organic contaminants such as dioxins the measured bioconcentration factor is used in XtraFood to calculate muscle, liver, kidney concentrations from concentrations in the feed. For other contaminants in the appropriate Kow range, the Travis and Arms equations were used. Concentrations in egg fat of foraging chickens is calculated from concentrations in soil (see Annex for mathematical model description). Concentrations of dioxins in milk is calculated using the carry-over-rates.

Biokinetic (dynamic) models
Under certain circumstances, the steady-state assumption may not be valid, e.g., for transfers in cows that take longer times than the time of exposure (as might be the case in nonlactating cows) or in case the exposure changes rapidly in time (incidents, sudden changes in emission rates). To account for this status of nonequilibrium, dynamic models have been developed. McLachlan (1994) presented a fugacity-based model consisting of three compartments, i.e. the gastro-intestinal tract, blood and fat deposits. Data from a PCB clearance experiment were used to parametrise the model. Freijer et al. (1999), based on earlier work of Olling et al. (1991; 1995), presented their Physiologically Based PharmacoKinetic (PBPK) model for lipophilic contaminants in domestic animals. The model was parametrised using concentration data of an injection experiment of 2378-TCDD into the rumen of lactating and nonlactating cows. Concentration measurements were used to estimate the initial body burden and the daily absorption.

An alternative model was programmed in XtraFood that describes non-steady state concentrations in milk fat, muscle tissue and egg fat (see Annex for formulation). The model assumes first-order kinetics and depends on the rate constants, available from feeding experiments where uptake and clearance of contaminants is monitored.

4.3.3.2 Validation of model calculations

The same dataset from McLachlan (1996) that was used for calculating pasture concentrations, was used to evaluate XtraFood predictions for milk concentrations of TCDD/TCDF congeners. Assuming a grass growing period of 30 days instead of 105 days decreased the calculated WHO-TEQ by 0.7 pg g^{-1} fat. The predictions somewhat overpredicted the measured concentrations in milk fat, but the results are satisfactory. The model predicts the trend in individual congener concentrations well.

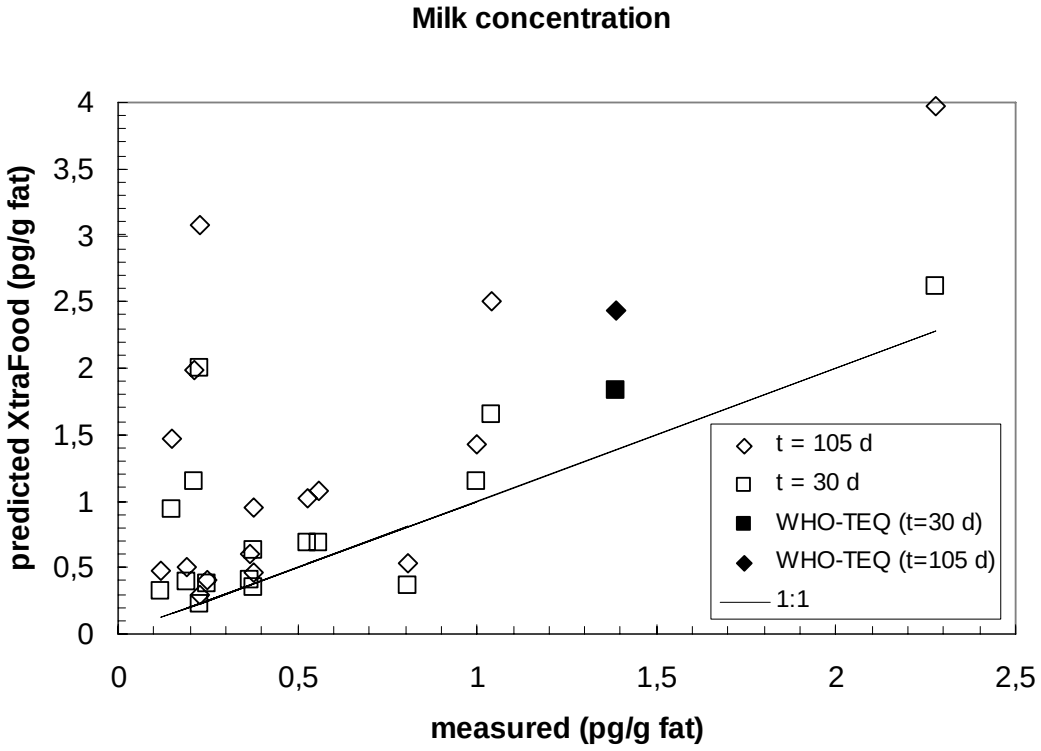


Figure 6: Measured PCDD/PCDF congener concentrations versus congener concentrations predicted by XtraFood

4.3.4 Pesticide residue modeling

4.3.4.1 Selection of relevant pesticides

In the frame of the project a selection of 19 pesticides was made, based on their physico-chemical and (eco)toxicological properties and on their sales figure. A further refinement has been made, taking into account the moment of application, the formulation type, the mode of action of the pesticide and the different cultures in which the pesticide can be applied. This refinement is necessary because in some cases, modelling the fate of pesticide residues on the leaf/fruit is not relevant. In Table 3, an overview is given of the use of the 19 pesticides. Since the final purpose of the pesticide model is the prediction of residues on fruit and vegetables after pesticide application and the possible impact on human health, a further pesticide selection can be made.

Table 3: Application details of the 19 selected pesticides

Active substance	***Type***	***Formulation***	***Moment of application***	***Crop***
amitrol	herbicide	liquid	-	apple, pear
atrazin	*No recognition in Belgium*			
benfluralin	herbicide	liquid	before sowing	scorzonera, lettuce, endive, chicory, bean, pea, succory
chloorpyrifos	insecticide	granule	when necessary	strawberry, broccoli, cauliflower, Brussels sprouts, cabbage, kohlrabi
cypermethrin	insecticide	liquid	when necessary	scorzonera, broccoli, cauliflower, cabbage, potato
dichlobenil	herbicide	granule	before sprouting	red/white/black currants, fruit trees
dimethoate	insecticide	liquid	when necessary(except: asparagus: after harvest)	(black) cherry, carrot, onion, shallot, cabbage, chicory, asparagus, potato
diuron	*No recognition for agricultural use in Belgium*			
endosulfan	*No recognition in Belgium (except for ornamentals in greenhouse)*			
fenarimol	fungicide	liquid	when necessary (every 7 days)	strawberry, currants, cucumber
fentinhydroxide	*No recognition in Belgium*			
fluazinam	fungicide	liquid	when necessary (every 10 days)	onion, shallot, potato
imidacloprid	insecticide	liquid	1 after flowering and 1 after harvest	apple, currants
lambda-cyhalothrin	insecticide	liquid	when necessary	apple, pear, (black) cherry, strawberry, blackberry, raspberry, red beet, carrot, celeriac, radish, scorzonera, kohlrabi, turnip, gherkin, courgette, broccoli, cauliflower, cabbage, lettuce, endive, spinach, celery, bean, pea, potato
		wettable granules	when necessary	apple, pear, (black) cherry, prune, celery, radish, scorzonera, gherkin, pea, potato
lenacil	herbicide	wettable powder	before sowing	spinach
lindane	*No recognition in Belgium*			
linuron	herbicide	liquid	before rising or during the first leaf stages	fruit trees, carrot, celery, pastinake, chervil, parsley, bean, pea, asparagus, celery, fennel, potato
prosulfocarb	herbicide	liquid	before rising	potato
triticonazole	*No recognition in Belgium (except for seed treatment)*			

Remark: Data source www.fytoweb.be (Pesticide database of the Belgian government)

The following restrictions are set:

- Pesticides which do not have a recognition in Belgium any more, are not relevant for further calculations and/or case studies
- Pesticides, formulated as granules, are supposed to reach the ground. No residues will be found on the leaf or fruit.

Pesticide treatments before sowing/rising or after harvest are not relevant for the model calculations, since they will not cause any direct risk for human health.

Putting those restrictions, includes that, in stead of 19 relevant pesticides, the selection will be refined to 8 relevant pesticides: amitrol, cypermethrin, dimethoate, fenarimol, fluazinam, imidacloprid, lambda-cyhalothrin and linuron.

Further pesticide residue calculations will be based on those active substances.

4.3.4.2 Review of modeling approaches and selection of the model

The task of Ghent University in the project was modelling the residues on leafs and fruits after pesticide application. This does not include the uptake of residues by roots and transport through the plant. The fate of pesticide residues depends upon different processes, which are shown in Figure 7.

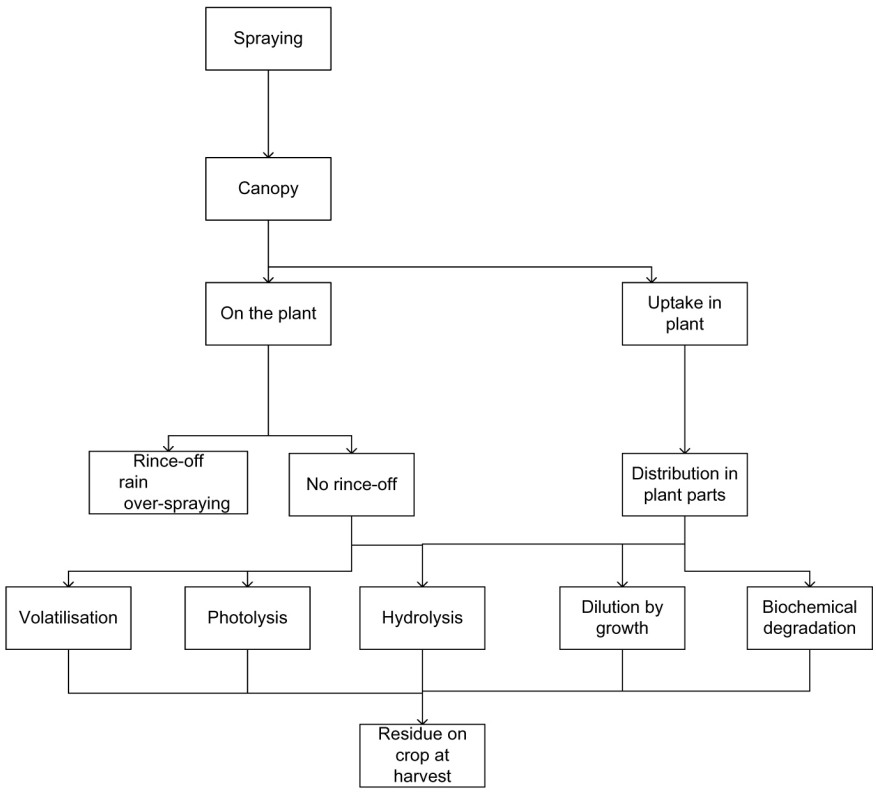


Figure 7: Fate of pesticide residues after spray application

A first-order kinetic model, based on the initial dose on the plant after application, has been selected, taking into account multiple applications during the growth season. (See Annex for formularium).
The following parameters are needed for the calculation of the concentration of residues in fruit/vegetables at harvest: C_0 (initial concentration), k (degradation factor), i (interval between two applications), n (number of applications) and t (time between the last application and harvest).

The degradation factor (k)

The degradation factor (k) is the pesticide outflux, depending on diffusion, growth, absorption, transport, runoff, volatilisation, photodegradation and chemical breakdown (d^{-1}).

$$k = \left(\frac{1}{k_{diff}} + \frac{1}{k_{growth}} + \frac{1}{k_{absorption}} + \frac{1}{k_{transport}} + \frac{1}{k_{runoff}} + \frac{1}{k_{volatilisation}} + \frac{1}{k_{photo}} + \frac{1}{k_{\deg r}}\right)^{-1}$$

Literature review has shown that the impact of most processes is very important in the first hours after the pesticide application. In frame of the impact of residues on human health, it can be set that the most important factor for long-term residue decline, is the biochemical degradation. Therefore, equation 4, can be rewritten as

$$k = k_{degr} = \frac{\ln(2)}{t_{1/2}} \ (d^{-1})$$

Where $t_{1/2}$ is the foliar/fruit half-life time (d).

Foliar half-life times were obtained from Willis *et al*. (1980) and Willis and McDowell (1987). For most pesticides, the foliar half-life is much less than the soil half-life due to enhanced volatilization and photodecomposition. While values for half-life were available for some pesticides, the majority of the foliar half-life values were calculated using the following rules:

1. Foliar half-life was assumed to be less than the soil half-life by a factor 0.5 to 0.25, depending on the vapour pressure and sensitivity to photodegradation
2. Foliar half-life was adjusted downwards for pesticides with vapour pressures less than 10^{-5} mm Hg
3. The maximum foliar half-life assigned was 30 days

The initial pesticide concentration (C_0)

C_0 is the initial pesticide concentration on the leaf/fruit, directly after spraying. Literature study has revealed several approximations. Two calculation methods have been taken into consideration.

Method 1

The first method calculates the initial concentration as follows:

$$C_0 = \frac{C_{ai} * A * F_{int} * GC}{10000 * B_0} \ (mg/kg)$$

Where C_{ai} is the concentration of active substance in the formulation (mg a.i./l), A is the pesticide application rate (l/ha), F_{int} is the crop interception factor, GC is the plants ground cover (m² plant/m² soil) and B_0 is the initial plant biomass (kg plant/m²).

Parameters such as C_{ai}, A and F_{int} are easily found in literature. The problem is the uncertainty about GC and B_0. For most pesticides, no experiments have been carried out yet and parameter values cannot be found in literature. Working with default values might be a solution, but it is very difficult to find an acceptable value. After all, biomass and ground cover depend on the time of application, the growth stage of the plant, the climatic conditions, the way of planting, …

It has to be concluded that the equation gives a good approach of the initial leaf/fruit pesticide concentration, on condition that all parameters are known. Working with default values might cause a serious under- or overestimation.

Method 2

A critical point in the estimation of consumers' exposure to pesticides trough the intake of food, is the prediction of the amount of pesticide reaching the plant at the moment of spraying or the initial plant concentration after a single application.

The European Commssion has worked out a document (Guidance document on risk assessment for birds and mammals under council directive 91/414/EEC, Sanco/4145/200), in which a first-tier approach for estimating the initial pesticide concentration on the plant has been described.

The method is based on research carried out by Hoerger and Kenaga in 1972 in which they analysed data on residues of 28 plant protection products in 60 different crops. They provided maximum and "typical" (mean values of the maximum for each crop/pesticide combination) values that can be expected immediately after spraying on vegetation (Table 4).
The main idea is that the residues are not the result of the compound but of the crop and that the initial concentration increases proportional with increasing dose.

Table 4: Relationship between "typical" and maximum residue concentrations on plants or plant parts (mg/kg fresh weight) and the dose (D) of plant protection producs (kg active substance/ha) immediately after spraying (according to the nomogram of Kenaga).

Plant/plant parts	Typical values	Maximum values
short grass	112*D	214*D
long grass	82*D	98*D
leaves and leafy crops	31*D	112*D
small seeds/forage crops	29*D	52*D
pods	2.7*D	11*D
cereals	2.7*D	8.9*D
fruit	1.3*D	6.3*D

Recently, several studies have been carried out, in the first place to check whether the results of 1972 are still valid nowadays (different compounds, low volumes, etc.) In particular, a study, carried out by Fletcher et al. (1994) is important in frame of this work.

The study of Fletcher re-examines the Kenaga nomogram using information compiled at the University of Oklahoma. Pesticide residue levels on days 0 and 1 after application were examined for 72 plant species and 68 chemicals. Most residue data pertained to leaves and leafy crops, legume foliage and fruit. In Table 5, the maximum and typical data of Kenaga are presented, the percentage of measurements found by Fletcher that were higher than the values of Kenaga (% of exceeding), the mean values found by Fletcher and the 95th percentile values, estimated as the mean plus 1.6 times the standard deviation.

Table 5: Residue values (normalised for an application rate of 1 kg active ingredient per ha); typical and maximum values according to Kenaga, mean and 95th percentile values according to Fletcher et al. and the percentage of values found by Fletcher et al. above the maximum values of Kenaga (% of exceeding).

Plant/plant parts	Kenaga "typical"	Kenaga maximum	Fletcher mean	Fletcher 95thpercentile	Fletcher % exceeding Kenaga
short grass	112	214	76	164	0 (0)
long grass	82	98	32	92	4 (2)
leaves and leafy crops	31	112	31	98	3 (0)
forage crops/small seeds	29	52	40	121	22 (9)
pods/large seeds	2.7	11	4	13	8 (4)
fruit	1.3	6.3	5	20	19 (7)

Fletcher et al. propose to use higher maximum values for small seeds/forage crops and fruit, 121 instead of 52 and 13 instead of 6.3, respectively. They propose to combine two categories pods/large seeds and fruit to one with a maximum value of 13 and one category for leaves/leafy crops and forage crops/small seeds and for the category of fruit. The lineair relationship that the Kenaga nomogram has between application rate and residue amounts is consistent with the findings of Fletcher et al.
No indications were found to treat one particular compound group differently from the others. No correlation was found for morphological differences (e.g. surface texture, leaf shape).

Because the database used by Fletcher et al. is much larger and more a reflection of the state of the art than the one used by Hoerger and Kenaga, preference is given to the Fletcher et al. database. It is recommended tot use four plant categories:

- short grass
- long grass
- leaves, leafy crops, forage crops and small seeds
- fruit, pods and large seeds

Further investigation suggests that the data probably are lognormally distributed (ECOFRAM report, 1999) and that the sample size must be taken into account (Aldenberg and Jaworska, 2000).

The European commission recommends that in case of acute exposure the 90th percentile of the initial concentration should be used. For short-term exposure, averaging of residues will occur and therefore arithmetic means are taken for residues in vegetation. For long-term exposure a further adjustment for degradation in time is recommended (time-weighted average).
Table 6 gives the values which will be used in case of acute, short-term and long-term exposure to estimate the initial residue concentration on the plant.

Table 6: Summary of the residue values (Fletcher et al., 1994), directly after application used in the calculation of acute, short-term and long-term exposure (normalised for an application rate of 1 kg active ingredient/ha).

Plant/plant parts	Mean	90th percentile
short grass	62	142
long grass	21	69
leaves and leafy crops + forage crops/small seeds	25	87
fruit/pods/large seeds	2,3	11

Interval (i), number of applications (n) and time between application and harvest (t)

Most of the information concerning those parameters was found on the website of the Belgian Government (www.fytoweb.fgov.be). The values for i, n and t vary between different crops and the mode of action of the different active substances. In case no values were found on Fytoweb, the internet and literature studies were consulted.

4.3.4.3 Validation

The model has been validated by comparing the results with literature data (results of supervised residue trials). Most of the data were obtained by the FAO (US). Some results for dimethoate are given in Table 7.
The current model gives satisfying results. In most of the cases the model calculations are an overestimating of the real situation. A possible explanation is that in reality the degradation on fruits and leaves starts very quickly and then slows down the next days. In fact, the degradation can be described with two degradation factors: one for the first hours/days and one for the following days. In the model, only one degradation factor has been taken into account, resulting in a slight overestimation. Nevertheless, it is a useful tool in predicting the human intake of pesticide residues by food.

Table 7: Validation exercise for dimethoate (FAO, 1998)

AS	Crop	Form	Country	AR (kg as/ha)	n	t (days)	TRIAL residue (mg/kg)	MODELLING residue (mg/kg)
dimethoate	cherries	EC	Germany	0,72	3	14	0,14	0,48
						21	<0,05	0,34
						28	0,05	0,25
						35	<0,05	0,20
dimethoate	cherries	EC	Germany	0,8	1	4	1	0,96
						7	1	0,73
						10	0,58	0,57
						14	0,66	0,43
						21	0,19	0,30
dimethoate	cherries	EC	Germany	0,8	2	4	3,38	1,15
						10	3,84	0,69
						14	1,64	0,52
						21	1,48	0,36
dimethoate	cherries	EC	Germany	0,6	4	14	0,37	0,41
						21	0,06	0,28
dimethoate	onion	EC	Germany	0,04	2	7	0,31	0,59
						14	0,14	0,36
						21	0,04	0,25
dimethoate	onion	EC	Germany	0,24	1	7	0,2	0,69
						28	0,05	0,21
						7	0,1	0,69
						28	<0,01	0,21
dimethoate	cauliflower	EC	UK	0,32	2	7	0,1	0,44
						14	0,13	0,26
						21	0,05	0,18
dimethoate	cauliflower	EC	UK	0,4	3	7	0,04	0,56
						14	<0,02	0,34
						21	<0,02	0,23
dimethoate	cauliflower	EC	UK	0,3	1	7	0,3	0,34
						14	0,18	0,20
						21	0,1	0,14
dimethoate	cauliflower	EC	UK	0,4	6	3	0,44	0,82
						7	0,34	0,57
						14	0,21	0,34
						21	0,11	0,23
dimethoate	Brussels sprouts	EC	Germany	0,32	2	7	0,12	0,43
						14	0,06	0,26
						21	0,02	0,18
						28	<0,02	0,14
dimethoate	Brussels sprouts	EC	Germany	0,24	3	3	0,11	0,49
						7	0,08	0,34
						14	<0,05	0,20
						21	<0,05	0,14
dimethoate	Brussels sprouts	EC	Germany	0,24	3	3	0,14	0,49
						7	<0,05	0,34
						14	<0,05	0,20
						21	<0,05	0,14

4.4 Human exposure via food

4.4.1 Food consumption data

4.4.1.1 Food consumption surveys

Recent data for food consumption by the Belgian population were expected from the Belgian National Food Consumption Survey (BNFCS, Nutrition information Center, 2006; http://www.nice-info.be). The BNFCS study was conducted in 2004-2005 and included 3200 persons older than 15 year. The BNFCS study was based on a 24-h recall food consumption questionnaire and recorded daily consumption of ± 2200 food products. Daily food consumption of average, median, 5^{th} -, 25^{th} , 75^{th} and 95^{th} percentile of the total population (including consumers + non-consumers) and consumers-only were investigated. However, due to a delay in the publication and availability of results of the BNFCS (not available before March 2006) the data of the BNFCS study could not be incorporated in the current database and calculations. It is intended to implement the results of the BNFCS study in a later version of Xtrafood.

