



2-FUN

*Full-chain and UNcertainty Approaches for Assessing Health Risks in
FUture ENvironmental Scenarios*

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REVIEW OF FEATURES, EVENTS AND PROCESSES INCORPORATED IN EXISTING MODELS FOR PLANTS AND ANIMALS

PROPOSAL OF THE CONCEPTUAL AND MATHEMATICAL 2-FUN MODEL FOR ASSESSING TRANSFER OF CHEMICALS TO PLANTS AND ANIMALS

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Contents

INTRODUCTION.....	4
1. MATERIAL AND METHODS	5
1.1 Perimeter of the 2-FUN modelling tool.....	5
1.2 Sub-systems of the environment.....	5
1.3 Mass-balance concepts	5
1.4 The Interaction Matrix methodology	6
1.5 List of reviewed models for the plant and animal system.....	6
2. THE PLANT AND ANIMAL SYSTEM – REVIEW OF MODELS.....	8
2.1 Interaction matrices.....	8
2.2 Compartments.....	16
2.3 Inputs/outputs.....	17
2.4 Intercompartment transfers	20
3. THE PLANT AND ANIMAL SYSTEM - DEFINITION OF THE 2-FUN INTERACTION MATRIX.....	21
3.1 Compartments.....	21
3.2 Inputs/outputs.....	22
3.3 Intercompartment transfers	23
4. THE PLANT AND ANIMAL SYSTEM – DEFINITION OF THE MATHEMATICAL MODEL FOR ORGANIC CHEMICALS.....	27
4.1 Root.....	27
4.2 Tuber.....	28
4.3 Leaf.....	31
4.4 Grain	35
4.5 Fruit.....	36
4.6 Animal	39
4.7 Milk.....	42
5. THE PLANT AND ANIMAL SYSTEM – DEFINITION OF THE MATHEMATICAL MODEL FOR METALS.....	43
5.1 Plants.....	44
5.2 Animals.....	49
References	51



INTRODUCTION

The main objective of 2-FUN's WP2 is to build a software based on multimedia models and associated databases for assessing the exposure to chemicals through indirect routes (e.g. through the food chain). The specifications of this final product can be summarized as follows:

- to date, the simultaneous and comparative exposure assessment of various chemicals is difficult because: (i) models are generally dedicated to one specific family of chemicals (e.g. metals, or pesticides) or one type of emission/environmental media (e.g. soil); (ii) the representation of the macro- and micro-environments governing behaviour of chemicals in the environment and subsequent human exposure is not homogeneous among models; (iii) the level of mathematical simplification/sophistication and the mathematical description of common processes (e.g. physical processes which are independent of the stressor) can differ a lot among models. To overcome these limitations, the 2-FUN tool intends to allow a **homogeneous assessment of various chemicals, released in various systems and reaching humans through various routes**.
- environmental conditions differ in space and time, with temperature and region and so forth. Human behaviour differs with group, region, age, gender et cetera. Besides, there is real uncertainty, based on ignorance ("no-know") of processes or events. In exposure and risk assessment, this uncertainty is only indirectly considered by constructing typical ("generic"), conservative or "worst-case" scenarios. This may give estimates "on the safe side", but does not allow a quantification of this safety. However, environmental variations (space, time, temperature, region) can in many cases be quantified and described, e.g. by probability density functions on key parameters. The same holds for differences in human behaviour. The objective of the 2-FUN tool is then to incorporate **distributed input data for the exposure assessment** (stored in an ad-hoc database), yielding a **distributed output**. The 2-FUN tool would then allow the quantification of the probability of an individual to be exposed, allowing a safety concept that substitutes the 'conservative' concept.
- To date, research on the **exposure profiles of children** to identify the most important routes of exposure are scarce. To incorporate specific children's pathways in exposure models, a review of the existing literature on children's exposure routes (e.g. epidemiological studies aiming at identifying exposure routes of organics, lead or radionuclides) will be conducted and relevant pathways (e.g. physiological parameters, behavioural parameters and time-activity data for different age groups) will be introduced into the multi-media model(s).

This report is the first stage to the construction of the 2-FUN's homogeneous and integrated software for the assessment of indirect exposures. Features, Events and Processes (FEPs) occurring within and/or between environmental compartments of interest for humans were reviewed considering existing models/frameworks/methodologies currently used for conducting human risk assessments. This report is specific to FEPs occurring in plants and animals¹.

A systematic method for the visualization of FEPs contained in each model (i.e. the Interaction matrix method) was used to compare models. The relevance of each FEP for its eventual incorporation into the 2-FUN model was studied. Finally, a list of relevant compartments and associated FEPs to be included into the 2-FUN modelling system will be proposed. Then the mathematical model for describing the transfer of chemicals to/within/from plants and animals is described in detail.

¹ A report related to freshwaters was already published and reports will be published on other sub-systems of the environment (soil and groundwater, atmosphere humans).



1. MATERIAL AND METHODS

1.1 Perimeter of the 2-FUN modelling tool

The 2-FUN modelling tool will focus on the detailed description of the transfer of chemicals through the human food chain. Thus, the 2-FUN modelling tool considers a region of investigation (a 'box') for which inputs at its frontiers are known. In other words, the 2-FUN model will use as input data:

- monitoring data directly collected at the frontier of the investigated region in surface water, air and/or soils;
- data produced by models simulating the physical transport (e.g. advection/diffusion/dispersion) of pollutants in the air or in water bodies from the release point(s) to the frontier of the investigated region, and providing concentrations of pollutants in air, soil and/or water entering the investigated region.

According to available data related to the contamination in water, air and/or soil at the assessment point, the 2-FUN modelling tool will consider:

- steady-state conditions, when permanent discharges into the environment are assumed;
- dynamic conditions, if time-dependent data are available (e.g. incidental/accidental discharges).

1.2 Sub-systems of the environment

The first step in the development of a biosphere model is the construction of a conceptual model defining the biosphere system components, e.g. air, water, soil, crops, animals etc, eventually sub-divided in several sub-compartments, as well as the relations between these components (i.e. transfers governed by physical, chemical and/or biological processes). Thus, compartments taken into account into multimedia models are the media in which chemicals may migrate or accumulate.

For facilitating the analysis of existing models and proposing an integrated framework for the further development of the 2-FUN modelling tool, five main sub-systems were defined:

- the 'surface freshwater' system;
- the 'soil' and 'groundwater' system;
- the 'air' system, including outdoor atmosphere and indoor air;
- the 'plant and animal' system;
- the 'human activity' system.

The present report focuses on the plant and animal subsystem. The freshwater system was reviewed in an already published report (Deliverable 2.1 on the freshwater system).

Besides, a specific analysis and associated reports will be produced for specific exposure pathways for children (Deliverable 2.2: review of relevant exposure pathways for children; Deliverable 2.7: Parameterisation of relevant exposure pathways for children).

1.3 Mass-balance concepts

The 2-FUN model was built to maintain a mass balance in the whole system, as well as in each of the sub-systems previously defined. When applied to a specific compartment, the mass balance approach implies that, for a given time period, the amount of chemical in the compartment at the end of the period results from the amount present at the beginning plus the gains occurring during the time period minus the chemical lost from the compartment.

The geometry of the investigated region is assumed to be known by the end-user, i.e. the length, width and height of the river/lake system, the surface of the soil system, as well as the distribution of the occupancy of the soil system by different culture types.

1.4 The Interaction Matrix methodology

Interaction Matrices, an expert qualitative method to identify multiple interactions among biotic and abiotic components of the biosphere, are a useful tool to develop conceptual models simulating the behaviour of chemicals in a complex environment. This systematic approach facilitates a comprehensible identification and visualization of the exposure pathways and allows classification of the role of different ecosystem components in terms of transfer relationships.

An Interaction Matrix is a table which describes the conceptual model by tabulating the interactions between the compartmental media. The main compartments of the biosphere system are identified and listed in the leading diagonal elements (LDEs) of the matrix; the interactions between the LDEs are listed in the off-diagonal elements (ODEs) (Figure 1).