Table 8: Overview of Belgian food consumption surveys used in Xtrafood

	teenager survey	young children survey	women survey
period	February- March 1997	winter 2002-2003	2002
no of participants	341	697	641
participation ratio	72.7 %		
gender males (%) females (%)	 62 38	 51 49	 0 100
population age categories	13-18 year -	3-6 year -	15-40 year 18-23 year 24-29 year 30-35 year 36-41 year
available statistics	average, median, P5, P95 of consumers-only and total population	average, median, P5, P25, P75, P95 of consumers-only and total population	average, median, P5, P25, P75, P95 of consumers-only and total population
region	region of Ghent	Flanders	region of Ghent
methodology	7-day estimated food record	3-day food record	2-day food record
classification of foods	list of 754 food products in 30 main classes and 229 subclasses	list of 937 food products in 30 main classes and 166 subclasses	list of 1084 food products in 30 mainclasses and 178 subclasses
scope of the study/ remarks	international research in new methodology related to food safety	monitoring food and nutrients intake by Flemish children; focus on Ca-intake	assessment of Fe-intake of not-pregnant women

The currently used data for food consumption of the Belgian population are based on 3 earlier performed food consumption surveys in Belgium (Table 8):

- teenager survey (GASTON, Ghent Adolescent Study on Nutrition; Matthys *et al*, 2003)
- young children survey (UGhent; Nutrition information Center, 2004)
- women survey (UGhent, Matthys *et al.*, 2004)

Features of these 3 studies are listed in Table 8.

4.4.1.2 Food classification

The data of the 3 different surveys (Table 8) were harmonized by means of one single food classification system for the data of the 3 studies. Food products were divided into 28 main classes, 109 subclasses category 1 (C1) and 215 subclasses category 2 (C2).

Table 9: classification system of vegetables

main class : vegetables (code 02)

code subclass C1	name subclass
0201	cabbages
0202	peas
0203	beans
0204	cumcumber and related
0205	corn and related
0206	tomatoes
0207	plump berryfruits
0208	flower vegetables
0209	foliage vegetables (no lettuce, endives or spinach)
0210	lettuce
0211	spinach
0212	endive
0213	asparagus
0214	fennel and related
0215	celery
0216	leek
0217	root vegetables (no carrots, parsnip or salsify)
0218	parsnip and salsify
0219	carrots
0220	bulbous plant
0221	edible fungi
0222	other vegetables
0223	sprouts

code sublclass C2	
020801	uncooked
020802	cooked

↓

cauliflower cooked
broccoli cooked
artichoke cooked

Main classes were vegetables, fruit, fish, milk(products), cheese,… Further grouping into subclasses was according to:

- plant properties (root, foliar,…), preparation method (vegetables)
- plant properties, preparation method, origin (fruit)
- vegetable or animal origin, fat content (fat)
- animal type, fat content (meat, cheese)
- fat content, preparation method (milkproducts)

An example of vegetable classification is given in Table 9.

4.4.1.3 Gender/age categories

The methodology of food consumption survey is generally designed to evaluate the nutritional level by food intake of a specific target group (e.g. young children, women) and uses short-term (a few days – weeks) food records. In contrast, the current study is focused on **exposure of contaminants** by food intake which requires lifetime dietary data. Therefore, data of food consumption for different gender/age categories are needed. Food consumption for 18 gender/age categories were extrapolated from the 3 above mentioned study (Table 10).

Table 10: gender/age categories for food consumption

category	gender/ age	code categories	gender/ age
F-1	female 3-5 year	M-1	male 3-5 year
F-2	female 6-9 year	M-2	male 6-9 year
F-3	female 10-14 year	M-3	male 10-14 year
F-4	female 15-20 year	M-4	male 15-20 year
F-5	female 21-30 year	M-5	male 21-30 year
F-6	female 31-40 year	M-6	male 31-40 year
F-7	female 41-50 year	M-7	male 41-50 year
F-8	female 51-60 year	M-8	male 51-60 year
F-9	female > 60 year	M-9	male > 60 year

4.4.1.4 Compilation and extrapolation food consumption data

Food consumption data for categories F-1, F-2, F-3 and M-1, M-2, M-3 and M-4 were assessed by extrapolating the data from the studies related to young children (average age: 4.5 year) and teenagers (average age: 15.5 year). Hereto, a linear increase (for most food products) or decrease (for typical children food products such as milk) with age was assumed. Food consumption data for categories F-4, F-5 and F-6 were extrapolated in a similar way from the 4 age categories of the women study. Additionally, food consumption for category F-4 was also calculated according to the extrapolation model based on the combined dataset of young children and teenagers. Generally, these 2 extrapolation models predicted similar food consumption for F-4, which confirms the presumption that the 3 studies are comparable.

Food consumption data for Belgian women > 40 year (F-7, F-8 and F-9) are lacking. To fill these gaps, a food consumption survey from the Netherlands (Nevo-study; (Nederlandse Zuivel Organisatie, 2005, available at zuivelengezondheid.nl).was used as a reference That Dutch Nevo-study, performed in 1998, handled the same methodology as the Belgian National Food Consumption Study and reports food consumption for age categories 1 – 4, 4 – 7, 7 – 10, 10 – 13, 13 – 16, 16 – 19, 19 – 22, 50 – 65 and 65 – 75 year, separately for males and females. It was first checked whether food consumption for the considered food product was similar for Belgian and Dutch women for age classes below 40 year. In case of similarity for age categories between 4 – 40 year, it was assumed that food consumption for women > 40 years is also equal between Belgian and Dutch women. Data of the Dutch Nevo-survey for women 50 – 65 year and 65 – 75 were then used for respectively F-8 and F-9. If food consumption by Belgian women below 40 year was lower or higher than for Dutch women in the corresponding age category, the relative changes in food consumption with age instead of the absolute food consumption values were derived the Dutch study and applied for the estimation of categories F-8 and F-9. The Dutch Nevo-study did not include a category corresponding to F-7. Therefore, food consumption for F-7 was calculated as the average of F-6 and F-8.

Data and extrapolation models for food consumption by men > 18 year are lacking for Belgium.
Food consumption data for M-6 were estimated from

i) data for Dutch men (22- 50 year) reported in the Nevo-survey
ii) data for M-4 and the food consumption – age trend for Dutch men, or
iii) data for M-4 and the food consumption – age trend for Belgian women

The choice for i), ii) or iii) was made for each food product individually. The first approach i) was generally applied, except for food products that showed large differences between Belgian and Dutch children and teenagers (e.g. French fries), as for these products differences between the 2 countries are also expected for older age categories. In that case, relative food-consumption – age trends instead of absolute values were used and applied for derivation of food consumption for M-6 based (approach ii) on data for M-4 and increases/decreases with age. For typical gender-specific products (e.g. beer) food consumption – age trends for Dutch men were applied for calculation of food consumption by Belgian men, while in other cases, the calculation were based on food consumption – age trend for Belgian women (approach iii).
Food consumption for M-5, M-7, M-8 and M-9 were estimated analogously to respectively F-5, F-7, F-8 and F-9.

In addition to the extrapolation of average food consumption, median, 5^{th} , 25^{th} , 75^{th} and 95^{th} percentiles of food consumption were derived analogously for each gender/age category.

4.4.1.5 Food consumption database: examples

An example of food consumption among different age categories is given for average consumption of cooked + fried potatoes for females (Figure 8*).*

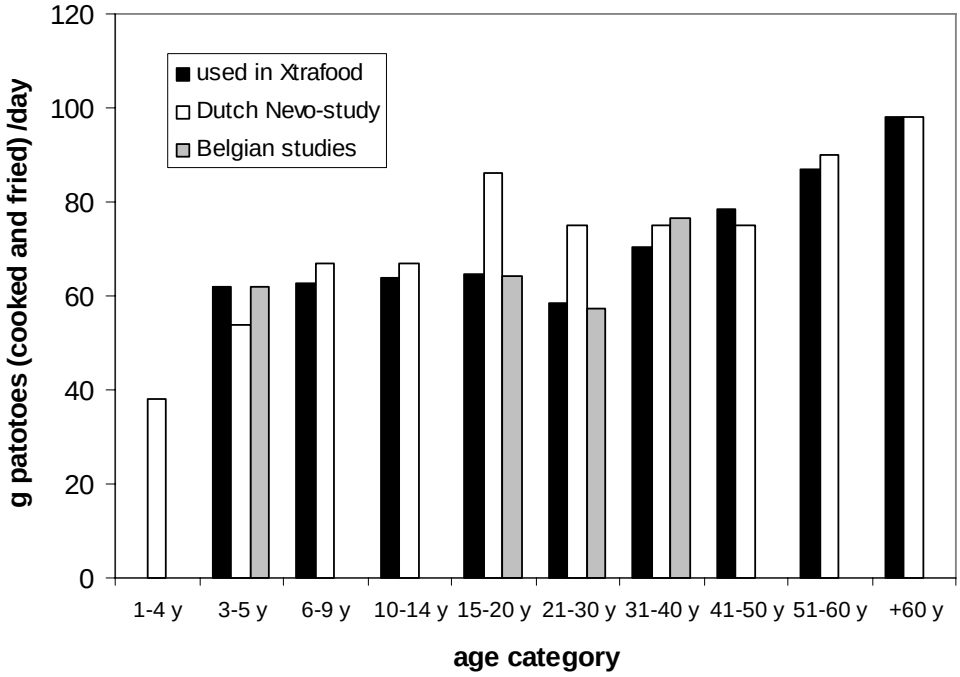


Figure 8: Estimated average consumption of potatoes (cooked + fried) for different (female) age categories in Xtrafood. Average consumption of the studies on which these estimates are based, i.e. the Belgian young children, teenager and women surveys and.the Dutch Nevo survey are given for illustration.

Average food consumption patterns for 5 age categories (men and women) are listed in Table 11
In Table 11, consumption of individual products is grouped by main classes of food products for summarization of food consumption. Contaminant exposure calculations (see below) through food

chain are executed at the finest detail level, i.e. for each food subclass C2 category separately (details see below).

Average total food consumption is higher for males than for females at corresponding age. Main products with a pronounced higher consumption by men than by women are potatoes, juices, sugar and confectionery, fats, bread and alcoholic drinks. On average, women consume more fruit than men. Regardless of gender, food consumption increases with age, from childhood to maturity, and also over different adults categories, food consumption increases with increasing age. Main exception is the decreasing consumption of milk and milk products with increasing age.

Table 11: Average food consumption for 10 selected gender/age categories in Xtrafood

	daily average consumption (g/day)									
food product main class	F-1	F-3	F-5	F-7	F-9	M-1	M-3	M-5	M-7	M-9
potatoes and other tubers	77	97	92	95	103	81	132	155	146	149
vegetables	60	95	186	245	272	64	110	166	235	276
fruits	98	109	131	184	224	104	91	100	133	151
juices	170	149	109	85	80	182	152	153	161	196
soups	59	29	48	84	92	59	32	48	84	91
sugar and confectionery	26	34	37	32	30	25	44	50	50	46
fats	7	17	14	21	33	8	26	34	37	60
sauces	8	11	22	15	10	8	13	17	13	6
non-alcoholic drinks	326	674	1249	1368	1337	343	769	1138	1066	994
alcoholic drinks	1	4	94	132	72	0	4	267	331	222
sojaproducts	9	3	10	15	15	29	9	10	15	15
bread and bread products	71	124	118	123	106	77	159	201	181	152
breakfast cereals	7	7	11	4	5	9	12	12	7	12
cereal products	41	36	52	46	46	46	43	38	37	43
rice	5	13	20	13	7	6	14	29	32	18
pasta	11	19	33	32	7	10	22	42	44	5
flour, binders and other grain products	1	1	2	2	2	1	1	1	1	1
wheat flour	0	1	1	1	1	0	1	2	2	2
meat	54	95	98	105	97	55	133	124	132	123
kidney and liver	1	1	1	1	1	1	1	1	1	1
poultry	17	22	25	27	27	19	27	31	33	34
game	0	0	0	0	0	0	0	0	0	0
meat substitute	0	1	6	4	4	1	1	1	1	1
milk and milk products	419	294	256	221	235	439	322	224	207	244
cheeses	14	23	31	43	40	13	22	31	36	30
eggs	5	8	9	8	8	5	8	11	12	11
composed foods	16	19	43	19	14	12	26	46	46	24
fish and shellfish	8	14	27	36	36	9	16	35	48	48

4.4.2 Incorporation of transfer to primary food products and food consumption data

Deliverables of the above described transfer models are contaminant concentrations in vegetables, fruit, cereals, meat, liver, kidney, milk and eggs. Combination of these concentrations with food consumption data (human diet) results in total daily intake (TDI) of a contaminant. A flow scheme of integration of food consumption data and farm transfer models into human exposure assessment in presented in Figure 9.

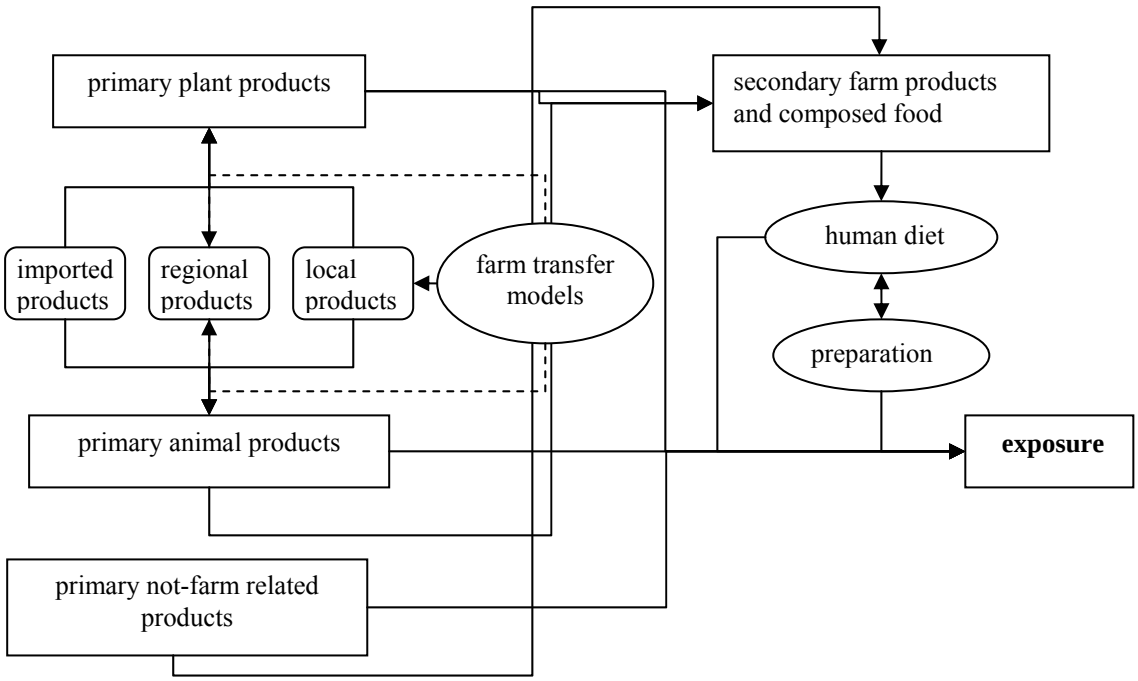


Figure 9: flow scheme of combination of biological transfer of contaminants and food consumption data for the assessment of human exposure to contaminants by diet.

4.4.2.1 Farm products versus human dietary products

The first step in the assessment of contaminant exposure through the diet involved matching food class C2 subcategories and farm products. Basically, all food products can be reduced to (a combination of) primary plant products, primary animal products or primary not-farm related products (Figure 9). Hereto, five major types of food classes (C2 subclasses) were identified:

1. type 1: single food classes that are products identical to one single primary farm product (e.g. milk, carrots,…)
2. type 2: single food classes foods that are secondary farm products which can be easily related to one single primary farm product. For example 1 kg cheese is, on average, manufactured from 10 liters milk.
3. type 3: not-farm related products (e.g. fish, tropical fruits,…). The current Xtrafood farm model does not include transfer models for animals and crops that are produced not produced in a more or less 'typical Belgian farm'. Contaminant concentrations in these products originate from concentrations reported in literature related to not contaminated situations.
4. type 4:composed food classes which can be split into different substances. These substances are then linked to single primary or secondary farm products, or not- farm related products.

A first type of a composed class (type 4a) is the food subclass C2 'flower vegetables, cooked) (food product code 020802); type 4a is a composed class of single products. Subclass C2 consists of 3 primary plant products, i.e. cauliflower, broccoli and artichoke. In order to link the food consumption data to the farm model, the contribution of the different primary plant products to the subclass is required. The contribution of the 2 major products was default set at 50 % for each when no information about that distribution was found. In the case of subclass 020802, it was assumed that 50 % was cauliflower and 50 % broccoli. That distribution over different products was highly speculative. However, it is expected to influence only marginally contaminant fluxes since products in one subclass are characterized by similar plant or animal properties and thus by similar contaminant transfer coefficients.

An second example of a composed class (type 4b) is food subclass C2 'cakes' (food product code 140100). For type 4b, not only the class itself is composed, but also the products in these classes are composed. The composed products are first split into different ingredients, which are related to primary farm products. In this example, flour is associated with wheat (primary plant product code C110100), sugar with sugar beet (primary plant product code C120100), eggs with primary animal product code A601110, butter with milk (primary animal product code A132211).
For example, biscuits consists of flour, eggs, butter, sugar and milk. The composition of a 'standard cake' was derived as the average of 5 common food products of the subclass C2 'cakes'.

Table 12: composition of a 'standard cake'

food product	composition				
	flour	eggs	butter	sugar	milk
cake	25%	25%	25%	25%	0,0%
biscuit	39%	17%	31%	14%	0,0%
pastry	41%	7%	31%	21%	0,0%
pancake	42%	41%	10%	7%	0,1%
waffle	50%	20%	17%	13%	0,1%
average ('standard cake')	**39%**	**22%**	**23%**	**16%**	**0,0%**

4.4.2.2 Import of farm products/ aggregation level (dilution)

The impact analysis of contaminants requires for each farm product the origin and distribution of that product. The origin of the food package is essential in the link between the farm model and contaminant exposure since the origin determines the environmental conditions, and thus the contamination level. For example, Cd exposure by home-garden carrots is, via the farm model linked with the environmental conditions of that home garden (soil Cd, soil pH, Cd deposition, surface ground water Cd,…). However, final Cd concentration of carrots in the food packet of people with a home garden with elevated Cd soil concentrations needs to be corrected for the fraction of home-garden grown carrots to the total amount of consumed carrots (in combination with Cd concentration of non-home garden grown carrots). In this way, Cd concentrations of carrots are 'diluted'. The pollution can also manifest at a larger, regional scale (e.g. the Kempen region or Flanders). Three aggregation levels were defined, i.e. local, regional and foreign level (imported products) (Figure 9). Concentrations of regional or imported products can be calculated in a similar way, using the farm model, with environmental conditions specific for that region.

The model also allows input of known (measured) instead of predicted concentration for regional or imported products. Input of measured concentrations is very useful for imported products that are not or poorly parameterized in the model (e.g. citrus fruit) and is necessary for products for which no transfer module was built in the Xtrafood model (e.g. fish).

The significance of dilution depends also on the *bulking properties* of the food product. For example, contaminated milk originating from one farm is readily mixed with not contaminated milk at the milk collector station; hence, milk sold at supermarkets contains not more than a small fraction of the contamination. Products with similar *bulking properties* are grain, rice,… This dilution is not applicable for not bulked products such as meat.

Consumption of home-grown vegetables depends on the individual situation of the consumer. Allocation of regional or imported products was assessed based on the FAO food balance data for 2002 (available at http://faostat.fao.org). Data of domestic supply (import, export, production) and domestic utilization for Belgium were used to asses import dilution (Table 13).
Import dilution was calculated based on supply balances (method A) and on utilization balances (method B):

$$import\ dilution = {import}\Big/{(production + import)} \qquad \text{(method A)}$$

$$import\ dilution = {import}\Big/{(export + feed + secondary\ processing + food)} \qquad \text{(method B)}$$

Table 13: Assessment of import dilution in Belgium for food products based on FAO Food Balance Sheets for Belgium (2002).

	domestic supply			domestic utilization			import dilution	import dilution
	production	import	export	feed	secondary processing	food	method A	method B
	1000 ton			1000 ton				
wheat	1675	4316	2374	1400	462	1033	0.72	0.81
potatoes	2909	1470	1898	800	89	946	0.34	0.34
sugar beet	6537	48	2		6302		0.01	0.01
vegetables	2274	1730	2158	379		1260	0.43	0.43
tomatoes	234	237	192			267	0.50	0.50
fruit	571	4456	4422	29	47	717	0.89	0.84
bananas		876	889			7	1.00	0.97
apples	349	607	679			236	0.63	0.63
meat	1761	420	1368	8		805	0.19	0.19
beef	305	50	152			203	0.14	0.14
sheep and goat	3	32	19			15	0.91	0.91
porc	1041	135	812			364	0.11	0.11
poultry	407	151	348		8	202	0.27	0.27
milk (excl. butter)	3469	3617	3831	665	68	2540	0.51	0.51
eggs	177	53	127			107	0.23	0.16

Both methods result in more or less the same import dilution factors. Fruit, especially tropical fruit, is mainly imported, while meat (porc and beef) is mainly from animals of Belgian farms (Table 13).
The Xtrafood model also allows to exclude dilution by import or to use user-defined import dilution factors and/or user-defined fraction home-garden grown products.

4.4.2.3 Influence of food preparation on contaminant fluxes

Figure 10 illustrates the influence of food preparation on contaminant fluxes through the human diet.