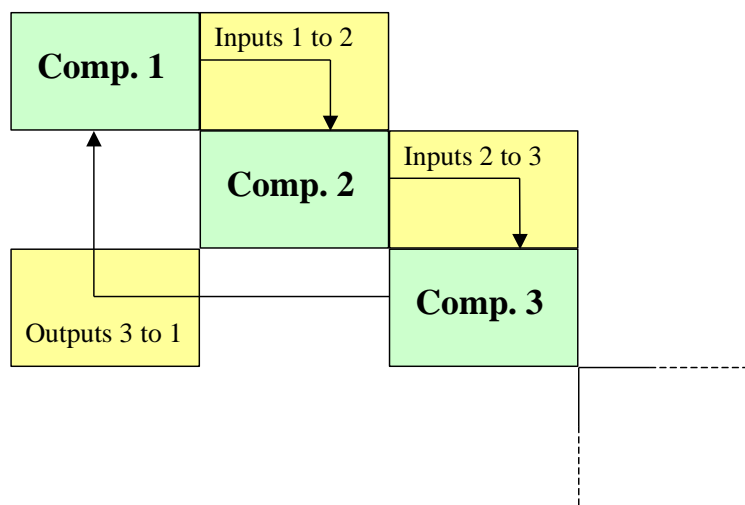


Figure 1 – The Interaction Matrix presentation

The Interaction Matrix will support the further mathematical implementation of the conceptual model²: the LDEs will usually be represented by compartments and the ODEs by transfer functions. Using the matrix as a complete representation of the conceptual model, it is relatively simple to cross-check it against a standard Features, Events and Processes (FEPs) list to ensure that the conceptual model is as complete as a specific context requires.

Obviously, there may be different alternative mathematical models for each FEP, as well as several numerical models for each mathematical model. Mathematical models describing the Interaction Matrices reviewed in the present document will not be detailed here. Only the final 2-FUN mathematical model is described in detail in Chapters 4 and 5.

1.5 List of reviewed models for the plant and animal system

For defining the 2-FUN conceptual model, existing models, frameworks and methodologies currently used for assessing transfer of chemicals to plants and animals were reviewed. A list of the reviewed material is presented in Tables 1 and 2. The reviewed models comprise empirical regressions and mechanistic models. Both of these approaches are used in the reviewed model frameworks applied for estimating the exposure of humans to chemicals. However, the list is not exhaustive; other models described in the scientific literature have been evaluated as well.

² the implementation will be conducted on the Ecolego® platform, specifically built for compartmental models described through an Interaction Matrix.



Only the part concerning uptake of chemicals in plants and animals was reviewed in the model frameworks. E.g. the transfer of chemical between soil and air has not been reviewed.

Table 1. List of reviewed models for the plant and animal system

Name	Description	References
T & A regressions	Bioconcentration of organic chemicals in beef, milk and vegetation	(Travis and Arms 1988)
Revised T & A regressions (Birak)	Evaluation of the T & A regressions for estimating bioconcentration of organic chemicals in beef, milk and vegetation	(Birak et al. 2001)
<i>RCF</i> (root concentration factor)	Two regressions for bioconcentration of chemicals in the root	(Briggs et al. 1982; Trapp and Pussemier 1991)
<i>TSCF</i> (transpiration stream concentration factor)	Several regressions for bioconcentration of chemicals in the xylem	(Briggs et al. 1982; Burken and Schnoor 1998; Dettenmaier et al. 2009; Hsu et al. 1990)
<i>SCF</i> (stem concentration factor)	One regression for bioconcentration of chemicals in the stem	(Briggs et al. 1983)
Three-compartment fugacity model	A three-compartment mass balance model of a plant developed to quantify the uptake of organic chemicals from soil and atmosphere	(Paterson et al. 1994)
Simplified three-compartment fugacity model	A simple three-compartment model using only readily available input data	(Hung and Mackay 1997)
Partition-limited model	A partition-limited model for the uptake of organic chemicals from soil or water	(Chiou et al. 2001)
Root model	A dynamic model for uptake of neutral lipophilic compounds from soil into roots	(Trapp 2002)
Potato model	A model for diffusive uptake of organic chemicals from soil into potatoes	(Trapp et al. 2007)
Leafy vegetables model	A differential mass-balance equation for the uptake of organic chemicals into the aerial plant compartment from soil and air	(Trapp and Matthies 1995)
Fruit tree model	A mathematical model to predict uptake of neutral organic chemicals from soil and air into fruits	(Trapp 2007)
Air to leaf deposition model	Basic equations describing gaseous and particle-bound deposition to vegetation	(McLachlan 1999)
Mother-child model	A coupled model for bioaccumulation of organic chemicals in breast-feeding mother and nursing infant. Here adapted to milk and beef cattle.	(Trapp et al. 2008)



Table 2. List of reviewed model frameworks for the plant and animal system

Name	Description	Institute	References
EU technical guidance document (TGD) on Risk Assessment	Models for uptake of organic compounds in roots, leafy vegetables, meat and milk.	EU	(EC 2003)
CSOIL	An exposure model for human risk assessment of soil contamination. Including models for roots and leafy vegetables.	RIVM (NL)	(Brand et al. 2007)
CLEA (the Contaminated Land Exposure Assessment Model)	The model estimates child and adult exposures to soil contamination for those potentially living, working and/or playing on contaminated sites over long time periods.	UK	(Jeffries and Martin 2008)
Xtrafood	Chain model for the impact analysis of chemicals in primary food products	VITO (B)	(Seuntjes et al. 2006)
ACC-HUMAN	Describes bioaccumulation of lipophilic organic chemicals to humans. Including fugacity-based models for grass, beef and milk cattle.	-	(Czub and McLachlan 2004)
OURSON	A dynamic model for assessing the transfer of several radionuclides in a food-chain.	EDF (F)	(Ciffroy et al. 2005; Queguiner et al. 2009)
NMF (new model framework)	A framework with crop-specific models for predicting the dietary intake of environmental chemicals from their background concentrations in soil and air	DTU (DK)	(Legind and Trapp 2009)

2. THE PLANT AND ANIMAL SYSTEM – REVIEW OF MODELS

The review of models and frameworks for modelling the transfer of chemicals to plants and animals focuses mainly on the following three issues:

- Compartments
- Inputs and outputs, and
- Intercompartment transfers

These points are depicted with the interaction matrix methodology described in Section 1.4. Also, possible gaps in the types of chemicals currently covered by the models are identified.

2.1 Interaction matrices

The interaction matrices of the reviewed models and model frameworks are presented in Figures 2 – 20.



T & A regression, plants

Soil	Bioconcentration
	Aboveground plant part

RCF (root concentration factor)

External solution	Bioconcentration
	Roots

Figure 2. Travis and Arms (T & A) regression, neutral organic chemicals ($\log K_{ow}$: 1.15 – 9.35) (Travis and Arms 1988) and root concentration factor (*RCF*), O-methylcarbamoyloximes and substituted phenylureas ($\log K_{ow}$: -0.57 - 4.6) (Briggs et al. 1982), N-methyl-arylcarbamates ($\log K_{ow}$: 1.16 – 3.21) (Trapp and Pussemier 1991).

T & A regression, beef and milk

Feed	Bioaccumulation	Bioaccumulation
	Beef	
		Milk

Figure 3. Travis and Arms (T & A) regression, neutral organic chemicals ($\log K_{ow}$: 1.5 – 6.5 (beef), $\log K_{ow}$: 3 – 6.5 (milk))(Travis and Arms 1988). (Birak et al. 2001) revised the regressions ($\log K_{ow}$: 1.4 – 8.8 (beef), $\log K_{ow}$: 1.5 – 8.8 (milk)).

TSCF (transpiration stream concentration factor)

External solution	Bioconcentration
	Xylem

SCF (stem concentration factor)

External solution	Bioconcentration
	Stem

Figure 4. Transpiration stream concentration factor (*TSCF*), O-methylcarbamoyloximes and substituted phenylureas ($\log K_{ow}$: -0.57 - 4.6) (Briggs et al. 1982), oxabicycloalkanes ($\log K_{ow}$: 0.96 – 5.29) (Hsu et al. 1990), mainly neutral organic chemicals ($\log K_{ow}$: 0.87 – 5.04) (Burken and Schnoor 1998), ($\log K_{ow}$: -0.8 – 5) (Dettenmaier et al. 2009) and *SCF* (stem concentration factor), O-methylcarbamoyloximes and substituted phenylureas ($\log K_{ow}$: -0.57 - 4.6) (Briggs et al. 1983).

Three-compartment fugacity model

Air	Diffusion			Diffusion	Advection
Diffusion	Soil	Xylem flow Diffusion			Degradation
Diffusion	Diffusion	Root	Xylem flow		Degradation Growth
		Phloem flow	Stem	Xylem flow	Degradation Growth
Diffusion			Phloem flow	Leaf	Degradation Growth
Advection					Sink

Figure 5. Three-compartment fugacity model, organic chemicals (Paterson et al. 1994). Leaf includes petiole and stem includes fruit, seed and tuber.



Simplified three-compartment fugacity model

Air				Diffusion	
	Soil	Xylem flow Diffusion			
		Root	Xylem flow		Degradation Growth Diffusion to soil
		Phloem flow	Stem	Xylem flow	Degradation Growth
			Phloem flow	Leaf	Degradation Growth Diffusion to air
					Sink

Figure 6. Simplified three-compartment fugacity model, organic chemicals (Hung and Mackay 1997). Stem includes fruit, nut and seed.

Partition-limited model

Soil	Partitioning
	Root

Figure 7. Partition-limited model, neutral organic chemicals (Chiou et al. 2001).

Root model

Soil	Xylem flow	
	Root	Degradation Growth Xylem flow to shoots
		Sink

Potato model

Soil	Diffusion	
	Potato	Degradation Growth Diffusion to soil
		Sink

Figure 8. Root model, neutral organic chemicals (Trapp 2002) and potato model, neutral organic chemicals (Trapp et al. 2007).

Leafy vegetables model

Air		Diffusion Particle deposition	
	Soil	Bioaccumulation Xylem flow Soil attachment	
		Leaf	Degradation Growth Diffusion to air
			Sink

Figure 9. Leafy vegetables model, neutral organic chemicals (Trapp and Matthies 1995) with particle deposition (Legind and Trapp, 2009).



Fruit tree model

Air			Diffusion	Diffusion Particle deposition	Diffusion Particle deposition	
	Soil	Xylem flow Diffusion				
		Root	Xylem flow			Degradation Growth Diffusion to soil
			Stem	Xylem flow	Xylem flow Phloem flow	Degradation Growth Diffusion to air
				Leaf		Degradation Growth Diffusion to air
					Fruit	Degradation Growth Diffusion to air
						Sink

Figure 10. Fruit tree model, neutral organic chemicals (Trapp 2007) with particle deposition (Legind and Trapp, 2009).

Air to leaf deposition model

Air	Diffusion Particle deposition	
	Leaf	Diffusion to air Particle erosion to air
		Sink

Figure 11. Air to leaf deposition model, SOCs (semivolatile organic chemicals) (McLachlan 1999).

Mother-child model adapted to cattle

Air			Inhalation	
	Soil		Ingestion	
		Water	Drinking	
			Grass	Ingestion
			Animal	Lactation Growth Metabolism Exhalation Outflux of lipids Urination
				Milk
				Sink

Figure 12. Mother-child model adapted to cattle, neutral organic chemicals (Trapp et al. 2008). Animals include milk and beef cattle. Offspring can be added.



Technical guidance document (TGD) on risk assessment

Air			Diffusion			
	Soil	Equilibrium	Bioaccumulation Xylem flow		Bioaccumulation	
		Water				
		Root				
			Leaf			Degradation Growth Diffusion to air
				Grass	Bioaccumulation	
					Meat	
						Milk
						Sink

Figure 13. EU technical guidance document (TGD) on risk assessment, neutral organic chemicals (EC 2003)

CSOIL

Neutral organic contaminants

Air			Diffusion	
	Soil	Equilibrium	Bioaccumulation Xylem flow Soil attachment	
		Root		
			Leaf	Degradation Growth Diffusion to air
				Sink

Inorganic contaminants

Soil	$C_S = C_R$	$C_S = C_L$ Soil attachment
	Root	
		Leaf

Metals

Soil	Bioaccumulation	Bioaccumulation
	Root	
		Leaf

Figure 14. CSOIL, neutral organic chemicals, inorganic chemicals and metals (Brand et al. 2007).



CLEA (the contaminated land exposure assessment model)

Neutral organic contaminants

Soil	Xylem flow	Diffusion	Bioaccumulation	Xylem flow Phloem flow Bioaccumulation	
	Root				Degradation Growth Diffusion to soil
		Tuber			Degradation Growth Diffusion to soil
			Green vegetable		
				Fruit	Degradation Growth
					Sink

Inorganic contaminants

Soil	Bioaccumulation				
	Root	Bioaccumulation	Bioaccumulation	Bioaccumulation	Bioaccumulation
		Root store			
			Tuber		
				Green vegetable	
					Fruit

Figure 15. CLEA (the contaminated land exposure assessment model), neutral organic and inorganic chemicals (Jeffries and Martin 2008). Fruit includes tree, herbaceous and shrub fruit.

Xtrafood

Organic contaminants

Air			Diffusion Particle deposition						
	Soil	Equilibrium	Bio- accumulation Xylem flow		Bioaccumulation				
	Water								
		Root						Degradation Growth Diffusion to air	
			Aboveground plant part						
				Grass					
					Concen- trates	Bio- accumulation	Bio- accumulation	Bio- accumulation	
						Animal			
							Egg		
								Milk	
								Sink	

Figure 16. Xtrafood, organic chemicals (Seuntjes et al. 2006). Animal include fat muscle, very fat muscle, low-fat muscle, lean muscle, fat, liver, kidney and egg.



Xtrafood

Heavy metals

Air			Particle deposition				
	Soil	Bioaccumulation	Bioaccumulation			Bioaccumulation	
	Water						
		Root					
			Aboveground plant parts				
				Grass			
					Concentrates		
						Animal	
							Milk

Pesticides

Air	Spray application	
	Aboveground plant part	Degradation
		Sink

Figure 17. Xtrafood, organic chemicals, heavy metals and pesticides (Seuntjes et al. 2006). For metals root includes potato, scorzonera, celery and carrot, aboveground plant part include endive, cucumber, leek, french bean, lettuce, spinach, tomato, wheat and barley, and animal include meat, liver and kidney. For pesticides aboveground plant part include short grass, long grass, leaf and fruit.

ACC Human

Air			Diffusion Particle deposition	Inhalation		
	Soil		Xylem flow Bioaccumulation	Ingestion		
		Water		Drinking		
			Grass	Ingestion		Degradation Diffusion to air
				Animal	Lactation	Degradation Exhalation Urination
					Milk	
						Sink

Figure 18. ACC Human, lipophilic organic chemicals (Czub and McLachlan 2004). Animals include a separate digestive tract and there are two animal types: Milk and beef cattle.



OURSON

Air		Wet and dry deposition				Wet and dry deposition		Inhalation	
	Water	Irrigation				Irrigation		Drinking	
Re-suspension		Soil surface layer	Percolation					Ingestion	Erosion Run off
			Soil ploughing zone	Percolation		Root uptake			
				Soil cultivation zone	Percolation				
					Non-saturated zone				
						Plant foliar surface	Trans-location	Ingestion	
							Plant inner tissue		
								Animal	Metabolism
									Sink

Figure 19. OURSON, radionuclides (Ciffroy et al. 2005; Queguiner et al. 2009). Cereals, root and fruit vegetables have plant inner tissue in addition to plant foliar surface, whereas leafy vegetables, grass and maize silage have not. Animal includes beef and milk.

NMF (new model framework)

Air				Diffusion Particle deposition		Diffusion	Diffusion Particle deposition	Diffusion Particle deposition	
	Soil	Xylem flow	Diffusion	Xylem flow Soil attachment	Xylem flow Diffusion				
		Root1							Degradation Growth Xylem flow to shoots
			Potato						Degradation Growth Diffusion to soil
				Leaf1					Degradation Growth Diffusion to air
					Root2	Xylem flow			Degradation Growth Diffusion to soil
						Stem	Xylem flow	Xylem flow Phloem flow	Degradation Growth Diffusion to air
							Leaf2		Degradation Growth Diffusion to air
								Fruit	Degradation Growth Diffusion to air
									Sink

Figure 20. NMF (new model framework), neutral organic chemicals (Legind and Trapp 2009). Leaf1 includes cereal. The NMF uses the T & A regression for estimating concentrations in milk and meat.



2.2 Compartments

The plant part of the system can be analysed by considering two main sub-systems: the below and aboveground plant compartments. Only the partition-limited model of Chiou et al. (2001) has one generic plant compartment representing both the below- and aboveground plant. Since the 2-FUN modelling tool will focus on transfer of chemicals in the human food chain, the centre of attention will be edible plants.

- All plant models include at least one below ground plant compartment, except the leafy vegetables model, the air to leaf deposition model, the grass model and the T & A, *TSCF* and *SCF* regressions. Possible belowground plant compartments can be separated into root and tuber, because different processes account for the main transfer of chemicals to root and tuber, respectively. Advection with the xylem flow drives uptake into roots, whereas diffusion dominates the transfer of chemicals to potatoes (Trapp et al. 2007). Seven of the models have a single root compartment, the potato model has a single tuber compartment, and two model frameworks have two or more belowground compartments. The CLEA model has both a root and a tuber compartment, and in addition for metals, a root store compartment. The NMF model has two distinct root compartments, the second being part of a fruit tree, and a tuber compartment. Also, the Xtrafood model for metals divide the root compartment into potato, scorzonera, celery and carrot according to empirical regressions found for metal transfer to plants.

Question 1: How many compartments are needed to describe the below ground plant?