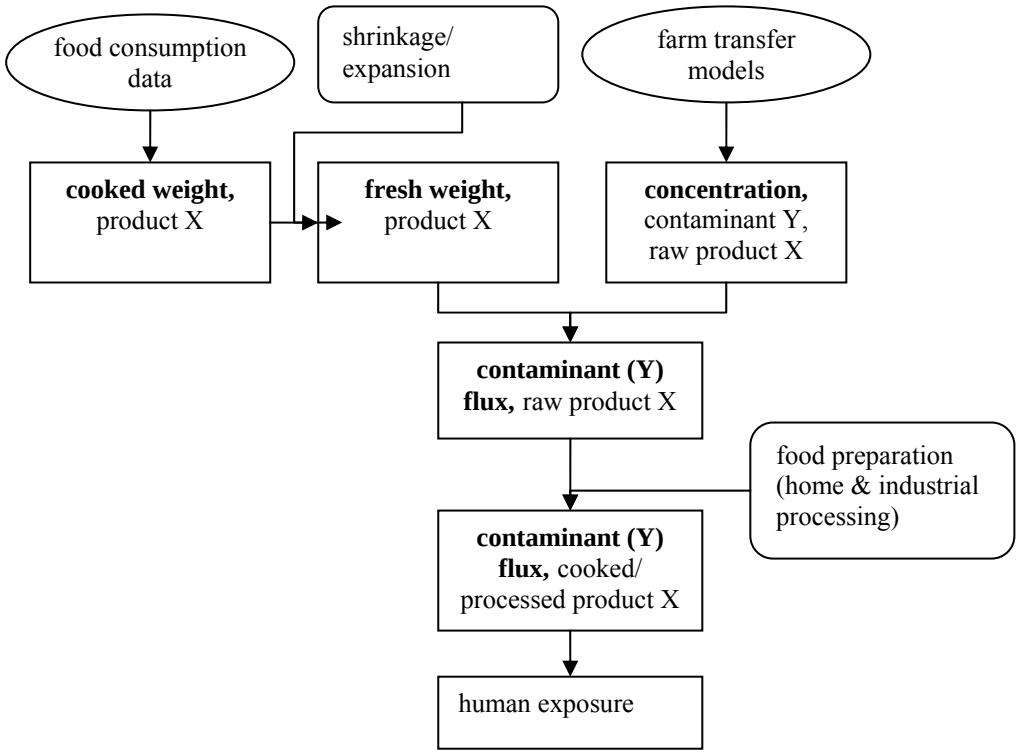


Figure 10: influence of food preparation on contaminant fluxes through the human diet

shrinkage/expansion

Calculations of contaminant fluxes use weights of consumed products and contaminant concentrations in primary farm or imported (not-farm) food products. Contaminant concentrations in primary farm products are expressed per unit fresh weight of raw product in the biological transfer models. Consequently, weights of consumed products have to be expressed on the same fresh weight basis. However, weights of food products reported in food consumption surveys are generally reported 'as eaten'. For cooked products, reported weights were converted to fresh weight by means of a shrinkage or expansion factor. Most products (vegetables, meat) lose weight by cooking, while some other products (e.g. rice) expand. Standard shrinkage (and expansion) factors reported in the document 'measures and weights: manual for standardized quantification of foods in Belgium' (Belgian Health Council, 2001) were used. Weight reduction by cooking of vegetables is, on average, 18 % and varies from 6 % (cauliflower) to 40 % (spinach). Each subclass C2 was assigned a shrinkage/expansion factor based on information that was found for products of that class. For example, the shrinkage factor for cauliflower was assigned to the whole subclass C020802 (cooked cauliflower, cooked broccoli and cooked artichoke).

Table 14: contaminant reduction factors for food preparation.

product	contaminant	process	reduction factor	reference
vegetables	Cd	washing	***0,75***	
spinach	Cd	washing	0,85	De Temmerman, 1999
lettuce	Cd	washing	0,65	De Temmerman, 1999
lambs' lettuce	Cd	washing	0,80	De Temmerman, 1999
endive	Cd	washing	0,50	De Temmerman, 1999
celery	Cd	washing	0,75	De Temmerman, 1999
kale	Cd	washing	0,70	De Temmerman, 1999
vegetables	Cd	boiling	**1,00**	Alberti-Fidanza et al., 2002
frozen french beans	Cd	boiling	0,95	Alberti-Fidanza et al., 2002
beans	Cd	boiling	0,85	Alberti-Fidanza et al., 2002
potatoes	Cd	frying	**1,11**	Alberti-Fidanza et al., 2002
rice	Cd	boiling	**0,52**	Morgan et al., 1999
red meat	Cd	frying	***1,03***	
sliced meat	Cd	frying	1,0	Alberti-Fidanza et al., 2002
hamburger	Cd	frying	0,9	Alberti-Fidanza et al., 2002
sausage	Cd	frying	1,05	Alberti-Fidanza et al., 2002
porc meat	Cd	frying	1,09	Alberti-Fidanza et al., 2002
Poultry	Cd	frying	***0,95***	
turkey	Cd	frying	1,11	Alberti-Fidanza et al., 2002
chicken	Cd	frying	0,80	Alberti-Fidanza et al., 2002
fish and shellfish	Cd	frying	***0,87***	
tilapia	Cd	frying	0,72	Atta et al., 1997
plaice	Cd	frying	1,02	Alberti-Fidanza et al., 2002
fish fingers	Cd	frying	1,05	Alberti-Fidanza et al., 2002
vegetables	dioxins	washing	***0,67***	
spinach	dioxins	washing	0,67	Tsutsumi et al., 2002
vegetables	dioxins	boiling	***0,41***	
spinach	dioxins	boiling	0,41	Tsutsumi et al., 2002
fruit	dioxins	washing	***1,00***	
apple	dioxins	washing	1,00	Müller et al., 1993
pear	dioxins	washing	1,00	Müller et al., 1993
fruit	dioxins	peeling	***0,51***	
pear	dioxins	peeling	0,51	Müller et al., 1993
red meat	dioxins	frying	***0,57***	
hamburger	dioxins	frying	0,55[a]-0,56[b]	[a]Petroske et al., 1998 & [b]Hori et al. 2005
beef	dioxins	frying	0,58	Hori et al., 2005
fish and shellfish	dioxins	boiling	***0,86***	
mackerel	dioxins	boiling	0,86	Hori et al., 2005
fish and shellfish	dioxins	frying	***0,62***	
fish	dioxins	frying	0,54	Zabik and Zabik, 1995
mackerel	dioxins	frying	0,69	Hori et al., 2005

food preparation: kitchen processing

The above described shrinkage/expansion factors account for changes in weight through cooking, under the assumption of conservation of contaminant fluxes. However, food preparation processes can largely reduce contaminant fluxes. Considered food preparation processes are washing, peeling, boiling and frying/grilling.

Contaminant reduction factors related to food preparation depend on:
- the contaminant
- the food product
- the preparation process

A summary of literature review on this topic is given in Table 14.
Dependent on the type of food preparation, contaminant and food product, the effect of preparation varied from no effect (e.g. dioxin concentration in fruit by washing), to more than 50 % reduction in contaminant concentration (e.g. dioxin concentration in spinach by boiling).

Table 14 shows that there was only patchy information available from literature on contaminant reduction due to food preparation. Based on the available data, we tried to extrapolate reduction factors to the whole package of food products in Xtrafood. Hereto, reduction factors for main classes that are derived as average of available data on food products of that class are marked in italic. Different products and different publications were given the same weight in average calculation. For some product/contaminant/process combination, this approach seems justified. For example, there is only very small variation on the 3 values for reduction factor for dioxins by frying meat, which originate from 2 different studies. Thus, it seems reasonable that the average reduction factor for red meat of 0.57 is applicable for other products in main class 'red meat'.
In contrast, the average reduction factor for removal of Cd by washing vegetables might be less suitable for a number of vegetables. In fact, most studies in the category 'vegetables' are foliage vegetables. It is plausible that for e.g. tomatoes reduction is less than for leafy vegetables. For the same reason, reduction of dioxins by washing or boiling might be overestimated since this factor is based on data for spinach.

The lack of a complete set of accurate contaminant reduction factors was taken into account in the Xtrafood model. The model includes the option to ignore contaminant reduction factors for food preparation. That option enables comparison of contaminant exposure between conservative scenario calculations (i.e. ignorance of all reduction factors) and scenario calculations using reduction factors in Table 14.

In addition, also more refined scenario's can be calculated as the option to use or ignore a contaminant reduction factor can be selected separately for each combination of food product/process/contaminant.

Considering the use of contaminant reduction factors, one should also pay attention to the way contaminant concentrations have been analyzed (or on which basis these are calculated). Some measuring protocols prescribe the washing or peeling of crops prior to further sample analysis. If such sample treatment is already included in the protocol, one should avoid the use of an extra reduction factor in order not to account twice for the reduction factor.

Regardless of the exact value of reduction factors, one could also reject the use of reduction factors for meat or fish frying based on more detailed cooking procedures. Notwithstanding that frying partly removes dioxins from meat and fish, fats and pan juices produced upon frying become enriched with these dioxins. If these fats and pan juices are not discarded but eaten or used for preparation of sauce, reduction factors should not be used. However, it cannot be derived from food consumption date whether pan juices are discarded or not.

It is noted that reduction factors in Table 14 are reported for the overall group of dioxins and furans (expressed as 2.3.7.8-TCDD-toxic equivalent, TEQ) and not for each congener separately. Congener specific reduction factors for hamburger cooking reported by Petroske et al. (1998) did not show differences between 13 congeners (including common dioxins and furans such as TCDD, PeCD, HxCD, HpCD, OCDF, PeCDF, HxCF and HpCF and OCDF). Only for OCDD, a slightly smaller reduction than for TEQ was reported.

food preparation: industrial preparation

Analogously to kitchen processing, industrial food processing might influence contaminant concentrations. An example of such industrial preparation is the production of cheese or butter. No literature related to contaminant reduction/enrichment factors for such industrial processes was found. For dioxins, it was assumed that the reduction/enrichment factor was proportional to changes in fat content. For Cd, it was assumed that Cd concentration in milk and cheese were equal.
For other industrial processes that resemble kitchen processes such as preparation of ready-to-eat meals, deepfreezing vegetables, manufacturing of cakes and biscuits,… the above described 'kitchen preparation' factors were used.

4.5 Exposure assessment and risk characterization

4.5.1 Exposure assessment

The XtraFood model provides as output the concentrations in specified food groups, food intake data and resulting contaminant intake, seggregated into age and gender categories. Exposure can be calculated as being representative for a population (group) or separately for local and background intake. In the latter case, the proportion of local intake to total intake allows the calculation of overall intake from local and background sources. All these intakes are linked to the output of the farm model. Additional inputs are provided to allow for concentration data in non-farm related foods (e.g. fruit juice, fish, …).

However, if we want to estimate the health risks and get insight in the importance of the food exposure pathway associated with the exposure from a certain contaminant, it is necessary to address exposure from all relevant pathways (including inhalation exposure, oral exposure like from dust, dermal exposure). This approach is called aggregate exposure and is now generally accepted as the way to proceed in human health risk assessments. If necessary from a toxicological point of view, cumulative exposure (i.e. exposure from multiple contaminants) should also be addressed.

In order to allow for aggregate exposure, input fields for intakes by other routes are provided with the same seggregation (age/gender) as for the food intake. Inhalation exposure, soil/dust exposure and dermal exposure is provided as a default input possibility. Other exposures can be defined on a case-by-case basis (as these are sometimes contaminant specific). The non-food related exposures are not calculated in detail within the model, the intake data should be estimated outside the model environment and put into the XtraFood model. An example of an output table is given in Table 15. This table is made for each age and gender group. A summary table provides the output per pathway for each age and gender group. Exposure is calculated as dose in units of µg/d and as dose in units of µg/kg body weight.d. The latter is the preferred metric for comparison with toxicological reference data. Body weights for Flemish children (age 2 – 20 years) per age and gender are available from the VUB (2004). Body weight for the Belgian population can be obtained from WIV (data to be ordered); at present a default value of 60 kg for women and 75 kg (for men) is used.

Table 15: Example of an output table for the exposure calculations

		LOCAL			BACKGROUND			TOTAL	
pathway	consumption (g/d)	concentration (µg/kg)	intake (µg/d)	intake (µg/kg.d)	concentration (µg/kg)	intake (µg/d)	intake (µg/kg.d)	fraction local	intake (µg/kg d)
FOOD									
food group 1									
food group 2									
…									
food group n									
total food									
AIR	-	-			-				
SOIL/DUST	-	-			-				
DERMAL	-	-			-				
OTHER									

The EC proposes the classification of age and gender as shown in Table 16. The classification used in XtraFood differs somewhat from the EU classification because of a 1 year shift, less detail at the 15-20 years of age and more detail above 20 years of age. XtraFood misses the 1-3 years group as no data on food consumption in Belgium were available for this group.

Table 16: Age-gender classification groups by the European Commission (from: Kroes et al., 2002)

children	men	women
1-3 years		
4-6 years		
7-10 years		
	11-14 years	11-14 years
	15-17 years	15-17 years
	18+ years	18+ years
		pregnant, lactating

EFSA (2005b) recommends that the dietary intake be based on:

- the whole population or preferably for "consumers only";
- the mean and the median intakes;
- the intake by individuals highly exposed (either due to high consumption of some foods or due to highly contaminated food).

If occurrence is in food items consumed by almost all of the population, the estimates can be based on the whole population. If occurrence is in foods consumed by a small part of the population, preference is given to consumer only exposure assessments. Confidence intervals on the intake should be provided.

With the present food consumption data, a difference between consumers and non-consumers can not be made yet; this will be provided in the near future with the BFCS. Exposure is first calculated for average and median food consumption (but could, if data are available, make use of variability information on concentrations). To account for high exposure, subsequent runs can simulate high intakes to food groups leading to higher exposure, by using the higher percentiles for these food

groups. Taking the highest percentiles for all food groups in one run would lead to overestimates in exposure, as food groups are not independent with regard to quantities consumed.

4.5.2 Risk characterization

The risk characterization process consists of the comparison of the exposure data with the hazard information and the dose-response relationships. Risk characterization should take into account:

- aggregate exposure;
- critical health effects;
- threshold / non-threshold mode of action;
- differences in toxicity by exposure pathway;
- sensitive groups.

Aggregate exposure and sensitive groups (by sensitivity to effects because of e.g. developmental processes; or by high exposure patterns) are taken into account in the exposure assessment. The results provide adequate detail to account for age and gender influence in sensitivity.

Risk charactization options in XtraFood are provided for chronic exposures. Acute exposure and risk characterization is not yet taken up in the model.

4.5.2.1 Hazard identification – dose response characterization

To be able to characterize human health risks, dose-response relationships should be derived. These dose-response relationships are typically provided at the external dose level (dose at the border of the human body). However, if information is available on the critical effect level as an absorbed dose or at a specified target organ, and on the pharmacokinetics, it is possible to use internal doses as the exposure metric.

For noncarcinogenic substances or carcinogenic substances with a nongenotoxic mode of action, the presence of a threshold is generally assumed (although in some cases, the possibility of the absence of a threshold, like for lead, is proposed). The maximum levels, which are assumed to be without risk for the human population, are generally derived from effect (LOAEL[2], BMD[3], BMDL[4]) or no effect levels (NOAEL[5]) in animal studies. Assessment factors to account for interspecies differences (extrapolation from animal to man), intraspecies differences (variability within the human population) are applied to these levels. Additional assessment factors can be used if only a LOAEL is available, or to account for differences in exposure times (e.g. extrapolation from subchronic data in animals to chronic exposure in humans) or limitations in the database. Typical default value per assessment factor is 10, lower values can be used if supported by information on toxicodynamics and toxicokinetics.

With regard to chronic exposure, following toxicological reference data can be used:

- TDI, ADI, RfD: reference dose below which it is assumed that long-time exposure will no lead to harmful effects; the value is based on the critical effect (leading to the lowest TDI, ADI or RfD)

[2] LOAEL: Lowest Observed Adverse Effect Level
[3] BMD: Bench Mark Dose, dose causing 5 or 10 % incidence above control; calculated by mathematical methods using the experimental dose-response data (US-EPA, 1995)
[4] BMDL: Bench Mark Dose lower limit: lower limits of a one-sided 95 % confidence interval on the BMD (EFSA, 2005b)
[5] NOAEL: No Observed Adverse Effect Level

– NOAEL or LOAEL values: levels observed in the toxicological studies; they can be expressed as external or internal doses; used to calculate a margin of exposure (MOE[6]).

For carcinogenic substances with assumed or proven genotoxic mode of action, the general assumption is the absence of a threshold of effects. This is based on the single-hit assumption, meaning that any extent of interaction of a direct-acting genotoxic substance with the genetic material could result in a finite probability of a response. As carcinogenic animal toxicity tests result in high cancer incidences (at high doses), extrapolation models are used to estimate the carcinogenic risk at low doses and low incidences (general population). All these models assume linearity in the low dose incidence range, but results can differ widely between the extrapolation models used.
Assuming no threshold for genotoxic carcinogens, the dose response relations for genotoxic carcinogens are expressed as a unit risk[7] or slope factor[8].

However, because of the fact that carcinogenesis is often not a single step process and the occurrence of repair mechanisms, there are suggestions for a practical threshold for genotoxic carcinogens (EFSA, 2005b). The extrapolation models often do not reflect biological processes and results can differ widely depending on the model used. Taking these considerations into accout, the Scientific Committee of EFSA explored the use of a margin of exposure (MOE) approach for genotoxic carcinogenic substances.

Comparing various approaches, the EFSA recommends the use of a BMDL10 (Benchmark Dose lower limit for 10 % response) if data are available; in case the data are insufficient, EFSA recommends the use of the T25[9] as reference point, as it is currently used in Europe for the setting of concentration limits for carcinogens in labelling of preparations.

4.5.2.2 Risk characterization

For noncarcinogens or non-genotoxic carcinogens, risk is often expressed as a risk index or a hazard quotient:

HQ or RI = D/TDI

If one uses the MOE concept, dose is divided by the NOAEL, BMDL or LOAEL. The acceptable MOE is based on the toxicological information.

The excess lifetime cancer risk under the assumption of the absence of a threshold for genotoxic carcinogens can be calculated as follows:

$$\text{Excess Lifetime Cancer Risk} = \sum \frac{D * ED}{AT} * SF$$

[6] MOE: ratio between a defined point on the dose-response curve for the adverse effect and the human intake (EFSA, 2005b); The LED_{10} or other point of departure divided by the actual or projected environmental exposure of interest (from: IRIS Glossary of Terms, http://www.epa.gov/iris/gloss8.htm#pagecontents)
[7] The upper-bound excess lifetime cancer risk estimated to result from continuous exposure to an agent at unit concentration (e.g. per µg/m³; per µg/l) (from: IRIS Glossary of Terms, http://www.epa.gov/iris/gloss8.htm#pagecontents)
[8] An upper bound, approximating a 95% confidence limit, on the increased cancer risk from a lifetime exposure to an agent. This estimate, usually expressed in units of proportion (of a population) affected per mg/kg-day, is generally reserved for use in the low-dose region of the dose-response relationship, that is, for exposures corresponding to risks less than 1 in 100 (from: IRIS Glossary of Terms, http://www.epa.gov/iris/gloss8.htm#pagecontents)
[9] T25: chronic dose rate in mg/kg.d, which will give 25 % of the animals tumours at a specific tissue site, after correction for sponaneous incidence, whichtin the standard liefe time of that species (from EFSA, 2005b)

in which D equals the dose (mg/kg.d), ED is the exposure duration (d), AT is the averaging time (d) and SF equals slope factor ($(mg/kg.d)^{-1}$). The acceptability of the estimated cancer risk is evaluated on the basis of accepted lifetime cancer risks (generally in the range of $1/10^5$ or $1/10^6$). The accepted lifetime cancer risk is generally based on a policy decision.
It is noted that the "Excess Lifetime Cancer Risk" methodology is currently not accepted by EFSA.

Using the methodology recently proposed by EFSA, it is assumend that genotoxic carcinogenic substances can also be assessed as having a threshold (below which cancer incidence is not increased). In contrary with non-carcinogens or non-genotoxic carcinogens, the threshold level can not yet be defined with current knowledge. For that reason, the MOE concept is introduced and the MOE is calculated as

MOE = (BMDL10 or T25)/D

The decision on the MOE which is associated with a low level of concern for long-term exposure depends on the availability of a BMD or a T25, the animal or human studies on which the point-of-departure is based and the overall quality of the database. As a rule of thumb, a MOE of 10,000 is considered adequate if a BMDL10 is available for animal studies. The final decision on the MOE should be taken by risk managers.

The Xtrafood model allows for risk charcterization at the level of the external dose or of the absorbed dose. The user of the model should provide the following input in order to perform the risk characterization:

- threshold or non-threshold approach;
- risk index or MOE approach;
- exposure duration and averaging time
- same critical endpoint for all exposure pathways or difference per exposure pathway;
- absorption (default = 1: risk characterization at the external dose level);
- TDI, slope factor, effect level.

In a first stage, the exposures are summed per route (oral, ingestion, dermal), possibly accounting for differences in bioavailability within a route (e.g. reduced oral bioavailability for contaminants in soil. If the assessment is done on the external dose level, the scheme as given in Figure 11 is followed; is the asssessment is done at the absorbed level, the dose for each route is multiplied by its appropriate absorption factor. The first distinction is made on the toxicological endpoints. If the critical endpoint is a systemic effect and the same endpoint applies to all routes, then the risk should be calculated on the aggregate exposure, but accounting for differences in toxicokinetics by route (as expressed by differences in toxicological reference values). Carcinogenic effects are considered the same endpoint, regardless of cancer type). If the effects are not systemic or the endpoints differ by route, the risk should be calculated per exposure route.