- The aboveground plant is included in all plant models except the *RCF* regression, root and potato model. Half of the plant models have a single leaf compartment representing the aboveground plant. Five of the plant models have two or more aboveground plant compartments. The three-compartment fugacity model and simplified three-compartment fugacity model have a leaf and a stem compartment. The CLEA model has a leaf and a fruit compartment, and the fruit tree and NMF model have all three: a leaf, a stem and a fruit compartment. However, the stem of plants is seldom eaten and the stem compartment in the fugacity models accounts also for fruit, nut and seed. The fruit compartment in the CLEA model is actually three compartments: the tree fruit, the herbaceous fruit and the shrub fruit compartment. However, the latter two are only modelled on a case-by-case basis, because no models are available to estimate the concentration of chemical in these (Jeffries and Martin 2008). In the Xtrafood model for metals, the aboveground compartment comprises empirical regressions for endives, cucumber, leek, french bean, lettuce, spinach, tomato, wheat and barley.

Question 2: Is it possible to describe the aboveground plant with a single compartment?

The animal part of the system can be analysed by considering both animals and animal products. All of the reviewed models that include animals have compartments for beef and milk.

- All of the models that contain an animal compartment choose to model the transfer of chemicals to cattle. However, the cattle compartment is defined differently in the various models and frameworks. The OURSON, T & A regression and the TGD (which uses the T & A regression) include beef cattle only in the cattle model, whereas the rest of the models (mother-child, Xtrafood and ACC Human) include both milk and beef cattle. However, the only difference being the bodyweight of the animal and the lactation rate. The ACC Human model for cattle is a two-compartment model including both a digestive tract and the rest of the cattle. The Xtrafood model distinguishes between fat muscle, very fat muscle, low-fat muscle, lean muscle, fat, liver and kidney. None of the models calculates the transfer of chemicals to other animal tissue than beef. However, in OURSON you can add lamb, poultry and eggs as separate compartments.



- Milk is the only animal product considered in the models, except for eggs, which are included in the Xtrafood model.

Question 3: How many compartments are needed to represent the animal system?

2.3 Inputs/outputs

There are three sources of chemicals for the plant in the models; these are external solution, soil and air:

- The *RCF*, *TSCF* and *SCF* regressions are based on the empirical relationships between concentration of chemical in external solution and plant tissue. Measurements are obtained from experiments with plants grown in hydroponic solutions containing the investigated range of organic chemicals. These regressions do not account for transfer of chemicals from air to plant. The concentration of chemical in external solution is in many models interpreted as the concentration of chemical in soil pore water.

Question 4: Can regressions based on measurements from experiments with plants grown in hydroponic solutions be used to model soil-plant systems?

- Except for the three aforementioned regressions based on experiments with plants grown in hydroponic solutions and the leaf to air deposition model, all plant models include the input of chemical from soil to plant. There are five inputs from soil to plant: water flow, diffusion, uptake from soil based on empirical regressions, soil attachment and equilibrium partitioning.
 - Water flow from soil is considered in two-thirds of the plant models under review. Only the empirical regressions, the partition-limited model and the potato model do not include a separate input with the water flow. The xylem flow in plants is soil water taken up by the roots and translocated in the plant with the transpiration stream. This is based on the transpiration flow rate and the chemical distribution between root and soil.
 - Diffusion from soil is considered in the three-compartment fugacity model, the simplified three-compartment fugacity model, the potato model, the fruit tree model, the CLEA model, and the NMF model. The fugacity models estimate diffusion as a fraction (5%) of the xylem flow, whereas the other models use the method outlined in the potato model for tubers, and the method in the fruit tree model for thick roots. The radial diffusion model is applied for potatoes. The diffusion coefficient in potato tissue is found from diffusion coefficients in water and air together with tortuosity factors that account for a slower diffusion in water and air pores of the potato than in pure water and air (Trapp et al. 2007). Partitioning from soil to potato tissue is calculated with partition coefficients. The same approach is applied for thick roots, but here the diffusion coefficient in root tissue is converted to permeability, the permeability of the root biomembrane is added and Fick's first law is applied instead of the radial diffusion model (Trapp 2007).
 - Uptake from soil based on empirical regressions is used in eight of the models. These are the T & A regression and 6 models which use a *TSCF* regression for modelling the chemical concentration in the xylem flow (leafy vegetables, grass, TGD, CSOIL, CLEA, and Xtrafood models). The prediction of metal transfer to plants from soil relies solely on empirically derived *TFs* (transfer factors) in the reviewed models (CSOIL, CLEA, OURSON and Xtrafood).
 - Soil attachment is only considered in three of the models (leafy vegetables, CSOIL and NMF models). Soil attachment is transport to plant surfaces by resuspended soil



particles. The chemical remains, even after washing. This is for all cases modelled by adding the chemical content in a fixed amount of soil assumed to adhere to plants.

- Equilibrium partitioning of the chemical between soil and root has been assumed for organic chemicals in three of the models. These are the TGD, CSOIL and Xtrafood models. Contradictory to this, the partition-limited model accounts for deviance from equilibrium by a 'quasi-equilibrium' factor.

Question 5: Is equilibrium partitioning of contaminants between soil and root a realistic assumption for all organic contaminants?

- Input of chemical to the plant system from air is included in half of the plant models under review. Only the empirical regressions, the partition-limited, the root, potato and CLEA models do not include input from air. There are three inputs from air to plant: diffusion, particle deposition, irrigation and spray application.
 - Gaseous diffusion of chemical from air to plant is considered in all plant models that contain an air compartment except for OURSON. This process pertains only to the fraction of chemical in air that is not adsorbed to particles. The gaseous concentration of chemical in air can either be calculated (aerosol to air partitioning is described in the deliverable related to the soil system) or directly put in the model. Either a fixed gas deposition rate (Trapp and Matthies 1995) used in the leafy vegetables, TGD and CSOIL model or calculated chemical specific permeabilities can be used to model gaseous diffusion. The fugacity, air to leaf deposition, grass and Xtrafood models consider air side and plant (cuticle) side resistances when calculating the transfer to leaves from air. In addition, the tree fruit and NMF models consider the stomata resistance for leaves, and for fruits also the tissue resistance calculated in the same way as for roots (Trapp 2007).
 - Particle deposition (wet and dry) is considered in seven of the models (leafy vegetables, fruit tree, Xtrafood, NMF, OURSON, air to leaf deposition, and grass models). The fraction of chemical in air that is adsorbed to particles can transfer to plants by particle deposition followed by diffusion into plant tissue. This is described with a particle deposition rate and the assumption of 100% transfer of chemical from particle to plant. Only the air to leaf deposition model (McLachlan 1999) and OURSON includes a first-order rate constant describing erosion of particle-bound chemical from the plant surface.
 - Irrigation by river water and dissolved metal species in rain is included in the OURSON model.
 - Spray application is considered for pesticides in the Xtrafood model.

Question 6: Is gas diffusion best described by a fixed gas deposition rate, or should the use of contaminant specific permeabilities for plant tissue be preferred?

Outputs from the plant system are the processes in the far right of the interaction matrices (Figures 2-20) leading to transfer of chemical out of the compartments into an imaginary sink, i.e. they do not add to the chemical pool in e.g. air and soil. These processes comprise: advection from air, degradation in soil and plant compartments, dilution by growth in all plant compartments, diffusion to soil from belowground plant parts, diffusion to air from aboveground plant parts, particle erosion to air, weathering and xylem flow from roots.

- Degradation is in all models described by a first order degradation rate constant, which is a chemical specific input to the model. Both biotic and abiotic processes are included. An example of an abiotic process is photodegradation of dioxins in aboveground plant parts. Biotic processes are metabolism in plants, which for most chemicals is unknown, so the degradation rate constant is an optional input to all models.



- Growth dilution, if considered, is like degradation modelled by a first order rate constant that can be added to the degradation rate constant. Growth dilution is an important process for compounds with a high K_{ow} , since these do not have enough time to equilibrate between e.g. soil and root during the growing period of the plant (Trapp 2002).

It should also be noted that some of the models reviewed for the soil system and described in Deliverable 2.5 (Proposal of the conceptual and mathematical 2-FUN model for assessing transfer of contaminants in soil and groundwater and associated indirect exposures) take into account particle deposition (dry and wet) onto leaves, and further transfer from leaves to soil, because these processes can act as a retardation process for the soil contamination. Thus, Deliverable 2.5 stated that:

‘Some models (e.g. SimpleBox, Caltox) consider that contaminants falling from the atmosphere under dry and wet deposits (as well as irrigation inputs) integrally and directly reach soil; the interception of a fraction of these contaminants by plants is then not taken into account in the mass balance model for soil surface. Instead, other models (e.g. OURSON, Cemos, TrimFate) explicitly consider that a fraction of deposits is intercepted by leaves and does not contaminate soil surface immediately. However, the simulation of interception processes, as well as of delayed leaves-to-soil transfer, differ among models:

- ✓ in TrimFate, the fraction of dry deposits that is intercepted by plants is assumed to be constant. Instead, the fraction of wet deposits that is intercepted by plants is calculated according to the Leaf Area Index (i.e. $m^2[\text{total leaf area}]/m^2[\text{underlying soil area}]$), a ‘vegetation-dependant leaf-wetting factor’ (i.e. a retention factor, in m) and amount of rainfall during a rainfall event;
- ✓ in OURSON, both the fractions of dry and wet deposits respectively are calculated taking into account an Interception coefficient (similar to the TrimFate’s ‘leaf-wetting factor’) and the aerial biomass (or Leaf Area Index). Aerial biomass is however a time-dependent variable because it is assumed to increase until harvest;

The intercepted fraction of contaminants can however reach soil with a retardation time through: (i) litter fall (indicated in Cemos and TrimFate as potential processes, but not appearing explicitly in the set of equations), and/or (ii) continuous transfer from leaves to soil by climate processes (wind, rain, etc), called ‘Wash-off’ in TrimFate and ‘Weathering’ in OURSON). In OURSON and TrimFate, this ‘weathering’ process is simulated through a constant weathering (or wash-off) loss rate, expressed in day⁻¹. In TrimFate, the loss rate is calculated to ensure that the particle mass on the leaves does not change (i.e. as much wet-deposited as is washed off).’

For maintaining homogeneity among the full chain modelling system, the formulations proposed for dry and wet interception in the soil model (Deliverable D2.5) will be applied for the 2-FUN model.

There are 3 main sources of chemicals for the animal part of the system. These are feed, water and air, but the transfer to the animal is handled differently in the 6 models.

- The T & A regressions for beef and milk are based on measurements (Travis and Arms 1988). Concentrations of chemicals in beef and milk are related to the amount of chemical ingested by the animal. This approach gives transfer factors (*TFs*) from feed to beef and milk.
- The TGD uses the T & A regressions.
- The Xtrafood model framework uses measured bio concentration factors (*BCFs*) that relate the concentration in the feed to the concentration in the animal tissue for estimating the transfer of organic chemicals to beef and eggs. If no *BCFs* are available, the *TFs* from Travis and Arms are employed. For modelling the transfer of organic chemicals to milk, the dietary absorption efficiency (McLachlan 1994), which is part of the ACC Human model, is applied. For metals, Xtrafood uses only measured *TFs* from feed to beef, milk and eggs.
- The mother-child model (Trapp et al. 2008) adapted to cattle is a mechanistic model that considers the animal as a flux-through system with input of chemical from feed, drinking water and inhalation of air. Feed is composed of grass and soil. The concentration of chemical



in the feed is estimated with the leafy vegetables model that calculates the concentration of chemical in leaves with attached soil. Concentration of chemicals in water and air are input.

- The ACC Human model (Czub and McLachlan 2004) for beef and milk is fugacity based and considers also the input of chemical to the animal from feed, drinking water and inhalation of air. Feed is composed of grass and air, and the concentration in grass is estimated with the grass model, that is part of ACC Human. Concentration of chemicals in soil, air and water are input. In addition, the ACC Human model estimates the dietary absorption efficiency, which is the ratio between the amount of chemical absorbed and the amount ingested, from K_{ow} .
- OURSON uses measured transfer factors from feed to beef and milk together with a biological half-life for radionuclides in meat and milk.

Outputs from the animal system are only present in the mother-child, ACC Human and OURSON models. Similar to the plant system these are the processes in the far right of the interaction matrices (Figures 2-20) leading to transfer of chemical out of the compartments into an imaginary sink, i.e. they do not add to the chemical pool in e.g. air and soil. These processes comprise: exhalation, urination, out flux of lipids, growth and degradation.

- Exhalation and inhalation is described with a respiration rate for cattle.
- Urination and drinking is described with a drinking rate.
- Outflux of lipids is only part of the mother-child model adapted to cattle and is calculated by assuming that 10% of the ingested lipids are being excreted. The amount of ingested lipids is found by multiplying the volume of grass eaten by the lipid content of the grass.
- Degradation is described by a first order degradation rate constant, which is a chemical specific input to the model. The ACC Human model distinguishes between three types of chemicals: persistent, semi-labile and labile.
- Growth dilution modelled as a first order rate constant that can be added to the degradation rate constant is only part of the mother-child model adapted to cattle. The ACC Human model for beef cattle includes growth by assuming a linear increase with time of the following parameters: cattle volume, respiration rate, grass ingestion rate, soil ingestion rate, drinking and urination rate.

Question 7: Is growth of animals best described by a fixed growth rate or parameters that increase with time (animal mass etc.)?

2.4 Intercompartment transfers

Transfer of chemicals between plant compartments is only relevant for the models with two or more plant compartments, i.e. half of the models described here. However, for organic chemicals, only 3 models (three-compartment fugacity, simplified three-compartment fugacity and fruit tree models) have included transfer processes between plant compartments. There are two processes for transfer between compartments: xylem and phloem flow.

- Xylem flows from root to stem and stem to leaf are included in the fugacity models. In addition, the fruit tree model includes xylem flow from stem to fruit. However, fruits are included in the stem compartment of the fugacity models. Xylem flow in the fugacity models is simulated by a fixed flow rate from root to leaf multiplied by the fugacity in the root or stem and the fugacity capacity of water (Paterson et al. 1994). In the fruit tree model there is a fixed flow rate from root to stem. This is multiplied with the concentration in the xylem of the root, found from the partition coefficient between root and water. Xylem flow to fruit and leaves differ and may be calculated by weighting the flow rate in the stem with surface areas of fruit and leaves (Trapp 2007). The concentration in xylem leaving the stem is found from a partition coefficient between stem and water, and the concentration at the top of the stem. The



concentration in the stem is a function of stem height and depends on adsorption in the stem and diffusion to and from air (Trapp 2007).

- Phloem flows from leaf to stem and stem to root are included in the fugacity models. In the fruit tree model, only phloem flow from stem to fruit is included. In the fugacity models phloem flow is modelled analogously to xylem flow, with a fixed phloem flow set to 5% of the xylem flow (Paterson et al. 1994). In the fruit tree model the phloem flow is found by assuming it identical to 10% of the dry matter content of the fruit divided by the growing period of the fruit (Trapp 2007).

Question 8: Is it essential to include phloem flow in the plant sub-system?

For inorganic chemicals, the CLEA model framework applies correction factors to account for internal plant partitioning with xylem and phloem flow. These factors give the fraction of chemical in the root that reaches the root store, tuber, green vegetable and fruit with xylem and phloem flow (Jeffries and Martin 2008). If available, they should be chemical specific.

The OURSON model includes translocation from plant foliar surface to plant inner tissue for cereals, root and fruit vegetables. This is modelled from the maximum translocation factor and the time during growth of the plant, when maximum translocation is reached (Ciffroy et al. 2005).

Transfer of chemicals between the plant and animal system is present in the Xtrafood model, where the amount of chemical ingested by the animal is found by adding all food sources, which includes roots and aboveground plants. The same is present in both OURSON and ACC Human, where the cattle feed on the grass.

Intercompartment transfers for the animal part of the system are present in the mother-child model adapted to cattle and the ACC Human model for beef and milk. This is the lactation of the milk cattle, which is described by a lactation rate.

The types of chemicals considered in the reviewed models are mainly neutral organic chemicals. Only the Xtrafood, OURSON, CSOIL and CLEA models include other compounds in their model frameworks, however with separate approaches. These are eight pesticides (partly ionic organic compounds) and heavy metals (Xtrafood), radionuclides and metals (OURSON), inorganic chemicals including metals (CLEA and CSOIL).

3. THE PLANT AND ANIMAL SYSTEM - DEFINITION OF THE 2-FUN INTERACTION MATRIX

The main questions identified from the model comparison are discussed in this section. This will lead to the definition of the 2-FUN interaction matrix for the plant system.

3.1 Compartments

Question 1: How many compartment are needed to describe the below ground plant?