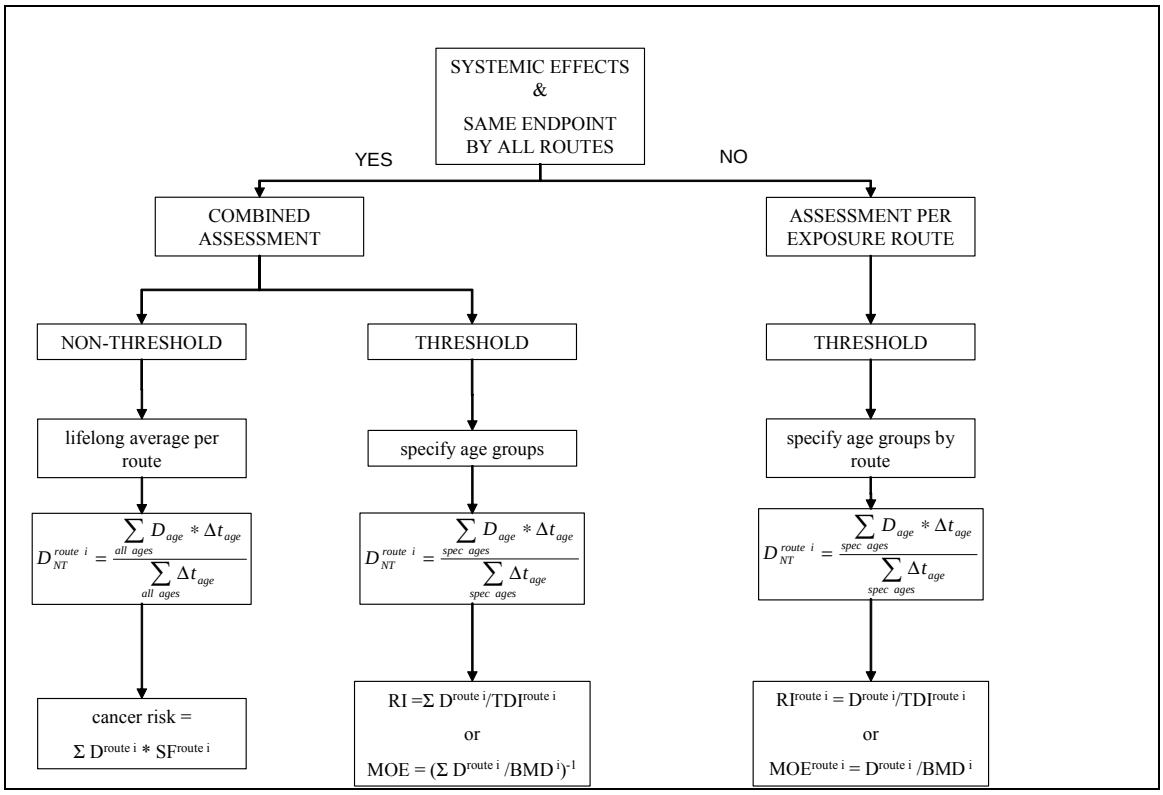


Figure 11: Risk characterization scheme for XtraFood

4.6 Programming XtraFOOD

4.6.1 Program structure transfer model in XtraFOOD

XtraFOOD is programmed in an SQL-environment, combining calculations in SQL language with databases constructed in MS-ACCESS. Figure 12 illustrates the conceptual structure of the model. The output of the atmosphere module is imported in the soil-plant module for transfer calculations in the soil-plant continuum. Predicted plant concentrations are used for calculation of levels in animal products in case the plants are used for feeding cattle or serve as output in case plants or edible plant parts are used for human consumption. If data on contaminant levels in the environment are available, they can be entered in the model to bypass calculations. On the other hand, measured contaminant levels will be used to validate the model calculations.

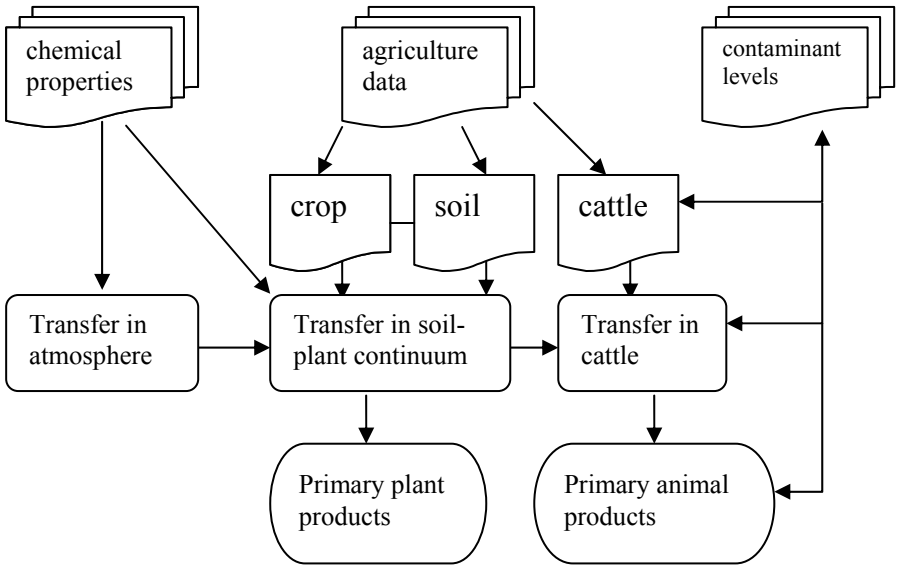


Figure 12:Structure of the transfer part of the XtraFOOD model

4.6.2 Program structure of the exposure part of the XtraFood model

The flow scheme in Figure 9 (see above) illustrates the conceptual structure of the exposure part of the Xtrafood model. The output of the transfer part module, i.e. chemical concentrations in crops or animal products are used as input in the exposure model. Additionally, data on chemical concentrations in non-farm food products (e.g. fish), chemical concentration in imported products, food intake records for different age/gender categories with statistical distributions, contaminant reduction factors related to food processing,.. are included in the database.

4.7 Parameter databases

4.7.1 Chemical properties of contaminants

Chemical data are taken from literature. Data on organic chemicals and heavy metals were gathered for human exposure assessment databases developed at VITO for the case of soil pollution and were stored in databases. Following data sources were used:
-Handbook of Environmental Data on Organic Chemicals (3rd ed.), by Verschueren, K.
-Illustrated Handbook of Physical-Chemical Properties and Environmental Fate for Organic Chemicals (volumes I – V), by Mackay, D.
-IUCLID CD-ROM, published by ECB (http://ecb.ei.jrc.it)
-Syracuse Research Corporation (SRC) (http://esc.syrres.com/)
-Chem finder, (http://www.chemfinder.com)

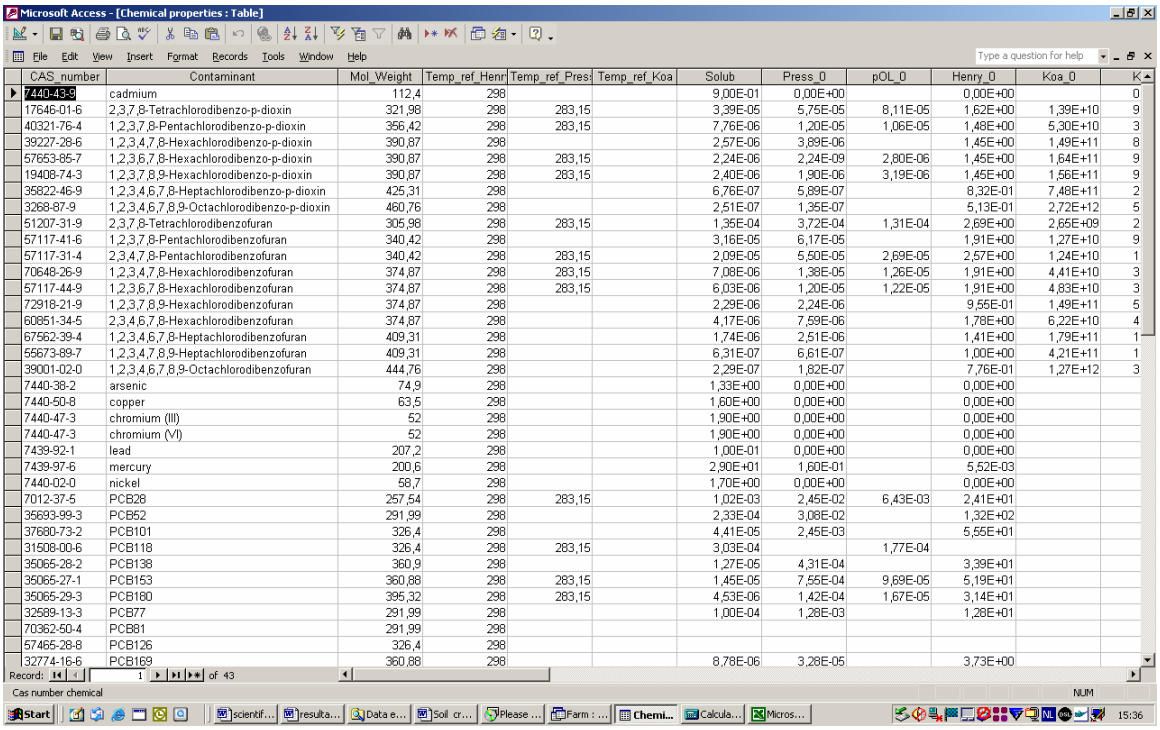
Data include: molecular weight, cas-number, solubility, vapour pressure, Henry coefficient, octanol-water partition coefficient, octanol-air partition coefficient, temperature correction coefficient, degradation constant, wash-out factor, biotransfer factor, bioconcentration factor, carry-over rate, diffusion constant in air and water (see Figure 13).

Similar data were collected for the selected pesticides in XtraFood (amitrol, cypermethrin, dimethoate, fenarimol, fluazinam, imidacloprid, lambda-cyhalothrin and linuron). In order to create an adequate model, predicting the fate of pesticide residues in/on the plant, it is necessary to know the physico-chemical properties of the active substances.

Those were collected based on the following hierarchy:

1. data from the European dossiers
2. data from the producers
3. pesticide database from CTB (The Netherlands)
4. the Pesticide Manual
5. Ecotoxnet/Toxnet
6. Other sources

Expert judgement has set up this list, based on their opinion on the “best available data”.



CAS_number	Contaminant	Mol_Weight	Temp_ref_Henr	Temp_ref_Pres	Temp_ref_Koa	Solub	Press_0	pOL_0	Henry_0	Koa_0	K
7440-43-9	cadmium	112,4	298			9,00E-01	0,00E+00		0,00E+00		0
17646-01-6	2,3,7,8-Tetrachlorodibenzo-p-dioxin	321,98	298	283,15		3,39E-05	5,75E-05	8,11E-05	1,62E+00	1,39E+10	9
40321-76-4	1,2,3,7,8-Pentachlorodibenzo-p-dioxin	356,42	298	283,15		7,76E-06	1,20E-05	1,06E-05	1,48E+00	5,30E+10	3
39227-28-6	1,2,3,4,7,8-Hexachlorodibenzo-p-dioxin	390,87	298			2,57E-06	3,89E-06		1,45E+00	1,49E+11	8
57653-85-7	1,2,3,6,7,8-Hexachlorodibenzo-p-dioxin	390,87	298	283,15		2,24E-06	2,24E-09	2,80E-06	1,45E+00	1,64E+11	9
19408-74-3	1,2,3,7,8,9-Hexachlorodibenzo-p-dioxin	390,87	298	283,15		2,40E-06	1,90E-06	3,19E-06	1,45E+00	1,56E+11	9
35822-46-9	1,2,3,4,6,7,8-Heptachlorodibenzo-p-dioxin	425,31	298			6,76E-07	5,89E-07		8,32E-01	7,48E+11	2
3268-87-9	1,2,3,4,6,7,8,9-Octachlorodibenzo-p-dioxin	460,76	298			2,51E-07	1,35E-07		5,13E-01	2,72E+12	5
51207-31-9	2,3,7,8-Tetrachlorodibenzofuran	305,98	298	283,15		1,35E-04	3,72E-04	1,31E-04	2,69E+00	2,65E+09	2
57117-41-6	1,2,3,7,8-Pentachlorodibenzofuran	340,42	298			3,16E-05	6,17E-05		1,91E+00	1,27E+10	9
57117-31-4	2,3,4,7,8-Pentachlorodibenzofuran	340,42	298	283,15		2,09E-05	5,50E-05	2,69E-05	2,57E+00	1,24E+10	1
70648-26-9	1,2,3,4,7,8-Hexachlorodibenzofuran	374,87	298	283,15		7,08E-06	1,38E-05	1,26E-05	1,91E+00	4,41E+10	3
57117-44-9	1,2,3,6,7,8-Hexachlorodibenzofuran	374,87	298	283,15		6,03E-06	1,20E-05	1,22E-05	1,91E+00	4,83E+10	3
72918-21-9	1,2,3,7,8,9-Hexachlorodibenzofuran	374,87	298			2,29E-06	2,24E-06		9,55E-01	1,49E+11	5
60851-34-5	2,3,4,6,7,8-Hexachlorodibenzofuran	374,87	298			4,17E-06	7,59E-06		1,78E+00	6,22E+10	4
67562-39-4	1,2,3,4,6,7,8-Heptachlorodibenzofuran	409,31	298			1,74E-06	2,51E-06		1,41E+00	1,79E+11	1
55673-89-7	1,2,3,4,7,8,9-Heptachlorodibenzofuran	409,31	298			6,31E-07	6,61E-07		1,00E+00	4,21E+11	1
39001-02-0	1,2,3,4,6,7,8,9-Octachlorodibenzofuran	444,76	298			2,29E-07	1,82E-07		7,76E-01	1,27E+12	3
7440-38-2	arsenic	74,9	298			1,33E+00	0,00E+00		0,00E+00		
7440-50-8	copper	63,5	298			1,60E+00	0,00E+00		0,00E+00		
7440-47-3	chromium (III)	52	298			1,90E+00	0,00E+00		0,00E+00		
7440-47-3	chromium (VI)	52	298			1,90E+00	0,00E+00		0,00E+00		
7439-92-1	lead	207,2	298			1,00E-01	0,00E+00		0,00E+00		
7439-97-6	mercury	200,6	298			2,90E+01	1,60E-01		5,52E-03		
7440-02-0	nickel	58,7	298			1,70E+00	0,00E+00		0,00E+00		
7012-37-5	PCB28	257,54	298	283,15		1,02E-03	2,45E-02	6,43E-03	2,41E+01		
35693-99-3	PCB52	291,99	298			2,33E-04	3,08E-02		1,32E+02		
37680-73-2	PCB101	326,4	298			4,41E-05	2,45E-03		5,55E+01		
31508-00-6	PCB118	326,4	298	283,15		3,03E-04		1,77E-04			
35065-28-2	PCB138	360,9	298			1,27E-05	4,31E-04		3,39E+01		
35065-27-1	PCB153	360,88	298	283,15		1,45E-05	7,55E-04	9,69E-05	5,19E+01		
35065-29-3	PCB180	395,32	298	283,15		4,53E-06	1,42E-04	1,67E-05	3,14E+01		
32589-13-3	PCB77	291,99	298			1,00E-04	1,28E-03		1,28E+01		
70362-50-4	PCB81	291,99	298								
57465-28-8	PCB126	326,4	298								
32774-16-6	PCB169	360,88	298			8,78E-06	3,28E-05		3,73E+00		

Figure 13: Chemical properties of selected chemicals and pesticides

4.7.2 Belgian agriculture

4.7.2.1 Farm bookkeeping

Bookkeeping data of typical farms in Belgium were collected at the level of an agricultural region, for each farm type, i.e., technological economical orientation (dairy farm, mixed farming, plant production farm, …) from the CLE-bookkeeping network (Centrum voor Landbouweconomie) and data . Typical data collected were:

- number of farms
- agricultural area
- number of animals
- total animal manure production
- use of fertilizers and manure
- excess of manure
- animal concentrates
- crop yield

The data were stored in a relational MS-ACCESS® database. They allow for calculating contaminant fluxes at the farm-level, for each type of farm and agricultural region. Within this project, no use is made of this option and contaminant transfer is calculated based on concentrations which were incorporated in the food consumption data.

4.7.2.2 Animal production

Specific data on animal production for various common animals (cows, pigs, sheep, chicken) were collected from BREFs on Slaughterhouses and Nubel, 1999. It concerns:

- animal housing
- milk production
- egg production
- fat content
- meat/offal production

4.7.2.3 Crop properties

The majority of the crop properties (lipid content, water content, interception fraction, growth period, surface area, crop volume, weathering constant…) were collected. Data on crop composition were obtained from Belgian and Dutch food composition data (fooddata.nl and Belgische voedingsmiddelenlijst).

4.7.2.4 Soil parameters

Data on soil properties were obtained from the AARDEWERK database (Van Orshoven and Vandenbroecke, 1993) containing information on basic soil profile properties gathered in intensive soil surveys largely conducted in the period between 1947 and 1971. The database contains information on basic soil properties (e.g., texture, organic matter content, clay content, pH, cation exchange capacity) from about 13000 soil profiles and approximately 70000 soil layers. The data were collected for the dominant soil types grouped per agricultural region and per land-use type (meadow or arable land).

4.7.3 Background contaminant levels in food and environment

Contaminant levels (heavy metals, pesticide residues, PCBs and dioxins in food products and animal feedstuffs were obtained from the European SCOOP report 3.2.1.1 ‘Assessment of the dietary exposure to arsenic, cadmium, lead and mercury of the EU Member States (March 2004), and completed with data from scientific literature (e.g. Focant et al., 2002; Baars et al., 2004, …)

5 MODEL DEMONSTRATION

5.1 Cadmium in the Kempen

5.1.1 Introduction

The Kempen is a heavy metal-contaminated area of about 2700 km^2 situated at both sides of the Dutch-Belgian border (see Figure 14). The area is contaminated by the emissions of former and operating zinc smelters during the past hundred years. As a result, the topsoil is contaminated with Cd and Zn to levels above intervention values close to the non-ferrous industries of Balen, Lommel (now closed) and Overpelt. Due to a relatively high mobility of the metals, this has resulted in increased levels of the metals in the groundwater and the food products.

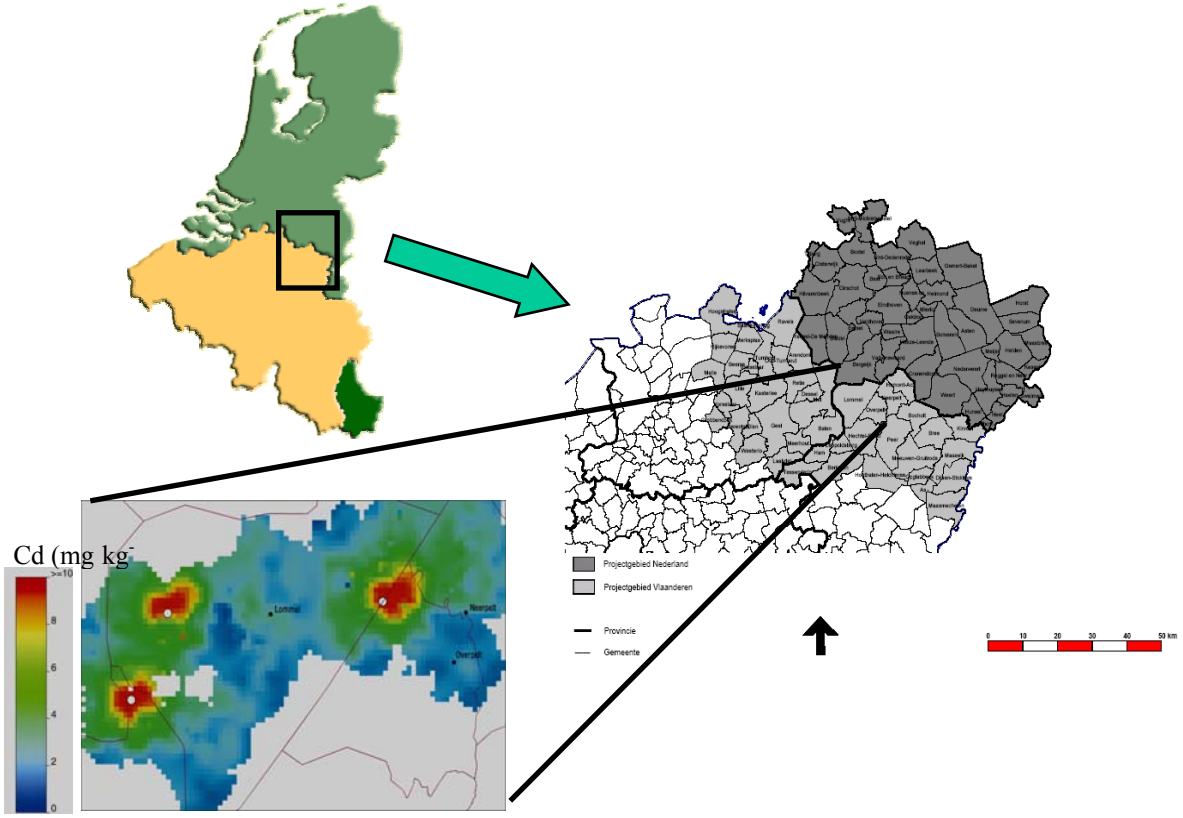


Figure 14:Location of the former and operating non-ferrous industries in the Kempen and map of cadmium contents in the topsoil.

The area is intensively investigated in terms of heavy metal concentrations, the various fluxes of metals to the soil and in the agro-ecosystem. We applied XtraFood to calculate primary food product concentrations of cadmium close to the industrial sites of Balen, Lommel and Overpelt and compared the predictions with results of an independent monitoring campaign held by by the Belgian Federal Agency for Food Safety (FAVV) in 2004 in the same region (FAVV, 2005).

5.1.2 Data on chemical concentrations in the Kempen

Data on concentrations in air, soil and water close to the non-ferrous industrial sites are compiled in Table 17. Elevated deposition data as compared to the background are largely due to resuspension of contaminated soil and dust, collected in the jars, and do not represent primary deposition.

Table 17: Chemical concentrations in the environment close to non-ferrous industry

	source data	stat. parameter	location measuring points	# data	period	data
						mg/m²/year
deposition	**Umicore (edge of sites)**	geomean	Balen & Overpelt	72	2000-2005	6,0
		median	Balen & Overpelt	72	2000-2005	6,0
		P5	Balen & Overpelt	72	2000-2005	1,3
		P25	Balen & Overpelt	72	2000-2005	2,9
		P75	Balen & Overpelt	72	2000-2005	8,0
		P95	Balen & Overpelt	72	2000-2005	11,7
	VMM, 2004	geomean	background (nature)	8	2004	0,07
		median	background (nature)	8	2004	0,07
		P5	background (nature)	8	2004	0,05
		P25	background (nature)	8	2004	0,07
		P75	background (nature)	8	2004	0,07
		P95	background (nature)	8	2004	0,10
						mg/m³
air (PM 10)	**VMM, 2004**	average	lommel & overpelt	227	2004	0,000001
		median	lommel & overpelt	227	2004	0,000001
		P10	lommel & overpelt	227	2004	0,000001
		P25	lommel & overpelt	227	2004	0,000001
		P75	lommel & overpelt	227	2004	0,000003
		P95	lommel & overpelt	227	2004	0,000012
		background	Knokke	300	2004	0,000001
						mg/l
ground water	**IHE, 1985**	*average*	kempen (restricted as test case)	2589	1983	0,0102
		median	kempen (restricted as test case)	2589	1983	0,0046
		P5	kempen (restricted as test case)	2589	1983	0,0006
		P25	kempen (restricted as test case)	2589	1983	0,0021
		P75	kempen (restricted as test case)	2589	1983	0,011
		P95	kempen (restricted as test case)	2589	1983	0,037
	source data	**stat. parameter**	**location measuring points**	**# data**	**period**	**data**
		background	Flanders			0,001
						mg/kg
soil	**VITO database, 2006**	*average*	kempen (restricted as test case)	1912	1980-1998	3,1
		median	kempen (restricted as test case)	1912	1980-1998	2,7
		P5	kempen (restricted as test case)	1912	1980-1998	0,5
		P25	kempen (restricted as test case)	1912	1980-1998	1,6
		P75	kempen (restricted as test case)	1912	1980-1998	4,4
		P95	kempen (restricted as test case)	1912	1980-1998	9,4
	CODA, 2000	background	Flanders, zandstreeks			0,32

5.1.3 Scenarios

In the calculations various scenarios using different percentiles of the statistical distribution (P5, P25, P50, P75 and P95) were used to calculate Cd concentrations in the primary food products. For example, the average scenario for the Kempen was calculated using average data for soil Cd, average deposition, average groundwater and average air data. The calculated concentrations were compared to measured data by FAVV (2005). The results are dispayed in Figure 15.