For organic chemicals there are two possible belowground plant compartments: root and tuber. They are two different plant organs. The root has uptake of chemical from soil water with the xylem flow, whereas the tuber has not. Instead, diffusion of chemical from soil to tuber becomes more important. Comparing the results from the root (Trapp 2002) and potato (Trapp et al. 2007) model for neutral compounds with varying K_{ow} gives a difference in chemical concentration up to a factor of 5 (Trapp and Legind 2009). The chemical concentration in roots is higher than in potato. Both the root and the tuber are in the 2-FUN context (edible plants) storage organs and receive nutrients from the phloem flux. However, this is not included in the above comparison between root and tuber. Since there is a measurable difference between xylem flow (root) and diffusion from soil (tuber) both a root and a



tuber compartment is included in the 2-FUN plant system. The tuber compartment covers mainly potatoes, which account for 39% of the consumption of vegetables in Denmark (Lyhne et al. 2005). For metals, the number of possible compartments depends on the availability of empirical data, but here it also seems reasonable to pool the belowground compartments into two compartments: root and tuber.

Question 2: Is it possible to describe the aboveground plant with a single compartment?

For organic chemicals the following aboveground plant compartments have been included in the reviewed models: leaf, stem and fruit. The leaf compartment is important, leafy vegetables are included in all model frameworks, so a leaf compartment is included in the 2-FUN plant system. In the NMF, the leaf model is also adapted to model uptake of organic chemicals in grains. This is done, because processes and parameters differ between leafs and grains, and cereal products constitute a large amount of our daily diet (in Denmark approximately 216 g/d is consumed by adults (Lyhne et al. 2005)). So a separate grain compartment is added to the 2-FUN plant system. Only for the fruit tree model, the stem is essential. This is because the concentration of chemical decreases with height of the stem. However, the stem is not a common part of the vegetable diet, so this compartment is neglected. Again, considering the composition of our daily diet, fruits should be included in the 2-FUN plant system. For pesticides, the major intake is in Denmark with apples (Fødevarestyrelsen 2008). But also processes between fruit and leaves differ. And a big difference between chemical concentrations in leaves and tree fruits are found, for sulfolane, *BCFs* for soil to leaves can be up to a factor of 230 larger than *BCFs* for soil to fruit (Chard et al. 2006). Leaves have generally a higher chemical load than fruits, due to a higher water flow to leaves and higher deposition from air.

Question 3: How many compartments are needed to represent the animal system?

The transfer of organic chemicals to animals and animal products are in the reviewed models all based on measurements and model estimations of the concentration of chemicals in cattle and milk. Therefore we choose to include two compartments for the animal part of the 2-FUN model: animal and milk. The animal is either beef or milk cattle. Looking at the consumption pattern for an average Dane this seems reasonable. An adult Dane consumes 113 g meat/d and 307 g milk/d, and only 27 g poultry/d, 29 g cheese/d and 16 g egg/d (Lyhne et al. 2005). However, meat includes pork as well as beef. So, differences between the transfer of chemicals to pigs and cattle should be resolved.

[3.2 Inputs/outputs](#)

Question 4: Can regressions based on measurements from experiments with plants grown in hydroponic solutions be used to model soil-plant systems?

TSCF regressions are the most widely applied relationships for predicting translocation of organic chemicals in plants from soil pore water. There are four regressions: Briggs et al. (1982), Burken and Schnoor (1998), Hsu et al. (1990) and Dettenmaier et al. (2009). However, the first three predicts a lower translocation for hydrophilic compounds ($\log K_{OW} < 1$) than the last one mentioned. Several experimental methods have been used to establish the *TSCF* regressions, e.g. the pressure chamber technique, which may lead to artificial results (Ciucani et al. 2002). Advancements in plant modelling replace the empirical regressions with a calculation using plant physiological parameters such as transpiration, growth rate and partitioning between root tissue and water (Trapp 2007). This approach and all of the regressions give similar results for lipophilic chemicals. For polar chemicals only the regression by Dettenmaier et al. (2009) and the new approach by Trapp (2007) predicts the same translocation. I.e. for polar chemicals ($\log K_{OW} < 1$) the ratio between the concentration in xylem and soil pore water remains high (i.e. close to 1). Trapp (2007) speculates that this is due to the formation



of root hairs in soil, which lead to better diffusive uptake of polar chemicals. Plants grown in hydroponics do not form root hairs to the same extent as plants grown in soil and the low translocation of polar compounds found in hydroponic experiments is perhaps an artefact. However, other arguments have also been suggested (Dettenmaier et al. 2009). For the 2-FUN plant system, the *TSCF* is replaced with the new modeling approach, which also relates the concentration of chemical in roots to the concentration in leaves.

Question 5: Is equilibrium partitioning of contaminants between soil and root a realistic assumption for all organic contaminants?

The equilibrium partitioning approach applied for the distribution of chemicals between soil and root (TGD, CSOIL and Xtrafood) have been questioned for lipophilic chemicals in some studies (Legind and Trapp 2009; Rikken et al. 2001; Trapp 2002; Trapp and Schwartz 2000). Comparing results from the equilibrium approach and the dynamic root model (Trapp 2002) to measured concentrations of benzo(a)pyrene in root crops shows that the equilibrium approach gives a concentration of benzo(a)pyrene in roots that is three orders of magnitude higher than measured. Furthermore, the estimate from the dynamic model lies in the same order of magnitude as the measured value (Legind and Trapp, 2009). For the 2-FUN plant system, uptake of chemical from soil to root is based on the transpiration flow rate and the chemical distribution between root and soil.

Question 6: Is gas diffusion best described by a fixed gas deposition rate, or should the use of contaminant specific permeabilities for plant tissue be preferred?

In three of the models, a fixed gas deposition rate is applied (leafy vegetables, TGD and CSOIL models), whereas other models (fugacity, air to leaf deposition, grass, Xtrafood, fruit tree and NMF models) estimate the gaseous diffusion by calculating chemical specific permeabilities of plant tissue. Diffusion of chemical between air and plant tissue is controlled by the permeability of the plant. Major resistances that control the exchange between air and plant are: air boundary layer, stomata and cuticle resistances (Riederer 1995). For the 2-FUN plant system, the permeability of these three layers (Trapp 2007) together with cell wall permeability (Trapp 2000) and aqueous layer permeability are calculated to model the diffusion between air and leaf or grain. For fruit, additional fruit tissue permeability is included in the overall conductance of plant tissue (Trapp 2007).

Question 7: Is growth of animals best described by a fixed growth rate or parameters that increase with time (animal mass etc.)?

Growth is included in the mother-child model and in the ACC human model for beef cattle. In the mother-child model a fixed growth rate is applied, and in the ACC human model for beef cattle six parameters are assumed to increase linearly with time from birth until slaughter. These parameters are: 1) volume of steer, 2) respiration rate of steer, 3) grass consumption rate of steer, 4) soil consumption rate of steer, 5) drinking rate of steer and 6) urination rate of steer. The two approaches give results in the same order of magnitude, so for simplicity reasons a fixed growth rate is applied in the 2-FUN model.

[3.3 Intercompartment transfers](#)

Question 8: Is it essential to include phloem flow in the plant sub-system?

Phloem flow is included in the fugacity models, but only with a flow rate that is estimated as 5% of the xylem flow rate. So the importance of this process is minor. In plants the total volume of xylem



flow is 50-100 fold greater than phloem flow (Bromilow and Chamberlain 1995). Only for fruits, the phloem flow dominates. So phloem flow is included in the fruit tree model (Trapp 2007). For polar, weak acids, phloem flow to all plant compartments might prove important. This is due to the ion trap. However, none of the reviewed models include the ion trap process. For the 2-FUN plant system only phloem flow to the fruit compartment is included, with the assumption that the concentration of chemical in phloem is equal to the concentration in xylem.

Considering the analysis above, the 2-FUN interaction matrix for the plant system was designed (Figure 20).



2-FUN interaction matrix for the plant and animal sub-system

Air				Particle deposition* Diffusion		Diffusion		Particle deposition* Diffusion	Inhalation <i>TF</i>	<i>TF</i>	
	Soil	Xylem flow <i>TF</i>	Diffusion <i>TF</i>	Soil attachment <i>TF</i>	Xylem flow <i>TF</i>	Soil attachment <i>TF</i>	Xylem flow <i>TF</i>	<i>TF</i>			
		Water		Irrigation		Irrigation			Drinking <i>TF</i>	<i>TF</i>	
			Root _L	Xylem flow _L							Degradation Growth
				Tuber							Degradation Growth Diffusion to soil
				Leaf					Ingestion <i>TF</i>	<i>TF</i>	Degradation Growth Diffusion to air
					Root _G	Xylem flow _G					Degradation Growth Xylem flow to top
						Grain					Degradation Growth Diffusion to air
							Root _F	Xylem flow _F Phloem flow _F			Degradation Growth Xylem flow to top
								Fruit			Degradation Growth Diffusion to air
									Animal	Lactation	Growth Degradation Exhalation Outflux of lipids Urination
										Milk	
											Sink

Figure 21. 2-FUN interaction matrix for the plant and animal sub-system, L means leaf, G means grain and F means fruit. For inorganic chemicals, only particle deposition from air (*) and empirical transfer factors (*TF*) are employed.