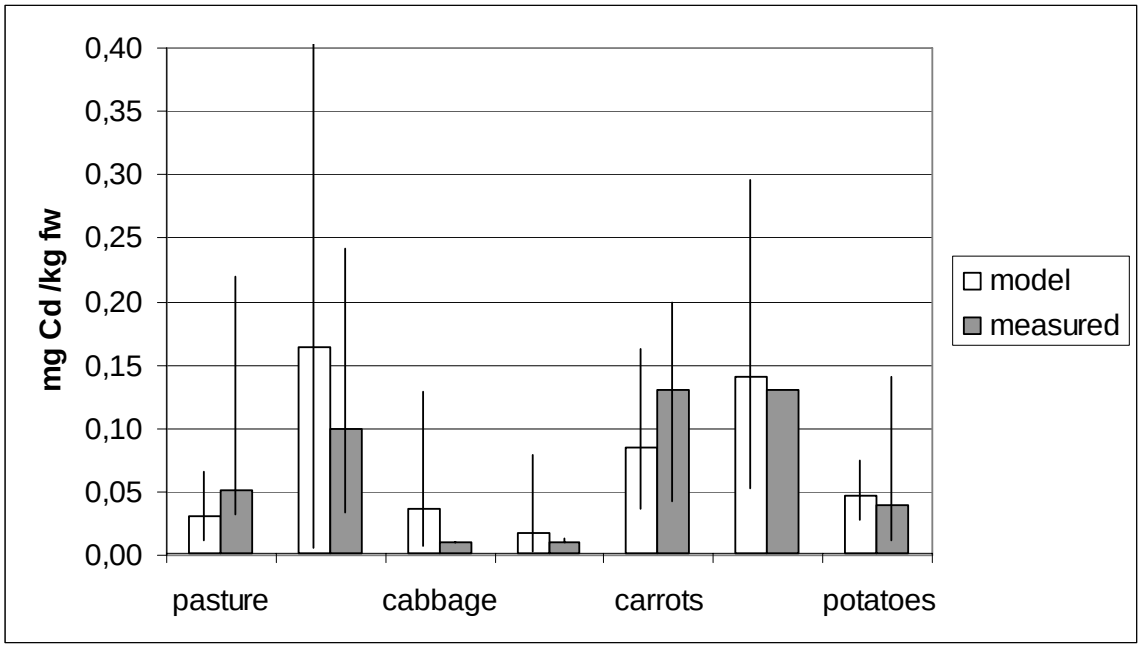


Figure 15: Measured versus predicted Cd concentrations in animal feed crops (pasture, maize, on dry weight basis)) and food crops (cabbage, beans, carrots, leek and potatoes, on wet weight basis). Bars represent median concentrations. Error bars represent minimum and maximum for measured concentrations and P5 and P95 for calculated concentrations.

Among all crops, there was a wide range in measured Cd concentrations in the Kempen. The overlap of error bars of predicted Cd concentrations with error bars of measured concentration suggests a realistic prediction of Cd crop concentration. Concentration for the median environmental contamination in the Kempen are below maximum levels in foodstuffs set by the European Commission for potatoes (0,10 mg Cd/kg fw), cabbage and beans (0,05 mg Cd/kg fw). In contrast, these Cd crop limits were exceeded for leek and carrots (0,10 mg Cd/kg fw). Cadmium concentrations in animal feed crops were below maximum levels for animal feed (maize & pasture: 1 mg Cd/kg feedstuff with a moisture content of 12%).
Limit exceeding is predicted for beans and cabbage under a worst case scenario (P95 environmental contamination), though these exceedings are not confirmed by measured data. The reverse is true for potatoes: the model does not predict limit exceeding under a worst case scenario P95, whereas it was observed in the measured dataset.

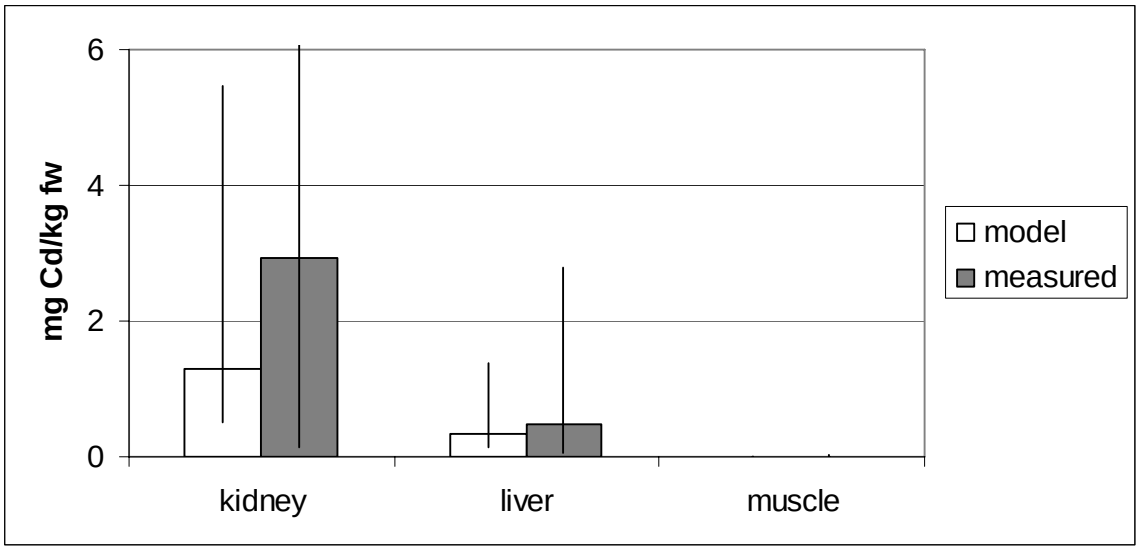


Figure 16: Measured versus predicted Cd concentrations in animal products. Bars represent average concentrations. Error bars represent minimum and maximum for measured concentrations and P5 and P95 for calculated concentrations

Average Cd concentrations in muscle were below the detection limit for Cd (0,01 mg/kg). Model calculations were also below 0,01 mg Cd/kg (P95: 0,004 mg Cd/kg). There was a wide range in measured Cd concentrations in kidney. Predicted Cd concentrations for kidney fell in that range. Cadmium concentrations in liver were lower than in kidney; this trend was also predicted with the Xtrafood model. A wide variety in measured concentrations was also observed for liver. The model predicts for average Cd environmental contamination in the Kempen Cd concentrations in in kidney above the EU limit of 1 mg Cd/kg for kidney (European Commission, 1997). Maximal level of Cd in kidney samples of the Kempen exceeded more than 10-fold this limit. Average prediction Cd in liver is below the limit of 0,5 mg Cd/kg, but might be exceeded in a worst case scenario, and exceeding of the limit was also observed in the Kempen (Figure 16).

5.1.4 Exposure to Cd by food intake in the Kempen

Exposure to Cd by food intake in the Kempen was assessed by combining the food consumption records for the Belgian population (see 4.4.1) with Cd concentrations in farm-bound foods predicted with the Xtrafood transfer module using environmental conditions specific for the Kempen (methodology: 4.4.2). Exposure was assessed by combining food consumption and Cd concentration at the finest detail level of the food consumption records, i.e. at subclass C2 level (see 4.4.1). Cadmium concentrations in non-farm bound foods (e.g. fish) were derived from literature. In below described calculations, Cd reduction factors related with peeling, washing, frying and boiling were ignored. This conservative approach was preferred since the reduction factors were rather insecure for a number of food products (discussed above).

Cadmium exposure by food was calculated according to the following scenarios (see also table

a) **average** Cd contamination of soil, air, groundwater and deposition (Table 17). In this case, it was assumed that all eaten farm-bound foods were grown under these environmental conditions. Exposure was calculated for an average food consumption pattern.

b) **background** Cd contamination of soil, air, groundwater and deposition for the sandy region (i.e. excluding the contaminated region in the Kempen). It was assumed that all eaten farm-bound foods were grown under these environmental conditions. Exposure was calculated for an average food consumption pattern.

c) **average** Cd contamination of soil, air, groundwater and deposition. In this case, it was assumed that 25 % of eaten farm-bound foods were grown under these environmental conditions and that 75 % was grown under background Cd conditions (case b). This is a more realistic scenario than case b. According to data from the Kempen (personal communication Tim Nawrot), the average is around 25% with large variation. This corresponds with values from France (CIBLEX). Exposure was calculated for an average food consumption pattern for 21-30 years old men (ML5).

d) same scenario as case c, except food consumption pattern. In the current case, P95 consumption of bread and breadproducts was considered.

In Table 18 these scenarios for 21-30 years old men (ML5) are displayed. Results (µg Cd uptake by food per day, and daily food consumption) are summarized by main food class. Case c is also shown for 21-30 years old women (VL5).

Table 18: Cd exposure by food intake in the Kempen for an average contamination scenario for different cases of consumption of locally grown food and food consumption patterns. (cases: see text)

	ML5								VL5	
	case a		case b		case c		case d		case c	
food product	weight g/day	Cd µg/day	weight g/day	Cd µg/day	weight g/day	Cd µg/day	weight g/day	Cd µg/day	weight g/day	Cd µg/day
potatoes and other tubers	155	6,92	155	3,5	155	4,34	155	4,34	92	2,57
vegetables	166	17,39	166	3,3	166	6,83	166	6,83	186	7,21
fruits	100	5,04	100	0,7	100	1,76	100	1,76	131	2,05
juices	153	0,73	153	0,4	153	0,46	153	0,46	109	0,40
soups	48	2,41	48	0,7	48	1,11	48	1,11	48	1,11
sugar and confectionery	54	0,27	54	0,3	54	0,27	54	0,27	41	4,58
fats	34	0,15	34	0,2	34	0,15	34	0,15	14	0,07
sauces	17	0,01	17	0,0	17	0,01	17	0,01	22	0,01
non-alcoholic drinks	1138	0,32	1138	0,3	1138	0,32	1138	0,32	1249	0,31
alcoholic drinks	267	0,10	267	0,1	267	0,10	267	0,10	94	0,04
sojaproducts	10	0,00	10	0,0	10	0,00	10	0,00	10	0,00
bread and bread products	201	31,83	201	11,4	201	16,53	344	28,53	118	9,71
breakfast cereals	12	2,13	12	0,8	12	1,10	12	1,10	11	1,03
cereal products	38	3,73	38	1,3	38	1,93	38	1,93	52	2,61
rice	29	2,52	29	2,5	29	2,52	29	2,52	20	1,69
pasta	42	4,25	42	1,5	42	2,20	42	2,20	33	1,65
flour, binders and other grain products	1	0,35	1	0,1	1	0,18	1	0,18	2	0,31
wheat flour	2	0,37	2	0,1	2	0,19	2	0,19	1	0,10
meat	124	0,15	124	0,1	124	0,08	124	0,08	98	0,06
kidney and liver	1	0,33	1	0,1	1	0,17	1	0,17	1	0,23
poultry	31	0,03	31	0,0	31	0,02	31	0,02	25	0,01
game	0	0,00	0	0,0	0	0,00	0	0,00	0	0,00
meat substitute	1	0,01	1	0,0	1	0,01	1	0,01	6	0,06
milk and milk products	224	0,28	224	0,3	224	0,28	224	0,28	256	0,40
cheeses	31	0,31	31	0,3	31	0,31	31	0,31	31	0,31
eggs	11	0,01	11	0,0	11	0,01	11	0,01	9	0,01
fish and shellfish	35	0,72	35	0,7	35	0,72	35	0,72	27	0,69
varia	1	0,01	1	0,0	1	0,01	1	0,01	0	0,00
composed foods	46	3,93	46	1,4	46	2,04	46	2,04	43	1,89
sum	2971	**84**	2971	**30**	2971	**44**	3113	**56**	2729	**39**

The relative contribution of the various food groups is given in Figure 17. Only food items which constitute more than 1 % of the Cd intake are included (the total amounts to more than 95% of the Cd intake). Intake is expressed per kg body weight. The body weight used for men is 80 kg and for women 64 kg (Health survey Belgium).

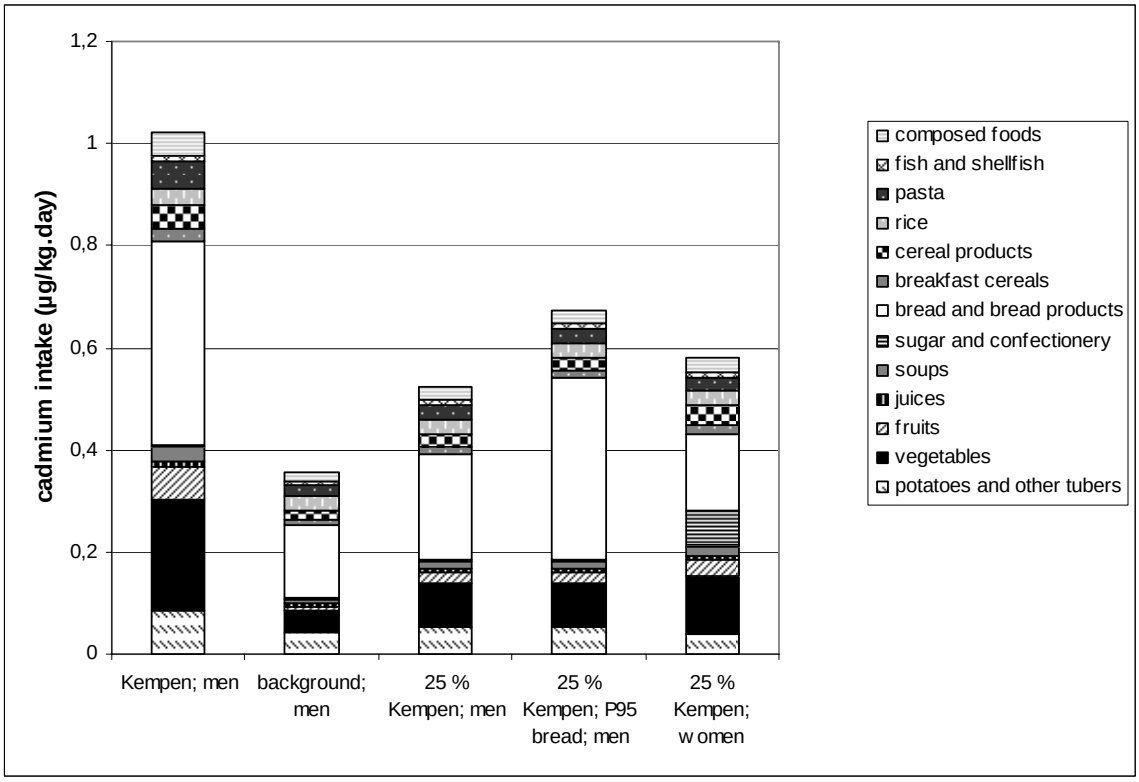


Figure 17: Relative contribution of food items to total cadmium intake

The main contribution comes from bread and bread products in all scenarios, followed by vegetables and potatoes. For women there seems to be a significant contribution from sweets. As it is assumed that cereals (bread and bread products), vegetables and potatoes are locally grown in the a and c scenarios, the contribution from the Kempen area is mainly seen in these food items.Assuming a 25 % contribution of food from the Kempen increases the Cd exposure in adults with about 50 %.

Case b (average environmental contamination the Kempen; 25 % locally grown food and average food consumption) was calculated for all age/gender categories in order to assess the lifetime exposure (Table 19).

Table 19: Cd exposure by food consumption (case b) for all age/gender categories for average Cd contamination in the Kempen

men			women		
cat.	total weight food g/day (including drinks)	µg Cd/day	cat.	total weight food g/day (including drinks)	µg Cd/day
ML1	1607	24	VL1	1515	22
ML2	1861	29	VL2	1682	26
ML3	2194	37	VL3	1901	31
ML4	2752	46	VL4	2223	35
ML5	2971	44	VL5	2729	39
ML6	3078	52	VL6	2881	41
ML7	3095	50	VL7	2966	42
ML8	3125	53	VL8	3065	43
ML9	2956	49	VL9	2906	40

The data from Table 19 were converted to doses on a body weight basis, using 50 percentile data from VUB and from the Belgian Health Survey (WIV). For adults, average and 50 percentiles do not show much difference. The dose per age group and the average dose calculated at 50 years of age (cumulative dose from 3 – 50 years divided by total number of years) are shown in Figure 18.

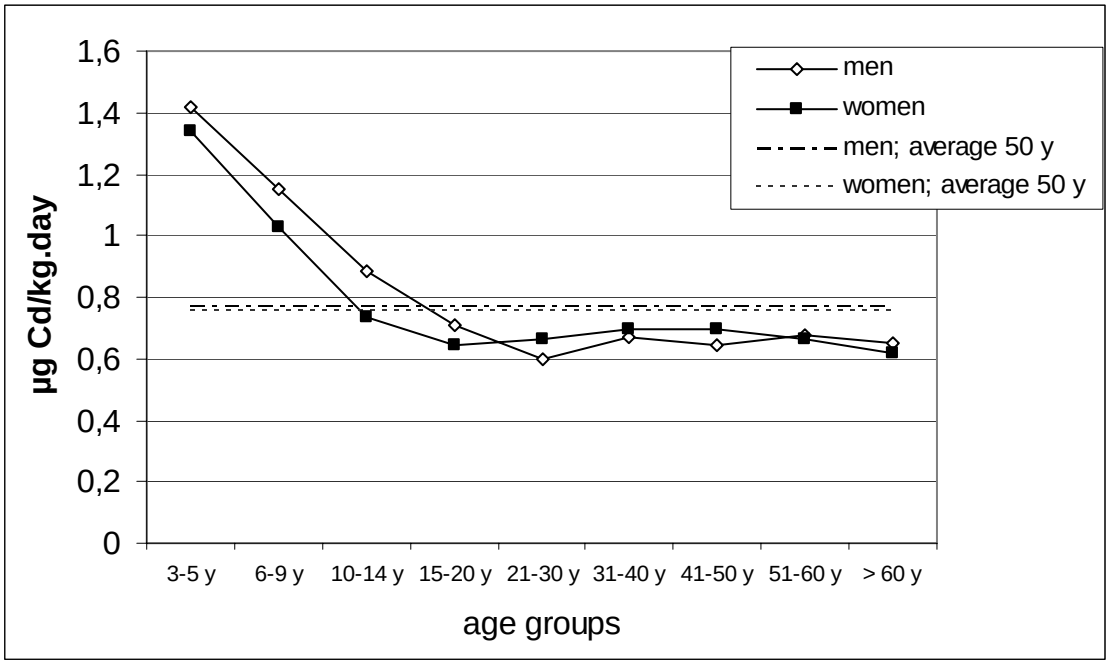


Figure 18: Cadmium intake per age group and cumulative cadmium intake at 50 year

From the curves, it is clear that children are higher exposed than adults; exposure levels off at the age of 15 – 20 years. Differences between men and women are seen, mainly at younger age. On a cumulative basis (average dose at 50 years) the difference is very limited. This high exposure at young age is a point of attention; however for cadmium the risk for renal effects (critical endpoint) is related to the cumulative dose at about 50 years.

Other sources of exposure to cadmium are inhalation of air, intake of soil (mainly by children) and smoking. Taking the data from the EU Risk Assessment Report for cadmium, the intake from air, soil and smoking is estimated to amount to the values displayed in Table 20.

Table 20: Estimated exposure from various routes compared to the calculated dietary exposure in scenario c

route	external dose (ng/kg.d)	internal dose (ng/kg.d)	absorption (from: RAR)
air[1]	1,3 - 4	0,3 – 1	25 %
dust[2]	8,4	0,25	3 %
smoking[3]	253	6,3 – 12,7	2,5 – 5 %
diet (scenario c)	770	23,1	3 %

[1]: concentration in air: 5 – 15 ng/m³ (from: RAR); [2]: soil concentration 7 mg/kg; [3]: 20 cigarettes/day, 1 – 2 µg Cd/cigarette (from: RAR)

5.2 Dioxins in Menen

5.2.1 Introduction

Deposition of dioxins due to emissions of an incinerator plant have elevated dioxin topsoil concentrations in Menen (Figure: see annex) around the this point source. At the moment, emissions from the incinerator plant are below the limit of 0,1 ng I-TEQ/Nm³. However, soil concentrations exceed background values on average by factor 10 and elevated dioxin concentrations in free range chicken eggs (and some crops, e.g. pumpkin) of home-gardens were measured (Nauwen et al., 2003).

Figure 19: Location of IMVO incinerator plant in Menen and sampling locations for soil, milk, eggs, vegetables and deposition measuring location points.

5.2.2 Data on chemical concentrations in the Menen

Data on concentrations in air, soil and deposition data in Menen are summarized in Table 21.

Table 21: Chemical concentrations in the environment close to incinerator plant in Menen

	source	stat. parameter	location measuring points	# data	period	data
						pg I-TEQ/m²/day
deposition	**VMM, 2004**	average	Menen	68	1998-2004	10,4
		median	Menen	68	1998-2004	10,6
		P5	Menen	68	1998-2004	2,6
		P25	Menen	68	1998-2004	5,2
		P75	Menen	68	1998-2004	14,5
		P95	Menen	68	1998-2004	43,6
		background				4,0
						I-TEQ fg/m³
air (total)	**VMM, 2004**	average	Menen	1	2000	213
		background	Mol	9	1999	*27*
						I-TEQ pg/l
groundwater		average and background	*default: zero*	0	-	0
						ng I-TEQ/kg ds
soil	**Vito database, 2000**	average	Menen	35	1995-2002	22,3
		median	Menen	35	1995-2002	21,6
		P5	Menen	35	1995-2002	4,3
		P25	Menen	35	1995-2002	11,0
		P75	Menen	35	1995-2002	29,3
		P95	Menen	35	1995-2002	52,0
	Vito database, 2003	average	Menen	5	2003	19,0
		median	Menen	5	2003	16,7
		P5	Menen	5	2003	10,8
		P25	Menen	5	2003	11,9
		P75	Menen	5	2003	20,0
		P95	Menen	5	2003	33,9
	Vito report	background			2003	2,0

Two sets of soil data are listed. The first dataset included more (35) samples than the second one (5). However, we used the second one for transfer calculation since these 5 samples are collected at the same location as where crops were collected. The smallest dataset is also representative for the larger one.

Dioxin concentrations in Table 21 are reported in units of I-TEQ (toxic equivalent), i.e. as the sum of 17 dioxin congeners. In that sum, congener concentrations are weighted for toxicity relative to the most toxic congener 2, 3,7,8-TCDD.

Transfer calculations were performed for each dioxin congener individually (details not shown in Table 21) since transfer depends on congener-specific properties. However, deposition (and air) data were available as the sum of total dioxins and not individually for each congener. Therefore, the average distribution of congeners in soil was used as partitioning key for deposition. Rationale for this relies in the direct relation between deposition and soil contaminated. Dioxins are not naturally present in the environment.

Table 22: relative contribution of different congeners in the total dioxin concentration (I-TEQ-units) in soils in Menen..

congener	fraction of total dioxins TEQ	standard deviation
1,2,3,4,6,7,8-H7CDD	4,1%	2%
1,2,3,4,6,7,8-H7CDF	2,8%	1%
1,2,3,4,7,8,9-H7CDF	0,3%	0%
1,2,3,4,7,8-H6CDD	3,0%	0%
1,2,3,4,7,8-H6CDF	6,6%	0%
1,2,3,6,7,8-H6CDD	4,3%	1%
1,2,3,6,7,8-H6CDF	6,2%	0%
1,2,3,7,8,9-H6CDD	3,9%	1%
1,2,3,7,8,9-H6CDF	1,7%	0%
1,2,3,7,8-P5CDD	27,1%	3%
1,2,3,7,8-P5CDF	1,7%	0%
2,3,4,6,7,8-H6CDF	7,2%	0%
2,3,4,7,8-P5CDF	27,5%	3%
2,3,7,8-T4CDD	4,6%	1%
2,3,7,8-T4CDF	2,9%	1%
O8CDD	0,2%	0%
O8CDF	0,0%	0%

5.2.3 Scenarios

In the calculations various scenarios using different percentiles of the statistical distribution (P5, P25, P50, P75 and P95) were used to calculate dioxin concentrations in the primary food products. The calculated concentrations were compared to measured data by Vito (2003). Transfer was calculated for each dioxin congener separately and than summed. Prediction of the total sum of dioxins in endives, courgettes, carrots and pumpkins are presented in Figure 20. In addition, more details on distribution over the 6 major congeners that were present in carrots are given in Figure 21. Prediction of the total sum of dioxins in animal products (meat, milk and eggs) are given in Figure 22 and distribution the 6 major congeners that were present in eggs are given in Figure 23.

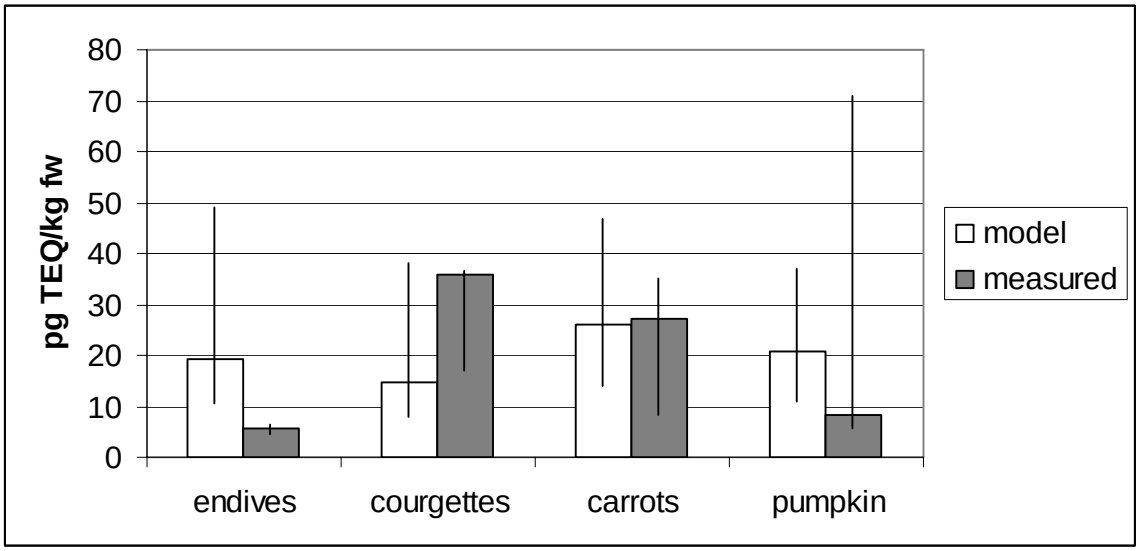


Figure 20: Measured versus predicted dioxin concentrations (expressed as TEQ-equivalent, i.e. concentrations expressed on toxic equivalent basis relative to the most toxic congener 2,3,7,8-TCDD) in food crops (endives,courgettes, carrots and pumpkin; on wet weight basis). Bars represent median concentrations. Error bars represent minimum and maximum for measured concentrations and P5 and P95 for calculated concentrations.

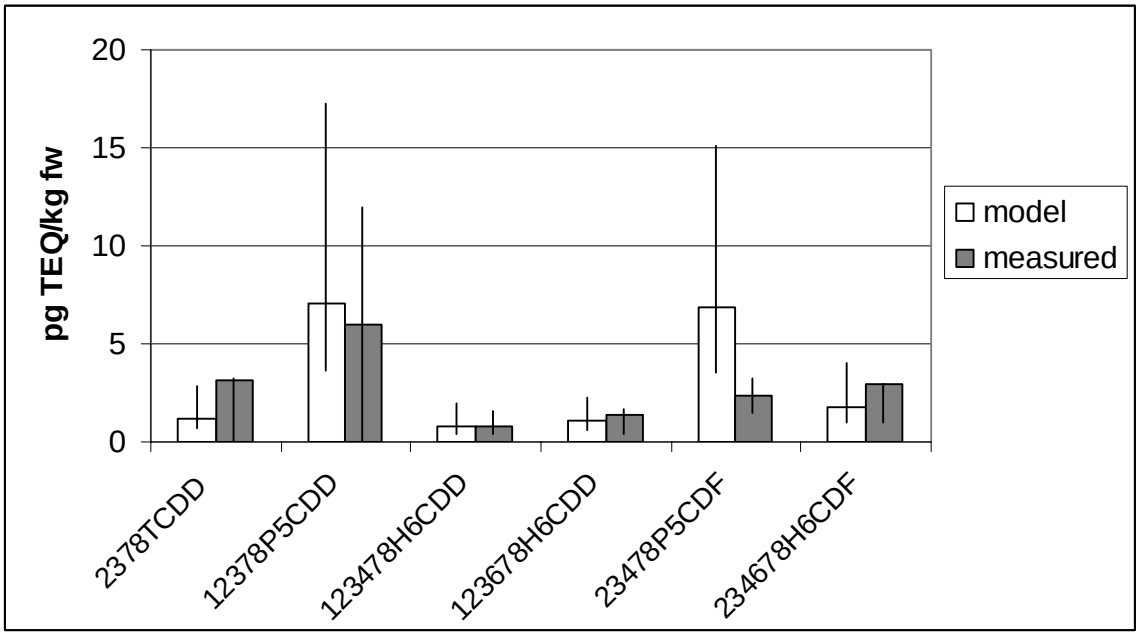


Figure 21: Measured versus predicted concentrations of 6 dioxin congeners in carrots in Menen. The 6 selected congeners were the ones with the largest contribution to total TEQ. Bars represent median concentrations. Error bars represent minimum and maximum for measured concentrations and P5 and P95 for calculated concentrations

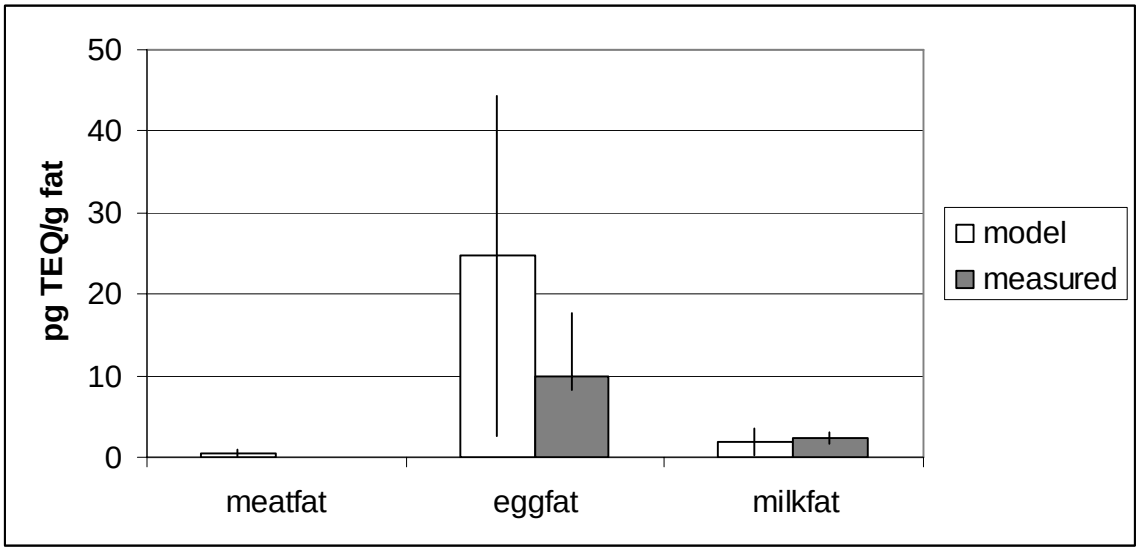


Figure 22: Measured versus predicted concentrations of total sum of dioxin congeners animal products in Menen. (expressed on fat basis). Error bars represent minimum and maximum for measured concentrations and P5 and P95 for calculated concentration. No validation data for dioxins in meat in Menen were available.

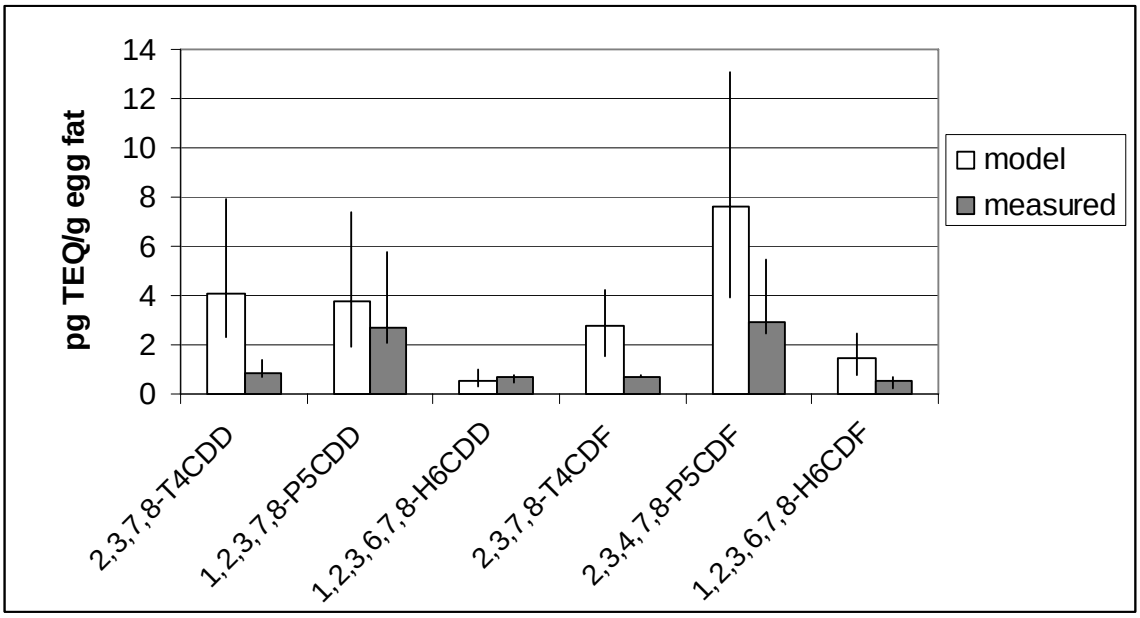


Figure 23: Measured versus predicted concentrations of 6 dioxin congeners in free range eggs in Menen. The 6 selected congeners were the ones with the largest contribution to total TEQ. Bars represent median concentrations. Error bars represent minimum and maximum for measured concentrations and P5 and P95 for calculated concentrations

The Xtrafood model predicted dioxin concentrations excellent for carrots, reasonably well for courgettes and pumpkins, but overpredicted transfer to endives. Predictions of individual congener concentrations in carrots were in agreement with measurements. The major contribution of congeners 2,3,4,7,8 P5CDF and 1,2,3,7,8 P5CDD in soil is reflected in the dioxin congener profiles in carrots.

Irrespective of the environmental contamination scenario (average or worst case), predicted and measured concentrations of dioxins are all below limits and action levels of 0,4 pg WHO-TEQ/g fresh weight (~ 0,3 pg I-TEQ/kg) for dioxins in fruits and vegetables (European Commision, 2001).

Transfer of dioxins to animal fat is largest for egg fat, followed by milk and, and lowest for meat fat. The Xtrafood model overpredicted transfer to egg fat by factor 3, while the match between model and measured data was better for milk. No validation data for dioxins in meat in Menen were available. Concentrations in meat fat (here: cow) were close to concentrations reported for beef in Belgium (1,56 pg TEQ/g fat; Focant *et al.,* 2002). Congener profiles in egg fat are also similar to congener profiles in soils. Mainly concentrations of the most toxic congeners, 2,3,7,8-TCDD and 2,3,7,8-TCDF were overpredicted by the Xtrafood model.

The overprediction of dioxins in eggfat by the current Xtrafood model is probably related with the selection of BCF_{egg} factors from a literature survey. For each dioxin congener, one average BCFegg factor was used in the Xtrafood model and this value was derived as the average of different values found in literature. However, chicken housing conditions and 'chicken density' (i.e. number of chickens per unit area) are known to affect BCF_{egg}. (Schuler et al.,1997). Gathering information related to these conditions for the specific cases of Menen and refinement of the Xtrafood model with 'chicken density' dependent BCF_{egg} factors could probably reduce the discrepancy between model and measured dioxin concentration in eggfat.

Predicted and measured median concentrations in egg fat largely exceed the maximum limit of 3 pg WHO-TEQ/g fat.

5.2.4 Exposure to dioxins in Menen

Since the contaminated area of Menen is rather small (compared to the Kempen case), it is not useful to calculate food exposure for the complete food package for people in Menen. It is not realistic that people living in Menen drink only milk from a local farm in Menen, and that all animal products originate from that small area. Milk of a single farm (on average 1000 l) is mixed with milk produced outside the dioxin contaminated region of Menen in collector tanks of 250000 liter.

For the Menen case, assessment of dioxins exposure of home-garden free range chicken eggs and home-garden vegetables, in combination with background dioxin levels of not-garden grown foods would be more meaningful. However, for some important (home-garden) crops (e.g. potatoes) in the food package the current Xtrafood model predicts rather high dioxins levels in Menen. No validation for potatoes could be performed for Menen, since no measured data were available for potatoes in Menen. However, predicted concentrations were > 20-fold above concentrations reported in literature (3,9 pg TEQ/kg fresh weight). Exposure calculations with these overpredicted dioxin levels in potatoes overestimates the dioxin flux via potatoes by food exposure to unrealistic values. Focant *et al.* (2002) reported that major food classes contributing to dioxin dietary intake in Belgian foodstuffs were 1) fish and seafoods (39%), 2) meat and meatproducts (31%) and 3) milk and diary products (30 %). A recent Vito study (Dioxine problematiek in Menen, 2003) also showed that consumption of home-grown crops in Menen should not be restricted since it this pathway only marginally contributed to dioxin dietary intake. The only home-garden related product with major contribution to dioxin dietary exposure are eggs. Focant *et al.* (2002) reported a dietary intake of 7,34 pg TEQ/day by consumption of eggs (2,76 pg TEQ/ g fat for an 'average belgian egg'), accounting for 11 % of total (average) dioxin dietary intake (65 pg TEQ/day) for Belgian adults. Under the assumption of the same egg consumption rate and 100 % contribution of free-range chicken eggs in Menen (median: 9,86 pg TEQ/g fat) to the total egg consumption, dioxin dietary exposure of 26 pg TEQ/day via egg fat is expected and could increase the dioxin dietary exposure from 65 to 84 pg TEQ/ day.
It is noted that the risk assessment of consumption of free-range chicken eggs in Menen should be not only investigate the dioxin exposure, but also risks related to PCBs should be evaluated. Toxicity of

PCBs and dioxins is synergetic and these compounds often . Transfer of PCBs to crops and and animals was however beyond the scope of the current Xtrafood model.

6 CONCLUSIONS

6.1 Task A: Transfer in the agro-ecosystem

The objectives of Task A were to develop:
-mass balance model for soils
-transfer model to primary food products

The objectives were met. The project resulted in a complete transfer model for calculating contaminant transfers in a farm system. The developed model is capable of calculating concentrations of contaminants in primary food products based on concentrations in the environment (soil, water, air) and on concentrations in various other inputs such as animal feed, specific applications of contaminants, input from fertilizers and manure. The mathematical model descriptions are obtained from literature representing the state-of-the-art in modeling contaminant transfer in the environment-plant-cattle pathway. Both inorganic and organic contaminants can be modeled. Various subparts of the model chain were evaluated with either data from the literature or from the demonstration cases. This has resulted in a validated transfer model.

The model is generic in the sense that transfer of new chemicals can be calculated based on physical-chemical properties of the chemical. This enables the user to use the model to calculate transfer when an incident happens and the impact on food quality needs to be assessed. One limitation of the model is that it cannot deal with ionic organic contaminants. Their behaviour is fundamentally different from the apolar organic chemicals and was beyond the scope of the project. New versions of the model should be adapted to allow for calculating transfer of ionic substances.

A specific residue model for pesticides was developed within the XtraFood framework. The pesticide model calculates dissipation of pesticides after application. The model takes into account the way of application, the properties of the pesticide, the properties of the plant, the effect of multiple applications. The model was validated against data from the residue database and proved to be valuable for worst case predictions.

6.2 Task B: Human exposure and impact analysis

The objectives of part B were to:
-estimate human exposure to primary food products and risk characterization
-estimate health impacts (including costs)
Human exposure is assessed using existing studies on food consumption and not from the new belgian food consumption survey, since the results arrived late for this project. The structure of the model allows data from the new food consumption survey to be incorporated. An extensive food consumption data package was defined taking into account variability between ages and between gender. The food products were aggregated in such a way that coupling between the farm model and the human diet could be made. The model allows to incorporate dilution factors to extrapolate from the farm products to the human diet. Provisions to assess the effect of preparation on contaminant fluxes were made in the model.
A methodology is developed to perform a risk characterization of contaminated food. Risk characterization options in XtraFood are provided for chronic exposures.
The objectives of Part B were partially met. The model allows to make a risk characterization for chronic exposures, but not for acute exposure. Risks are characterized by means of comparison of exposure through the human diet and acceptable toxicological levels. It was already agreed upon that impact assessment was not to be included in the final model.

6.3 Task C: Integration of transfer and exposure in XtraFood

The objective of Task C was to develop an integrated calculation tool for performing targeted calculations.

The objective of Task C was met. A lot of effort was put to the coupling of the transfer model to the human exposure assessment within the SQL based XtraFood code. This has resulted in a more user-friendly software environment where contaminant concentrations are calculated for a variety of food products and where the calculated concentrations are automatically imported in the food consumption database to calculate human exposure. The user can introduce contamination events such as incidents in some parts of the food chain.

6.4 Task D: Demonstration

The objective of Task D was to demonstrate the model for three cases:
-cadmium in the Kempen
-dioxins
-pesticides
The objectives were partially met. For Cadmium, the full chain was demonstrated and risks were characterized. For dioxins, calculations of human exposure were performed. For pesticides, the transfers were calculated and compared to pesticide residues from measurement databases. Given the complexity of human exposure to pesticides and the scientific debate and uncertainty in estimating risks from exposure to pesticides, it was felt that a full risk characterisation was impossible within the scope of the project. The proposed methodology does not allow for characterization of acute effects, which is important for pesticides.

6.5 Variability and uncertainty

At various steps within the project, the issue of variability and uncertainty is addressed.

Variability is an intrinsic property of the system or process under study. In case of modeling food exposure by transfer through the primary food chain it refers to:
-variability in contaminant concentrations in the agro-food chain;
-variability in parameters related to transfer of chemicals in the primary food chain, i.e., soil properties, crop properties, cattle properties, …;
-variability in parameters related to human exposure, i.e., human behaviour, human sensitivity to contaminants, food intake, …
Uncertainty is a lack of knowledge about a process, a parameter, a model. In our case it refers to:
-uncertainty about measurements, parameters and variables, i.e., a measured environmental contaminant concentration, uncertainty about a value of food intake, …
-uncertainty about processes and models, i.e., a steady state model for transfer of chemicals to animal or crop products, …;
How we dealt with variability within this project:
-we constructed databases of model input parameters and variables, containing ranges of values that can be used to calculate percentiles or do scenario analyses;
-we calculated with a percentile value of a parameter that corresponds to a reasonable worst case scenario (e.g., biotransfer factor, food intake value, …);
-we calculated with a minimum and maximum value of the variable to obtain minimum and maximum exposure or effect values; preliminary check on the sensitivity of the system to variation in model parameters;
-we did not perform a full sensitivity and uncertainty analysis that use Monte-Carlo sampling techniques that exploit the full range of information related to the statistical distribution of the

variable; if the information is available, it can be coupled to the model using specific software such as Crystal Ball. The Monte-Carlo techniques are well-known in studies estimating exposure to food contaminants (see e.g. EU 5FP Monte-Carlo project, teenager exposure by Ugent, …)
How we can deal with uncertainty:
-take into account measurement uncertainty; labs that report numbers of contaminant levels in various environmental matrices, need to specify the measurement uncertainty according to their accreditation; this is not taken into account within the project;
-try to assess model uncertainty by comparing predicted and observed variables or by comparing models (this is what has actually been done in the selection of the models);
-similar scenario analyses or Monte-carlo simulations can be performed; to discern between variabilty and uncertainty, advanced 2D-modeling techniques are available that are beyond the scope of the project.
To conclude, established protocols and software is available to take into account uncertainty and variability. The databases, the transfer and exposure model developed in this project, aim to provide a reliable estimate of the risk associated to contaminated primary food products. We have been applying implicit and explicit methods to deal with uncertainty, but a full uncertainty analysis is beyond the scope of the project.