The main principles of this conceptual model are summarised below:

Compartments:

- Two belowground plant compartments: root and tuber
- Three aboveground plant compartments: leaf, grain and fruit (for inorganic chemicals, the leaf and fruit compartments have two sub compartments: one that receives chemical from air, and one that receives chemical from soil)
- Each aboveground compartment is connected to a separate root compartment (there are no crops where leaves, grains and fruits are harvested together) (only organic compounds)
- One animal compartment comprising both beef and milk cattle
- A milk compartment

Inputs/outputs:

- Water flow from soil to root
- Diffusion from soil to tuber
- Transfer from soil to leaf, grain and fruit (only inorganic chemicals)
- Soil attachment on leaf and grain (only organic compounds)
- Diffusion from air to leaf, grain and fruit (only organic compounds)
- Inhalation and exhalation of air by animal (exhalation: only organic compounds)
- Drinking of water by animal and urination (urination: only organic compounds)
- Transfer from air and water to milk (only inorganic chemicals)
- Particle deposition from air to leaf and fruit
- Irrigation from water to leaf and grain
- Weathering of particles from leaf and fruit to soil (only inorganic chemicals)
- Metabolism of chemicals in all plant and animal compartments (only organic compounds)
- Growth of all plant and animal compartments (except milk cattle)
- Xylem flow to top plant parts other than grain and fruit (only organic compounds)
- Outflux of lipids from animal (only organic compounds)

Intercompartment transfers:

- Xylem flow from root to leaf, grain and fruit (only organic compounds)
- Phloem flow from root to fruit (only organic compounds)
- Ingestion of leaves by animal
- Transfer from leaves to milk (only inorganic chemicals)
- Lactation by animal (only organic compounds)



4. THE PLANT AND ANIMAL SYSTEM – DEFINITION OF THE MATHEMATICAL MODEL FOR ORGANIC CHEMICALS

This section describes the equations behind the interaction matrix for the 2-FUN plant system for organic chemicals (Figure 21). Time-dependent concentrations or masses of chemicals in each of the plant, animal and milk compartments are derived from inputs, outputs, and intercompartment transfers previously selected.

4.1 Root

The change of chemical concentration in thick roots can be described as follows: influx with xylem water minus outflux with xylem water, growth and degradation. Diffusive uptake is not considered since it usually only makes a small change in the concentration in roots. Also, it is assumed that the root is peeled before consumption. Hydrophobic chemicals only reach the peel of the root by diffusion.

$$(1) \quad \frac{dC_R}{dt} = \frac{Q}{M_R} K_{WS} C_S - \frac{Q}{M_R K_{RW}} C_R - k C_R$$

where

- C_R (mg kg fw⁻¹) is the concentration of chemical in root
- Q (L d⁻¹) is the transpiration stream
- M_R (kg fw) is mass of the root
- K_{WS} (kg ww L⁻¹) is the partition coefficient between soil pore water and bulk soil ($K_{WS} = C_W / C_S$) (described in the deliverable related to the soil system)
- C_S (mg kg ww⁻¹) is the concentration of chemical in bulk soil
- K_{RW} (L kg fw⁻¹) is the partition coefficient between root and water
- k (d⁻¹) is the sum of k_G (d⁻¹) the growth rate and k_{deg} (d⁻¹) the degradation rate

The equation for the change of chemical mass is the same for all root compartments. However, for the root compartment connected to grains, the outflow of chemical with the xylem flow can be described as the sum of flow to grains and flow to rest of the plant ($Q_R = Q_G + Q_{G,top}$). Similarly, for the root compartment connected to fruits, the outflow of chemical with the xylem flow can be described as the sum of xylem and phloem flow to fruits and xylem flow to the rest of the plant ($Q_R = Q_F + Q_{F,top}$).

The phase equilibrium between root and water considers sorption to root lipids and dissolution into the aqueous solution of root cells.

$$(2) \quad K_{RW} = W_R + L_R a K_{OW}^b + G_R K_{AW}$$

where

- W_R (L kg fw⁻¹) is the water content of the root



- L_R (kg kg^{-1} (ww)) is the lipid content of the root
- a equals $1/\rho_{\text{Octanol}}$ (1.22 L kg^{-1}) and is a correction for density differences between water and n-octanol
- K_{OW} is the octanol water partition coefficient
- b is an empirical correction factor for differences between solubility in octanol and sorption to plant lipids ($b = 0.77$ for roots (Briggs et al. 1982) and 0.95 for leaves (Briggs et al. 1983))
- G_R (L kg fw^{-1}) is the air content of the root
- K_{AW} is the partition coefficient between air and water

The generic parameterisation of the root model is given in Table 3.

Table 3. Parameters of the root (Trapp 2002; Trapp 2007).

Parameter	Symbol	Value	Unit
Transpiration	Q	1	L d^{-1}
Mass	M_R	1	kg fw
Growth rate	k_G	0.1	d^{-1}
Water content	W_R	0.89	L kg fw^{-1}
Lipid content	L_R	0.025	kg kg^{-1} (ww)
Correction factor	b	0.77	
Air content	G_R	0.1	L kg fw^{-1}
Root wet density	$\rho_{R,wet}$	1	kg fw L^{-1}
Root dry density	$\rho_{R,dry}$	0.11	kg dw L^{-1}
Growth period	t_{root}	120	d

4.2 Tuber

For tubers, a potato model that considers diffusion from soil into spherical potatoes, dilution by growth and degradation is applied.

$$(3) \quad \frac{dC_P}{dt} = k_I C_S - k_2 C_P - k C_P$$

where:

- C_P (mg kg fw^{-1}) is the concentration of chemical in potato
- k_I (d^{-1}) is the uptake rate
- k_2 (d^{-1}) is the depuration rate
- k (d^{-1}) is the sum of k_G (d^{-1}) the growth rate and k_{deg} (d^{-1}) the degradation rate



The depuration rate is deduced from a radial diffusion model

$$(4) \quad k_2 = \frac{23 D_P}{R^2}$$

where:

- D_P ($\text{m}^2 \text{d}^{-1}$) is the diffusion coefficient in potato
- R (m) is the radius of the potato

The diffusion coefficient in potato tissue is calculated from the diffusion in the water and air phases of the potato

$$(5) \quad D_P = T_W f_W D_W + T_G f_G D_G$$

where:

- T_W is the tortuosity in the water pores of the potato
- f_W is the fraction of the chemical dissolved in the water of the potato
- D_W ($\text{m}^2 \text{d}^{-1}$) is the diffusion coefficient in pure water
- T_G is the tortuosity of the air pores of the potato
- f_G is the fraction of the chemical dissolved in the air of the potato
- D_G ($\text{m}^2 \text{d}^{-1}$) is the diffusion coefficient in pure air

In porous solids such as plant tissue, the diffusion is hampered by a “labyrinth factor”, named the tortuosity. This is estimated by the method of Millington and Quirk (cited in Jury et al (1983)). The equations are not unit true.

$$(6) \quad T_W = \frac{W_P^{10/3}}{(W_P + G_P)^2} \quad T_G = \frac{G_P^{10/3}}{(W_P + G_P)^2}$$

where:

- W_P (L kg fw^{-1}) is the water content of the potato
- G_P (L kg fw^{-1}) is the air content of the potato

The fractions of chemicals dissolved in the water and air of the potato are equal to the ratios of concentration in water and air phase, respectively, of the plant tissue to total concentration in the potato.



$$(7) \quad f_w = \frac{W_P}{K_{PW}} \qquad f_G = \frac{G_P K_{AW}}{K_{PW}}$$

where:

- K_{PW} (L kg fw⁻¹) is the partition coefficient between potato and water

$$(8) \quad K_{PW} = W_P + f_{CH} K_{CH} + L_P a K_{OW}^b + G_P K_{AW}$$

where:

- f_{CH} (L kg fw⁻¹) is the fraction of carbohydrates in potato
- K_{CH} is the partition coefficient between carbohydrates and water. Chiou et al. (2001) assume K_{CH} to be 0.1 for compounds with $\log K_{OW} < 0$; 0.2 for $\log K_{OW} = 0.1-0.9$; 0.5 for $\log K_{OW} = 1.0-1.9$; 1 for $\log K_{OW} = 2.0-2.9$; 2 for $\log K_{OW} = 3.0-3.9$; and 3 for $\log K_{OW} \geq 4.0$.
- L_P (kg kg⁻¹ (ww)) is the lipid content of potato

The diffusion coefficients of chemicals can be related to the square root of the molar mass.

$$(9) \quad D_w = D_{O_2} \frac{\sqrt{32 \text{ g mol}^{-1}}}{\sqrt{M}} \qquad D_G = D_{H_2O} \frac{\sqrt{18 \text{ g mol}^{-1}}}{\sqrt{M}}$$

where:

- D_{O_2} is the diffusion coefficient of oxygen in water ($1.728 \times 10^{-4} \text{ m}^2 \text{ d}^{-1}$)
- M (g mol⁻¹) is the molar mass of the chemical
- D_{H_2O} is the diffusion coefficient of water vapour in air ($2.22 \text{ m}^2 \text{ d}^{-1}$)

The uptake rate k_I is calculated from phase equilibrium

$$(10) \quad k_I = k_2 \frac{K_{PW}}{K_{SW}}$$

The parameterisation of the potato model is given in Table 4.