6.6 Added value of the project for Belgian research and policy

The scientific added value is the development of a completely new integrated model that couples transfer models for the primary food chain to exposure models. Most research projects deal with either one of the themes, but fail on integrating them. The added value for the Belgian policy makers is that specific data on the Belgian agriculture, and exposure of the Belgian population are incorporated in the model. This allows users of the model to have specific calculations of contaminant transfer in the Belgian primary food production. It will support the Federal agencies dealing with food safety in performing realistic risk assessments for known and unknown chemicals.

7 ANNEXES

7.1 References

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7.2 Publications

XtraFood: an impact analysis model for contaminants in primary food production / P. Seuntjens, S. Claeys, A. Ruttens, C. Cornelis, W. Steurbaut, J. Vangronsveld.
EuroFoodChem XII: Strategies for safe foods - pg. 87- 90
KVCV, Belgie,
2003/IMS/P/0096

XtraFood: a model for the impact analysis of contaminants in primary food production / P. Seuntjens.
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Cornelis, C. 2004. XtraFood: a model for transfer of contaminants through the food chain. COST 859 Phytotechnologies, WG 4, UFZ Leipzig, Germany

The importance of plant transfer processes in the food chain model XtraFood / P. Seuntjens.
Cost 859 Phytotechnologies, Pisa, Italy, 2005-06-14 - 2005-06-16.
2005/IMS/M/0146

Xtrafood:a model for transfer and exposure of contaminants in the primary food chain / M. Van Holderbeke, C. Cornelis, P. Seuntjens.
Zware Metalen in het Leefmilieu Nieuwe inzichten, Nieuwe Wetten ?, Heverlee, Belgium, 2005-09-23.
2005/IMS/M/0243

XtraFOOD: an impact analysis model for contaminants in primary food production / M. Van Holderbeke, P. Seuntjens, C. Cornelis.
Themadag Aardwetenschappen in het Milieuwerkveld, Utrecht, The Netherlands, 2005-12-10.
2005/IMS/M/0312

Xtrafood: a model for the impact analysis of contaminants in primary food production / K. De Brouwere, M. Van Holderbeke, P. Seuntjens, C. Cornelis
International Satellite Congress of the Cluster Project 'Platform for Scientific Concertation: Food Safety', Belgium, Antwerp. 2006-16-05.
2006/IMS/M/0XXX

Zware metalen… zijn preventieve acties mogelijk? Presentatie van het ketenmodel voor de impactanalyse van contaminanten in de primaire voedselketen. K. De Brouwere
Seminarie rond contaminanten in AGF producten voor de leden van Belgapom, Vegebe, Nubelt en Nufeg. Affligem, 2006-06-22.
2006/IMS/M/0XXX

7.3 Members of the User Committee

The project has been stimulated by; and discussed with the user committee. The user committee consisted of agricultural and consumer representing instances and scientific and governmental institutions:

Belgapom/Vegebe/Nubelt – Beroepsvereniging voor Belgische handelaars en verwerkers van aardappelen/Beroepsvereniging voor groenteverwerking en handel in industriegroenten/Federatie van de groenten -en fruitexporteurs
Romain Cools

Bemefa - Beroepsvereniging van de mengvoederfabrikanten
Erik Hoeven

CODA – Centrum voor Onderzoek in Diergeneeskunde en Agrochemie – Departement Kwaliteit en Veiligheid
Luc Pussemier, Nadia Waegeneers

FOD Volksgezondheid, Veiligheid van de Voedselketen en Leefmilieu
Christine Vinckx, Sara Demuynck

Ministerie van Middenstand en Landbouw
Diederik Standaert

UGent, Vakgroep Maatschappelijke Gezondheidkunde
Stefaan De Henauw, Maaike Bilau

Venootschap Mechelse Veilingen
Luc Peeters

7.4 Summary of the agro-ecosystem transfer model

The following paragraphs summarize the selected model formulations for calculating contaminant transfer in the agro-ecosystem in XtraFood. The transfer model includes:

soil-plant-atmosphere transfer
transfer in soil
soil/crop – cattle transfer
pesticide residue modeling
agro – ecosystem transfer

7.4.1 Air partitioning

If the total air concentration is known, the gas phase and particle concentrations are calculated from gas/aerosol partitioning. The fraction of POP adsorbed on atmospheric aerosol particles is given by the Junge-Pankov model:

$$\phi = \frac{c \cdot \theta}{p_{OL} + c \cdot \theta}$$

where:

c is the Junge-Pankov constant [Pa.m]; $c = 0.17$
θ is the specific surface area of aerosol particles [$m^2.m^{-3}$]; $\theta = 1.5.10^{-4}$ for rural background; $\theta = 1.1.10^{-3}$ for urban conditions; $\theta = 4.2.10^{-5}$ for clean continental background
p_{OL} is the subcooled liquid vapour pressure [Pa], see Table

The subcooled liquid vapour pressure depends on temperature:

$$p_{OL} = p^0_{OL} \cdot \exp\left[-a_p\left(\frac{1}{T} - \frac{1}{T_0}\right)\right]$$

where:

T is the ambient temperature [K]
T_0 is the reference temperature [K]
p^0_{OL} is the value of pOL at the reference temperature T0 [Pa]
a_p is the coefficient of vapour pressure temperature dependence [K]

The choice of the formula depends on the availability of data. If few data on chemical properties are available, empirical formulas may be used. If the compound is a PCDD/PCDF, a PAH or an OCC (organochlorine compound), empirical constants a and b can be used to calculate the particle-gas partition constant K_p from K_{oa}:

$$\log K_P = a \log K_{OA} + b$$

where:

K_p is the particle-gas partition coefficient [$m^3.kg^{-1}$]
a, b are regression constants
K_{OA} is the octanol-air partition coefficient [$m^3.m^{-3}$]

The constants *a* and *b* depend on the class of chemicals. For PCDD/PCDFs *a*= 0.784 and *b*=-9.84, for PAHs *a*=0.79 and *b*=-10.01, and for OCC (incl. PCBs, …) *a*=0.55 and *b*=-8.23.

The temperature dependence of K_p is given by:

$$\log K_P = \left(m_T \cdot \frac{1}{T} \right) + b_T$$

where:

m_T and b_T are coefficients of temperature dependence
T is the ambient temperature [K]

The octanol-air partition coefficient is either given or can be calculated from:

$$K_{OA} = \frac{K_{OW} RT}{K_H}$$

where :

K_{OW} is the octanol-water partition coefficient
K_H is the Henry coefficient [Pa m^3 mol^{-1}]
R is the universal gas constant [Pa m^3 mol^{-1} K^{-1}]

The temperature dependence of K_{OA} is given by:

$$K_{OA} = K_{OA}^0 \cdot \exp\left[-a_k \left(\frac{1}{T} - \frac{1}{T_0} \right) \right]$$

where:

K^0_{OA} is the value of K_{OA} at the reference temperature T_0 [Pa]
a_k is the coefficient of K_{OA} temperature dependence [K]

$$K_H = \frac{K_{H0}}{RT} \exp\left[-a_H \left(\frac{1}{T} - \frac{1}{T_{H0}} \right) \right]$$

where:

K_{H0} is the Henry coefficient at reference temperature [Pa m^3 mol^{-1}]
R is the universal gas constant [Pa m^3 mol^{-1} K^{-1}] = 8,31451
T is the ambient temperature [K]
a_H is the Coefficient of the Henry coefficient temperature dependence
T_{H0} is the Reference temperature Henry constant [K]

The concentrations in either the gas phase or the particulate phase can be determined from the total air concentration:

$$C_{g,a} = (1 - \phi) \cdot C_{a,a}$$
$$C_{p,a} = \phi \cdot C_{a,a}$$
$$\phi = \frac{K_p \cdot TSP}{(TSP \cdot K_p + 1)}$$

where:

$C_{a,a}$ is the total concentration[10] in air [M m^{-3}]

[10] Concentration is expressed in mass units M that may range from pg or pg TEQ (dioxins) to mg (heavy metals)

$C_{g,a}$ is the gas phase concentration in air [M m^{-3}]
$C_{p,a}$ is the particle concentration in air [M m^{-3}]
TSP is the total suspended particles in air [kg m^{-3}]

7.4.2 Soil-plant-atmosphere transfer

Depending on the availability of air quality parameters, different process formulations are used to calculate plant concentrations from concentrations in air. It is assumed that heavy metals (except mercury) are deposited on plants by wet and dry particle deposition and that they do not partition between gas phase and particulate air phase. The soil-plant-atmosphere transfer is described by the PLANTX model (Trapp and Matthies, 1995), complemented with the atmosphere-plant particle deposition model of McLachlan (1999).

Organic chemicals

Aboveground plant parts

The concentration in the aboveground plant parts is calculated from:

$$C_v = C_{v,sg}(t) + C_{v,p}(t)$$

where:

$C_{v,p}$ (t) is the plant concentration at harvest time *t* due to particle deposition [M kg^{-1} fresh weight]
$C_{v,sg}$ (t) is the plant concentration at harvest time *t* due to uptake from soil and deposition from the gas phase [M kg^{-1} fresh weight]

Plant concentrations resulting from soil uptake and gas plant partitioning are given by:

$$C_{v,sg}(t) = C_{v,sg}(0) \times e^{-\alpha \times t} + \frac{b}{\alpha \times \rho_s} \times (1 - e^{-\alpha \times t})$$

where:

$C_{v,sg}$ (0) is the initial plant concentration [M kg^{-1} fresh weight]
t is harvest time [jr]
a is the first-order plant loss rate constant [yr^{-1}]
b is a source term for uptake from soil and atmosphere [M $m^{-3}jr^{-1}$]
ρ_s is the wet density of the stem [kg fresh weight m^{-3}]

Similarly, plant concentrations resulting from the wet and dry deposition (either measured as F_P or estimated from air particle concentration $C_{p,a}$), are given by:

$$C_{v,p}(t) = \frac{F_P \times I_V \times (1 - \exp[-k_w t])}{k_w \times Y_V} = \frac{C_{p,a} \times I_V \times ((V_d) + (R_n \times R_w \times W_p)) \times (1 - \exp[-k_w t])}{k_w \times Y_V}$$

where :

$C_{v,p}$ is the plant concentration due to particle deposition [M kg^{-1} fresh weight]
F_P is the contaminant particle deposition flux [M m^{-2} yr^{-1}]
I_V is the fraction of particles intercepted [-]
k_w is the plant weathering constant [yr^{-1}]
Y_V is the plant yield [kg fresh weight m^{-2}]
V_d is the dry particle deposition rate [m yr^{-1}]
R_n is the annual rainfall [m yr^{-1}]
R_w is the fraction retained after rainfall [-]
W_p is the washout factor [-]

The plant loss rate *a* is calculated from:

$$a = \sum \alpha_i = \alpha_{metabolism} + \alpha_{photolysis} + \alpha_{volatilization} + \alpha_{growth}$$

$$\alpha_{metabolism} = 0$$
$$\alpha_{photolysis} = 0$$
$$\alpha_{growth} = 12.8 yr^{-1}$$
$$\alpha_{volatilization} = \frac{A \times G_{pl}}{V \times K_{VG}}$$

where:

G_{pl} is the conductance [= 3.15e4 m yr^{-1}]
V is the plant volume [m^3]
K_{VG} is the gas-plant partition coefficient [m^3 m^{-3}]
A is the plant surface area [m^2]

$$K_{VG} = mK_{OA}^{n}$$

where:

m,n are plant specific regression constants
K_{OA} is the octanol-air partition coefficient [$m^3.m^{-3}$]

The plant source term *b* is calculated from :

$$b = C_{w,s} \times \frac{TSCF \times Q_{transp}}{V} + C_{g,a} \times \frac{v_G \times A}{V}$$

where:

TSCF is the transpiration stream concentration factor [-]
Q_{transp} is the transpiration rate [m^3 yr^{-1}]
V is the plant volume [m^3]
A is the plant surface area [m^2]
v_g is the gas deposition velocity [m s^{-1}]
$C_{w,s}$ is the soil pore water concentration [M m^{-3}]
$C_{g,a}$ is the gas phase concentration in air [M m^{-3}]

The transpiration stream concentration factor is calculated using:

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

where :

K_{ow} is the octanol-water partition coefficient. If log Kow > 4.5, then $TSCF = 0.038$.

$$v_G = \frac{1}{\left(1/v_{GG} + 1/K_{VG} v_{GV} \right)}$$

where:

v_{GG} is the mass transfer rate from atmosphere to plant surface [= 3.15e3 m yr^{-1}]
v_{GV} is the mass transfer rate from plant surface to plant reservoir [= 2.45e-4 m yr^{-1}]
K_{VG} is the gas – plant partition coefficient [m^3 m^{-3}]

Root crops

The concentration in the root crops is calculated from:

$$C_{v,s} = C_{w,s} \times \frac{K_{pl,w}}{\rho_r}$$

where:

$C_{w,s}$ is the soil pore water concentration [M m^{-3}]
$K_{pl,w}$ is the plant-water partition coefficient [m^3 m^{-3}]
ρ_r is the wet density of the root [kg fresh weight m^{-3}]

$$K_{pl,w} = \theta_{w,v} + \theta_{l,v} \times K_{ow}^{bol}$$

where :

$\theta_{w,v}$ is the volumetric plant water content [m^3 m^{-3}]
$\theta_{l,v}$ is the volumetric plant lipid content [m^3 m^{-3}]
bol is the octanol-lipid correction factor = 0.95
K_{ow} is the octanol-water partition coefficient

$$\theta_{w,v} = \frac{\rho_v}{1000} \times \left(1 - \frac{DM}{100} \right)$$

where :

ρ_v is the plant wet density [kg fresh weight m^{-3} wet plant]
DM is the dry matter content (% of fresh weight) of the plant:

$$\theta_{l,v} = \rho_v \times \frac{lipid\%}{100} \times \frac{1}{\rho_l}$$

where :

ρ_v is the plant wet density [kg fresh weight m^{-3} wet plant]
lipid% is the Lipid content (% of fresh weight)
ρ_l is the lipid density in plants [=700 kg lipid m^{-3} lipid]

Heavy metals

For describing soil-plant-atmosphere transfer of heavy metals, bioconcentration factors are used for modeling uptake from soil and particle deposition is assumed for modeling uptake from atmosphere.

Aboveground plant parts

The concentration in the aboveground plant parts is calculated from:

$$C_v = C_{v,sg}(t) + C_{v,p}(t)$$

For describing soil-plant transfer of heavy metals, bioconcentration factors are used. Plant concentrations can be calculated from total soil concentrations using:

$$C_{v,sg} = BCF \cdot C$$

where:

$C_{v,s}$ is the plant concentration due to soil-plant transfer [M kg^{-1} fresh weight]
BCF is the bioconcentration factor [kg soil dry weight kg^{-1} plant fresh weight]
C is the total soil concentration [M kg^{-1} soil dry weight]

$$\log BCF = a' + b' \times pH + c' \times \log C$$

where:

a', b' and c' are crop specific regression constants (see Table 2)

Particle deposition of heavy metals on aboveground plant parts is modeled using:

$$C_{v,p}(t) = \frac{F_P \times I_V \times (1 - \exp[-k_w t])}{k_w \times Y_V}$$

where:

F_P is the contaminant particle deposition flux [M m^{-2} yr^{-1}]
I_V is the fraction of particles intercepted [-]
k_w is the plant weathering constant [yr^{-1}]
Y_V is the plant yield [kg fresh weight m^{-2}]

Root crops

It is assumed that uptake in root crops occurs via soil only. In the model, the aformentioned BCFs for root crops are used.

7.4.3 Transfer in soil

The soil model calculates changes in concentrations in soil during the crop growing season.

The transfer in soil is described using a first-order kinetic model. The contaminant concentrations within a single homogeneous soil compartment are described by a linear first-order differential equation of the form:

$$\frac{dC}{dt} = -kC + I$$

where:

C is the total concentration in soil [M kg^{-1} dry weight]
k is the overall first-order rate coefficient [yr^{-1}]
I is the contaminant load to the soil [M kg^{-1} yr^{-1}]

The soil contaminant load may be the result of atmospheric deposition, irrigation, fertilizer application, pesticide application, sludge or biowaste application, etc..

The total soil concentration is the sum of the amount of contaminant in the solid, liquid and gas phases:

$$\rho C = \theta_{w,s} C_{w,s} + \rho C_{s,s} + \theta_{a,s} C_{a,s}$$

where:

ρ is the bulk soil density [kg m^{-3}]
$\theta_{w,s}$ is the volumetric soil water content [m^3 m^{-3}]
$C_{s,s}$ is the contaminant concentration in the soil solid phase [M kg^{-1}]
$\theta_{a,s}$ is the volumetric soil air content [m^3 m^{-3}],
$C_{a,s}$ is the contaminant concentration in the soil air phase [M m^{-3}]

Phase transition between water and solid phase and between water and air phase is modeled using equilibrium partition coefficients:

$$K_d = \frac{C_{s,s}}{C_{w,s}}$$

$$H' = \frac{C_{a,s}}{C_{w,s}} = \frac{K_H}{RT}$$

where:

K_d is the soil-water distribution coefficient [m^3 kg^{-1}]
H' is the air-water distribution coefficient [m^3 m^{-3}]
K_H is the Henry coefficient [Pa m^3 mol^{-1}]
H' is the dimensionless Henry coefficient or water-air distribution coefficient [-]

The analytical solution of Eq. is given by:

$$C = C_i e^{-kt} + \frac{I}{k}(1 - e^{-kt})$$

where:

C_i is the initial total contaminant concentration [M kg^{-1}]

Eq. shows that the predicted concentration is independent of space and valid for a known volume of soil. The model further assumes that contaminants are completely mixed in the soil. Contaminants are lost from the soil by a series of transport (advective solute leaching, diffusive volatilisation, run-off, root uptake) and transformation (degradation) processes that can be represented mathematically as first-order losses. The overall rate coefficient k in Eq. A.1 is the sum of the individual first-order rate coefficients:

$$k = k_v + k_r + k_p + k_b + k_l$$

where:

k_v is the volatilization coefficient [yr^{-1}]
k_r is the run-off coefficient [yr^{-1}]
k_p is the root-uptake coefficient [yr^{-1}]

k_b is the degradation coefficient [yr^{-1}]
k_l is the leaching rate coefficient [yr^{-1}]

The volatilisation coefficient is given by:

$$k_v = 2\frac{D_{eff}}{d^2}\frac{\theta_{a,s}H'}{(\rho K_d + \theta_{w,s} + \theta_{a,s}H')}$$

where:

d is the thickness of the soil profile [m]
D_{eff} is the effective diffusion coefficient in soil air [$m^2\ yr^{-1}$]

$$D_{eff} = \frac{\theta_a^{10/3}}{\theta_s^2}D_a$$

where:

θ_s is the saturated volumetric water content or porosity [$m^3\ m^{-3}$]
D_a is the molecular diffusion coefficient in air [$m^2\ yr^{-1}$]

The run-off coefficient k_r is given by:

$$k_r = \frac{A_s}{\rho d}$$

where:

A_s is the erosion soil loss [$kg\ m^{-2}\ yr^{-1}$]

The soil loss may be calculated using the Universal Soil Loss Equation, but is not considered in XtraFood (k_r=0).

The root-uptake coefficient k_p is given by:

$$k_p = BCF \cdot \frac{Y}{\rho d}$$

where:

Y is the plant yield [kg fresh weight $m^{-2}\ yr^{-1}$]

The degradation constant k_b is readily equivalent to the first-order biodegradation constant obtained in degradation experiments. Care should be taken to convert from a degradation constant k_w obtained in water to a degradation constant k_b based on total concentration:

$$k_b = k_w \frac{\theta}{\theta_{w,s} + \rho K_d + \theta_{a,s}H'}$$

Finally, the leaching coefficient is given by:

$$k_l = \frac{q}{d}\frac{1}{(\theta_{w,s} + \rho K_d + \theta_{a,s}H')}$$

where:

q is the infiltration rate [$m\ yr^{-1}$]

7.4.4 Pesticide residue model

The fate of pesticide residues on the leaf/fruit can be described as a first-order differential equation:

$$\frac{dC}{dt} = -k * C + J_{in}$$

or

$$C(t) = C_0 * e^{-k*t} + \frac{J_{in}}{k} * (1 - e^{-k*t})$$

Where C_0 is the initial concentration in/on the plant at time 0 (mg/kg plant), J_{in} is the input factor (mg/kg plant/day), k is the degradation factor (d^{-1}) and t is the time after application (d).

Since the model only considers the residues on leafs/fruits by spray application and not by atmospheric deposition or by uptake from the soil, the input factor (J_{in}) can be set as zero and the equation can be written as:

$$C(t) = C_0 * e^{-k*t}$$

In several cases, more than one application is done during the growth season. Therefore, it is obvious to insert a "multiple application factor" and to work with a "time weighted average" factor, which takes into account the time between two applications. (EC, SANCO/4145/2000-final, 2002)

The equation can then be rewritten as:

$$C(t) = C_0 * MAF * f_{twa}$$

The "multiple application" factor (MAF) is calculated by:

$$MAF = \frac{1 - e^{-nki}}{1 - e^{-ki}}$$

In which n is the number of applications, k is the degradation factor (d^{-1}) and i is the interval between two applications (d).

The "time weighted average" factor is given by:

$$f_{twa} = \frac{1 - e^{-kt}}{kt}$$

In which k is the degradation factor (d^{-1}) and t is the time between the last application and harvest (d).

7.4.5 Soil/plant/feed/water – cattle transfer

To calculate transfer to animal products, different types of transfer factors are used for heavy metals as compared to organic pollutants. XtraFood assumes that equilibrium exists between feed and animal product. Biotransfer factors for liver, kidney and meat are used for heavy metals. Bioconcentration factors are used for transfer of organic chemicals from feed to meat, liver and kidney and from soil to eggs. Carry-over-rates are used for transfer of organics from feed to milk.

Composition of the cattle feed

The feed is composed of soil, fodder crops, grass, concentrates and water. It is assumed that soil, fodder crops, grass and (ground)water originate from the farm itself. When the farm is not self-supplying in feed, the feed is imported from elsewhere.

$$J_{f,winter} = J_{soil,winter} + J_{fodder,winter} + J_{pasture,winter} + J_{conc,winter} + J_{water,winter}$$
$$J_{f,summer} = J_{soil,summer} + J_{fodder,summer} + J_{pasture,summer} + J_{conc,summer} + J_{water,summer}$$

$$J_{soil,winter} = q_{soil,winter} \times C$$
$$J_{fodder,winter} = \sum (q_{crop,winter} \times C_v)$$
$$q_{crop,winter} = q_{fodder,winter} \times f_{crop,winter}$$
$$for\ crop = voederbiet, wortelknol, voedermais, eenjarigvoedergewas, groenvoeder, hooi$$
$$q_{voederbiet,winter} = q_{fodder,winter} \times f_{voederbiet,winter}$$
$$q_{wortelenknolgew,winter} = q_{fodder,winter} \times f_{wortelenknolgew,winter}$$
$$q_{voedermaïs,winter} = q_{fodder,winter} \times f_{voedermaïs,winter}$$
$$q_{eenjarigvoeder,winter} = q_{fodder,winter} \times f_{eenjarigvoeder,winter}$$
$$q_{groenvoeder,winter} = q_{fodder,winter} \times f_{groenvoeder,winter}$$
$$q_{hooi,winter} = q_{fodder,winter} \times f_{hooi,winter}$$
$$J_{pasture,winter} = \sum (q_{grass,winter} \times C_{grass})$$
$$q_{grass,winter} = q_{pasture,winter} \times f_{grass,winter}$$
$$for\ grass = tijdelijkeweiden, blijvendgras$$
$$q_{tijdelijkeweiden,winter} = q_{pasture,winter} \times f_{tijdeljkeweiden,winter}$$
$$q_{blijvendgras,winter} = q_{pasture,winter} \times f_{blijvendgras,winter}$$
$$J_{conc,winter} = q_{conc,winter} \times C_{conc}$$
$$J_{water,winter} = q_{water,winter} \times C_{w,s}$$

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

$$J_{fodder,summer} = \sum (q_{crop,summer} \times C_v)$$

$$q_{crop,summer} = q_{fodder,summer} \times f_{crop,summer}$$

$$for\ crop = voederbiet, wortelenknol, voedermais, eenjarigevoedergewas, groenvoeder, hooi$$

$$q_{voederbiet,summer} = q_{fodder,summer} \times f_{voederbiet,summer}$$

$$q_{wortelknol,summer} = q_{fodder,summer} \times f_{wortelknol,summer}$$

$$q_{voedermaïs,summer} = q_{fodder,summer} \times f_{voedermais,summer}$$

$$q_{eenjarigvoedergewas,summer} = q_{fodder,summer} \times f_{eenjarigvoedergewas,summer}$$

$$q_{groenvoeder,summer} = q_{fodder,summer} \times f_{groenvoeder,summer}$$

$$q_{hooi,summer} = q_{fodder,summer} \times f_{hooi,summer}$$

$$J_{pasture,summer} = \sum (q_{grass,summer} \times C_{grass})$$

$$q_{grass,summer} = q_{pasture,summer} \times f_{grass,summer}$$

$$for\ grass = tijdelijkeweiden,\ blijvendgras$$

$$q_{tijdelijkeweiden,summer} = q_{pasture,summer} \times f_{tijdelijkeweiden,summer}$$

$$q_{blijvendgras,summer} = q_{pasture,summer} \times f_{blijvendgras,summer}$$

$$J_{conc,summer} = q_{conc,summer} \times C_{conc}$$

$$J_{water,summer} = q_{water,summer} \times C_{w,s}$$

$J_{f,\ winter}$ is the daily contaminant intake during winter [M d^{-1}]
$J_{f,\ summer}$ is the daily contaminant intake during summer [M d^{-1}]
$J_{soil,\ winter}$ is the daily contaminant intake due to soil intake during winter [M d^{-1}
$J_{soil,\ summer}$ is the daily contaminant intake due to soil intake during summer [M d^{-1}]
$J_{fodder,\ winter}$ is the daily contaminant intake due to fodder crop intake during winter [M d^{-1}]
$J_{fodder,\ summer}$ is the daily contaminant intake due to fodder crop intake during summer [M d^{-1}]
$J_{pasture,\ winter}$ is the daily contaminant intake due to grass intake during winter [M d^{-1}]
$J_{pasture,\ summer}$ is the daily contaminant intake due to grass intake during summer [M d^{-1}]
$J_{conc,\ winter}$ is the daily contaminant intake due to concentrate intake during winter [M d^{-1}]
$J_{conc,\ summer}$ is the daily contaminant intake due to concentrate intake during summer [M d^{-1}]
$J_{water,\ winter}$ is the daily contaminant intake due to water intake during winter [M d^{-1}]
$J_{water,\ summer}$ is the daily contaminant intake due to water intake during summer [M d^{-1}]
$q_{soil,\ winter}$ is the daily soil intake in winter [kg dry weight d^{-1}]
$q_{soil,\ summer}$ is the daily soil intake in summer [kg dry weight d^{-1}]
$q_{crop,\ winter}$ is the daily crop intake in winter [kg fresh weight d^{-1}]
$q_{crop,\ summer}$ is the daily fodder intake in summer [kg fresh weight d^{-1}]
$q_{fodder,winter}$ is the daily fodder intake in winter [kg fresh weight d^{-1}]
$q_{fodder,summer}$ is the daily fodder intake in summer [kg fresh weight d^{-1}]
$f_{voederbiet,\ winter}$ is the fraction voederbiet in the winterdiet (-)
$f_{wortelknol,\ winter}$ is the fraction wortelknol in the winterdiet (-)
$f_{voedermaïs,\ winter}$ is the fraction voedermaïs in the winterdiet (-)
$f_{eenjarigvoedergewas,\ winter}$ is the fraction eenjarigvoedergewas in the winterdiet (-)
$f_{groenvoeder,\ winter}$ is the fraction groenvoeder in the winterdiet (-)
$f_{hooi,\ winter}$ is the fraction hooi in the winterdiet (-)
$f_{voederbiet,\ summer}$ is the fraction voederbiet in the summerdiet (-)
$f_{wortelknol,\ summer}$ is the fraction wortelknol in the summerdiet (-)
$f_{voedermaïs,\ summer}$ is the fraction voedermaïs in the summerdiet (-)

$f_{eenjarigvoedergewas,\ summer}$ is the fraction eenjarigvoedergewas in the summerdiet (-)
$f_{groenvoeder,\ summer}$ is the fraction groenvoeder in the summerdiet (-)
$f_{hooi,\ summer}$ is the fraction hooi in the summerdiet (-)
$q_{grass,\ winter}$ is the daily grass intake in winter [kg fresh weight d^{-1}]
$q_{grass,\ summer}$ is the daily grass intake in summer [kg fresh weight d^{-1}
$q_{pasture,\ winter}$ is the total daily grass intake in winter [kg fresh weight d^{-1}]
$q_{pasture,\ summer}$ is the total daily grass intake in summer [kg fresh weight d^{-1}]
$q_{conc,\ winter}$ is the daily concentrate intake during winter [kg fresh weight d^{-1}]
$q_{conc,\ summer}$ is the daily concentrate intake during summer [kg fresh weight d^{-1}]
$q_{water,\ winter}$ is the daily water intake during winter [m^3 d^{-1}]
$q_{water,\ summer}$ is the daily water intake during summer [m^3 d^{-1}]
C is the total soil concentration [M kg^{-1} dry weight]
C_v is the fodder crop concentration [M kg^{-1} fresh weight]
C_{grass} is the grass concentration [M kg^{-1} fresh weight]
C_{conc} is the concentrate concentration [M kg^{-1} fresh weight]
$C_{w,s}$ is the soil pore water concentration [M m^{-3}]

$$J_{f,year} = TF_{summer} \cdot J_{f,summer} + TF_{winter} \cdot J_{f,winter}$$

$J_{f,\ year}$ is the daily average contaminant intake due to feed intake [M d^{-1}]
$J_{f,\ winter}$ is the daily contaminant intake during winter [M d^{-1}]
$J_{f,\ summer}$ is the daily contaminant intake during summer [M d^{-1}]
TF_{summer} is the time fraction the cattle is receiving a summer diet [-]
TF_{winter} is the time fraction the cattle is receiving a winter diet [-]

Transfer of heavy metals from feed to animal products

Concentrations in meat, liver, kidney and milk

Concentrations in animal products are calculated using biotransfer factors.

$$C_{meat} = BTF_{muscle} J_{f,year}$$
$$C_{liver} = BTF_{liver} J_{f,year}$$
$$C_{kidney} = BTF_{kidney} J_{f,year}$$
$$C_{milk} = (BTF_{milk} J_{f,year}) \times \frac{1000}{0.95}$$

C_{meat} is the concentration in animal muscle [M kg^{-1} fresh weight]
C_{liver} is the concentration in animal liver [M kg^{-1} fresh weight]
C_{kidney} is the concentration in animal kidney [M kg^{-1} fresh weight]
C_{milk} is the concentration in milk [M m^{-3}] (correction factor 0.95 voor s.w. milk and 1000 for l to m^3)
BTF_{meat} is the feed to muscle biotransfer factor [d kg^{-1} fresh weight]
BTF_{liver} is the feed to liver biotransfer factor [d kg^{-1} fresh weight]
BTF_{kidney} is the feed to kidney biotransfer factor [d kg^{-1} fresh weight]
BTF_{milk} is the feed to milk biotransfer factor [d kg^{-1} fresh weight]
$J_{f,\ year}$ is the daily average contaminant intake due to feed intake [M d^{-1}]

Transfer of organic chemicals from feed to animal meat products

Transfer of organic chemicals to animal products is calculated using measured bioconcentration factors. If no BCFs are available a relationship between Kow and BTF is used to calculate concentrations in animal products.

$$C_{meatf} = BCF_{musclef} \times C_{fe}$$
$$C_{meatvf} = BCF_{musclevf} \times C_{fe}$$
$$C_{meatlf} = BCF_{musclelf} \times C_{fe}$$
$$C_{meatl} = BCF_{musclel} \times C_{fe}$$
$$C_{liver} = BCF_{liver} \times C_{fe}$$
$$C_{kidney} = BCF_{kidney} \times C_{fe}$$
$$C_{fat} = 6.7 \times BCF_{kmusclef} \times C_{fe}$$

C_{meatf} is the concentration in fat animal muscle (10,1 – 20 g fat/100 g) [M kg^{-1} fresh weight]
C_{meatvf} is the concentration in very fat animal muscle (> 20 g fat/100 g) [M kg^{-1} fresh weight]
C_{meatlf} is the concentration in low-fat animal muscle (5,1 – 10 g fat/100 g) [M kg^{-1} fresh weight]
C_{meatl} is the concentration in lean animal muscle (< 5 g fat/100 g) [M kg^{-1} fresh weight]
C_{liver} is the concentration in animal liver [M kg^{-1} fresh weight]
C_{kidney} is the concentration in animal kidney [M kg^{-1} fresh weight]
C_{fat} is the concentration in animal fat [M kg^{-1} fresh weight]
$BCF_{musclef}$ is the bioconcentration factor from feed to muscle [kg feed fresh weight kg^{-1} muscle fresh weight]
$BCF_{musclevf}$ is the bioconcentration factor from feed to muscle [kg feed fresh weight kg^{-1} muscle fresh weight]
$BCF_{musclelf}$ is the bioconcentration factor from feed to muscle [kg feed fresh weight kg^{-1} muscle fresh weight]
$BCF_{musclel}$ is the bioconcentration factor from feed to muscle [kg feed fresh weight kg^{-1} muscle fresh weight]
BCF_{liver} is the bioconcentration factor from feed to liver [kg feed fresh weight kg^{-1} liver fresh weight]
BCF_{kidney} is the bioconcentration factor from feed to kidney [kg feed fresh weight kg^{-1} kidney fresh weight]

$BTF_{org} = 10^{\wedge(-7.7+1.03*\log10(Kow))}$ BTF=<0.1

$$C_{meatf} = BTF_{org} \times (FC_{musclef} / 0.25) \times J_{f\ year}$$
$$C_{meatvf} = BTF_{org} \times (FC_{musclevf} / 0.25) \times J_{f\ year}$$
$$C_{meatlf} = BTF_{org} \times (FC_{musclelf} / 0.25) \times J_{f\ year}$$
$$C_{meatl} = BTF_{org} \times (FC_{musclel} / 0.25) \times J_{f\ year}$$
$$C_{meatvf} = BTF_{org} \times (FC_{musclevf} / 0.25) \times J_{f\ year}$$
$$C_{kiver} = BTF_{org} \times (FC_{liver} / 0.25) \times J_{f\ year}$$
$$C_{kidney} = BTF_{org} \times (FC_{kidney} / 0.25) \times J_{f\ year}$$

$FC_{musclef}$ is the fat content in fat animal muscle (10,1 – 20 g fat/100 g) [kg fat kg^{-1} fresh weight],]
$FC_{musclevf}$ is the fat content in very fat animal muscle (> 20 g fat/100 g) [kg fat kg^{-1} fresh weight]
$FC_{musclelf}$ is the fat content in low-fat animal muscle (5,1 – 10 g fat/100 g) [M kg^{-1} fresh weight]
$FC_{musclel}$ is the fat content in lean animal muscle (< 5 g fat/100 g) [M kg^{-1} fresh weight],
FC_{liver} is the fat content in animal liver [M kg^{-1} fresh weight]
FC_{kidney} is the fat content in animal kidney [M kg^{-1} fresh weight]
C_{fe} is the feed concentration [M kg^{-1} fresh weight]

$$C_{fe} = \frac{J_{f,\,year}}{\sum q}$$

$$\sum q = (q_{fodder,\ winter} \times TF_{w\,int\,er}) + (q_{fodder,summer} \times TF_{summer}) + (q_{pasture,w\,int\,er} \times TF_{w\,int\,er}) +$$
$$(q_{pasture,summer} \times TF_{summer}) + (q_{conc,summer} \times TF_{summer}) + (q_{conc,w\,int\,er} \times TF_{w\,int\,er})$$
$$+ 1000 \times ((q_{water,w\,int\,er} \times TF_{w\,int\,er}) + (q_{water,summer} \times TF_{summer}))$$
$$+ (1 + \frac{\theta_{w,s}}{\rho_s}) \times ((q_{soil,\ winter} \times TF_{w\,int\,er}) + (q_{soil,\ summer} \times TF_{summer}))$$

$J_{f,\,year}$ is the daily average contaminant intake due to feed intake [M d^{-1}],
$q_{soil,\,winter}$ is the daily soil intake in winter [kg dry weight d^{-1}]
$q_{soil,\,summer}$ is the daily soil intake in summer [kg dry weight d^{-1}]
$q_{fodder,\,winter}$ is the daily fodder intake in winter [kg fresh weight d^{-1}]
$q_{fodder\,summer}$ is the daily fodder intake in summer [kg fresh weight d^{-1}]
$q_{pasture,\,winter}$ is the daily grass intake in winter [kg fresh weight d^{-1}]
$q_{pasture,\,summer}$ is the daily grass intake in summer [kg fresh weight d^{-1}]
$q_{conc,\,winter}$ is the daily concentrate intake during winter [kg fresh weight d^{-1}]
$q_{conc,\,summer}$ is the daily concentrate intake during summer [kg fresh weight d^{-1}]
$q_{water,\,winter}$ is the daily water intake during winter [m^3 d^{-1}]
$q_{water,\,summer}$ is the daily water intake during summer [m^3 d^{-1}]
$\theta_{w,s}$ is the volumetric soil water content [m^3 m^{-3}]
ρ_s is the Soil dry bulk density (kg soil/l soil)

Transfer to milk

$$C_{milk} = \frac{J_{milk}}{q_{milk}}$$

C_{milk} is the concentration in the milk [M m^{-3}]
q_{milk} is the daily milk production [m^3 d^{-1}]
J_{milk} is the contaminant flux in the milk [M d^{-1}]

To express the concentration in milk as a function of the fat content:

$$C_{milk,\,fat} = \frac{C_{milk}}{f_{fat}}$$

$C_{milk,fat}$ is the concentration in the milk fat [M g^{-1} milk fat]
C_{milk} is the concentration in the milk [M m^{-3}]
f_{fat} is the fat content of the milk [g fat m^{-3}] = 42.000 g fat m^{-3}

$$J_{milk} = COR \cdot J_{f,year}$$

J_{milk} is the contaminant flux in the milk [M d^{-1}]
COR is the carry-over-rate [-]
$J_{f,\,year}$ is the contaminant intake due to feed intake [M d^{-1}]

For dioxins en PCBs the following relationships were established:

$$\frac{1}{E_o} = 1.283 + 2.875e-8 \cdot K_{ow}$$

$$\frac{1}{1.283 + 2.875 \times e - 8 \times K_{ow}} = E_o = COR$$

E_M is the maximum fraction absorbed (labile contaminants that are metabolized)
E_o is the fraction absorbed (is equivalent to COR for persistent contaminants showing no transformation or metabolisation)
K_{ow} is the octanol-water partition coefficient

voor compounds that are metabolized (PAHs):

$$\frac{1}{E_M} = 1.2 + 2.875e - 8 \cdot K_{ow}$$

$$E_M = \frac{1}{1.2 + 2.875e - 8 \cdot K_{ow}} = COR_{PAK}$$

K_{ow} is the octanol-water partition coefficient

Transfer to eggs

$$C_{egg,fat} = f_{free-range} \times BCF_{egg} \times C_{soil} + \quad BTF_{egg} \times J_{year,corrected}$$

$f_{free-range}$ is the fraction of free-range chickens of all chickens
BTF_{egg} is the biotransferfactor egg
$C_{egg, fat}$ is the concentration in the egg fat [M g^{-1} egg fat]
BCF_{egg} is the soil-egg bioconcentration factor [kg soil dry weight g^{-1} egg fat]
C_{soil} is the total soil concentration [M kg^{-1} soil dry weight]
$J_{year,corrected}$ is the daily average contaminant intake due to feed intake, excluding soil intake:

$$J_{f,year,corrected} = TF_{summer} \times \left(J_{crop,summer} + J_{conc,summer} + J_{water,summer}\right)$$
$$+ TF_{winter} \times \left(J_{crop,winter} + J_{conc,winter} + J_{water,winter}\right)$$

If no BCF for eggs is available a BTF can be used:

BTF_{egg}=BTF = 10^(-7.7+1.03*log10(Kow)) BTF_{egg} is maximum 0.1

Biokinetic cattle models

In some cases, biokinetic models are preferred to calculate transfer. A simplified first-order model is proposed to calculate concentrations in animal products as a function of time:

$$C_{milk}(t) = C_{milk,0}e^{-k_{milk}t} + \frac{COR \cdot J_f}{q_{milk}}(1 - e^{-k_{milk}t})$$
$$C_{muscle}(t) = C_{muscle,0}e^{-k_{muscle}t} + BCF_{muscle} \cdot C_{fe}(1 - e^{-k_{muscle}t})$$
$$C_{egg}(t) = C_{egg,0}e^{-k_{egg}t} + BCF_{egg} \cdot C(1 - e^{-k_{egg}t})$$

where:
$C_{milk,0}$ is the concentration in the milk at time 0 [M m^{-3}]
$C_{muscle,0}$ is the concentration in the muscle at time 0 [M kg^{-1} fresh weight]

$C_{egg,0}$ is the egg concentration at time 0 [M g^{-1} egg fat]
k_{milk} is the first order rate constant for milk [yr^{-1}]
k_{muscle} is the first order rate constant for muscle tissue [yr^{-1}]
k_{egg} is the first order rate constant for egg fat [yr^{-1}]

Rate constants may differ from uptake stage to clearance stage. The biokinetic model has not been implemented in XtraFood so far.

7.4.6 Model default values

The Xtrafood model uses default values if information in the database records is lacking. Major default values are listed in Table 23.

Table 23: Default values in the Xtrafood model

TableName	ColumnName	DefaultValue	Unit
crop properties	conductance	31500	m/year
crop properties	CroppingCondition	2	(1=greenhouse;2=open air)
crop properties	dens_lipid	700	kg/m³
crop properties	dens_plant	800	kg/m³
crop properties	dry_matter	10	%
crop properties	fraction_retained_after_rainfall	1	-
crop properties	growth_period	0,4	year
crop properties	hor_surf_to_vol	2500	m²/m³
crop properties	interception	0,4	-
crop properties	leaf_surface_area	4,36	m²/m²
crop properties	m	17378	
crop properties	n	0,29	
crop properties	perc_air	20	%
crop properties	perc_lipid	0,01	%
crop properties	plant_height	0,5	m
crop properties	roughness	0,1	-
crop properties	shoot_vol	0,003	m³/m²
crop properties	surf_to_vol	5000	m²/m³
crop properties	transp_stream	0,365	/year
crop properties	weathering_constant	12	
Soil	pH	6	
animal production	eggs	0	number/animal/day
animal production	FC_kidney	0,04	kg fat kg/fw
animal production	FC_liver	0,04	kg fat kg/fw
animal production	FC_muscle_fat	0,15	kg fat kg/fw
animal production	FC_muscle_lean	0,04	kg fat kg/fw
animal production	FC_muscle_low_fat	0,075	kg fat kg/fw
animal production	FC_muscle_very_fat	0,22	kg fat kg/fw
animal production	kidney	0,002	-
animal production	liver	0,06	-
animal production	meat	0,375	-
chemical properties	a	0,784	
chemical properties	aH	10104	
chemical properties	ak	10104	
chemical properties	ap	10113	
chemical properties	b	-9,84	
chemical properties	bT	-15,1	
chemical properties	Diff_air	0,00000558	
chemical properties	Diff_water	6,53E-10	
chemical properties	mT	3700	
chemical properties	pOL_0	0,0000811	
chemical properties	Press_0	5,7544E-05	
chemical properties	Temp_ref_Henry	298	
chemical properties	Temp_ref_Koa	298	
chemical properties	Temp_ref_Press	283,15	
chemical properties	Washout	55000	