Table 4. Parameters of the potato (Trapp et al. 2007)

Parameter	Symbol	Value	Unit
Radius	R	0.04	m
Growth rate	k_G	0.139	d^{-1}
Water content	W_P	0.778	$L\ kg\ fw^{-1}$
Air content	G_P	0.04	$L\ kg\ fw^{-1}$
Lipid content	L_P	0.001	$kg\ kg^{-1}\ (ww)$
Carbohydrate fraction	f_{CH}	0.086	$L\ kg\ fw^{-1}$
Correction factor	b	0.77	
Potato wet density	$\rho_{P,wet}$	1	$kg\ fw\ L^{-1}$
Potato dry density	$\rho_{P,dry}$	0.222	$kg\ dw\ L^{-1}$
Growth period	t_{potato}	60	d

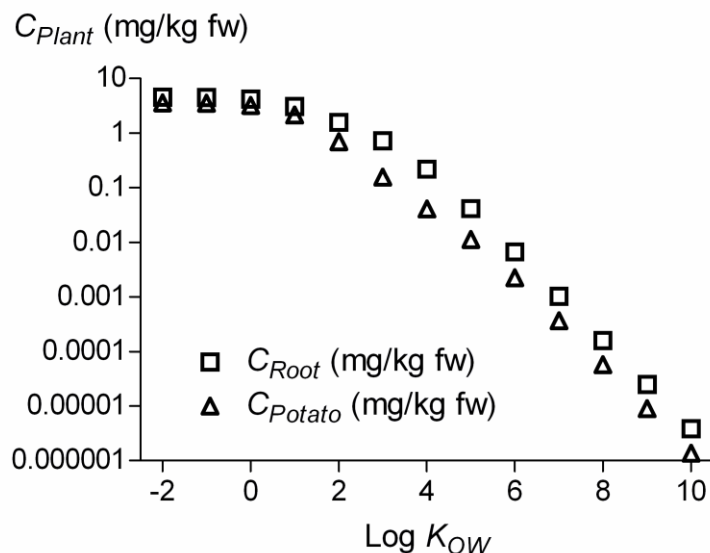


Figure 21. Steady state concentration of chemical in root and potato tissue as a function of lipophilicity, $C_{Soil} = 1\ mg/kg\ ww$.

The steady state concentrations of chemical in plant tissue, predicted with the root and potato model are compared in Figure 21. It is seen that the concentration of chemical in both root and potato tissue decreases with increasing lipophilicity of the chemical.

[4.3 Leaf](#)

The change of chemical concentration in leaves is influx with transpiration water plus gaseous and particulate deposition from air plus soil attachment minus diffusion to air, growth and degradation.



$$(11) \quad \frac{dC_L}{dt} = \frac{Q}{M_L K_{RW}} C_{R_L} + \frac{A_L g_L}{M_L} C_{A, gas} + \frac{(f_{wet} \Lambda_{part} Rain + f_{dry} v_{dep, dry}) S_{field}}{M_L} TSP_A C_{A, part} + \frac{f_{wet} Irr S_{field}}{M_L} C_{River} - \frac{A_L g_L}{K_{LA} M_L} C_L - k C_L$$

where:

- C_L (mg kg fw⁻¹) is the concentration of chemical in leaves
- M_L (kg fw) is the mass of leaves
- A_L (m²) is the area of leaves
- g_L (m d⁻¹) is the conductance of leaves
- $C_{A, gas}$ (mg m⁻³) is the gaseous concentration of chemical in air
- $C_{A, part}$ (mg g⁻¹) is the concentration of chemical at particles in air
- TSP_A (g m⁻³) is the total amount of particles in air
- Λ_{part} (m³ air m⁻³ rain) is the rainfall scavenging ratio for particles
- $Rain$ (m d⁻¹) is rainfall
- $v_{dep, dry}$ (m d⁻¹) is the dry deposition velocity of particles
- S_{field} (m²) is the surface area of the field
- Irr (mm d⁻¹) is the irrigation rate
- C_{River} (mg L⁻¹) is the concentration of chemical in river water
- ρ_L (kg fw m⁻³) is the density of leaves
- K_{LA} (m³ kg fw⁻¹) is the partition coefficient between leaves and air
- k (d⁻¹) is the sum of k_G (d⁻¹) the growth rate and k_{Loss} (d⁻¹) the degradation rate

The conductance of leaves is related to the permeability of leaves. The difference is that the permeability is related to concentrations in water, while conductance is related to concentrations in the gas phase.

$$(12) \quad g_L = \frac{P_L}{K_{AW}}$$

where:

- P_L (m d⁻¹) is the permeability of leaves

$$(13) \quad P_L = P_{c, total} + P_{stomata}$$

where:



- $P_{c,total}$ (m d^{-1}) is the total permeability of the cuticle pathway
- $P_{stomata}$ (m d^{-1}) is the permeability of the stomata in the leaf

$$(14) \quad P_{c,total} = \frac{1}{\frac{1}{P_{air}} + \frac{1}{P_{cuticle}} + \frac{1}{P_{water}} + \frac{1}{P_{cellwall}}}$$

where:

- P_{air} (m d^{-1}) is the permeability of the air boundary layer around the leaf
- $P_{cuticle}$ (m d^{-1}) is the permeability of the cuticle
- P_{water} (m d^{-1}) is the permeability of the water inside the leaf
- $P_{cellwall}$ (m d^{-1}) is the permeability of the cell wall (21.6 m d^{-1} (Trapp 2000))

A resistance of 200 m s^{-1} was estimated as typical for a chemical with a molecular mass of 300 g mol^{-1} for the air boundary layer (Thompson 1983).

$$(15) \quad P_{air} = \left(\frac{1}{200} \frac{\sqrt{300 \text{ g mol}^{-1}}}{\sqrt{M}} \right) (\text{m s}^{-1}) K_{AW} 86400 (\text{s d}^{-1})$$

A regression equation was derived for the permeability of citrus cuticles (Kerler and Schonherr 1988).

$$(16) \quad P_{cuticle} = 10^{0.704 \log K_{ow} - 11.2} (\text{m s}^{-1}) 86400 (\text{s d}^{-1})$$

The permeability of the water in leaves is calculated from the diffusion coefficient in water found from Equation 9.

$$(17) \quad P_{water} = \frac{D_w}{\Delta x}$$

where:

- Δx is the thickness of the water layer ($5 \cdot 10^{-5} \text{ m}$)

The permeability of the stomatal pathway can be calculated if the water loss by transpiration and the leaf surface area of the plant are known (Trapp 2007).



$$(18) \quad P_{Stomata} = \frac{Q \rho_w \sqrt{18 \text{ g mol}^{-1}} K_{AW} 461.9 (\text{N m kg K}^{-1}) (T + 273.15)}{610.7 \times 10^{\frac{7.5T}{237+T}} (\text{N m}^{-2}) A_L (1 - rh)}$$

where

- ρ_w is the density of water (1 kg L⁻¹)
- T (°C) is the temperature
- rh is the relative humidity (0.5)

The partition coefficient between leaves and air is found from the partition coefficient between leaves and water.

$$(19) \quad K_{LA} = \frac{K_{LW}}{K_{AW} 1000 \text{ L m}^{-3}}$$

where:

- K_{LW} (L kg fw⁻¹) is the partition coefficient between leaf tissue and water found from Equation 2 but with parameters for the leaf (Table 5)

The fraction of chemical in irrigation water and at particles that are intercepted by and transferred to the leaves, f_{wet} and f_{dry} , are found from the biomass and absorption coefficients:

$$(20) \quad f_{wet/dry} = 1 - \exp\left(\frac{-\mu_{wet/dry} B_{Aerial} \rho_{L,dry}}{\rho_{L,fresh}}\right)$$

where:

- $\mu_{wet/dry}$ (m² kg dw⁻¹) is an empirically derived absorption coefficient
- $\rho_{L,dry}$ (kg dw L⁻¹) is the leaf dry density
- $\rho_{L,fresh}$ (kg fw L⁻¹) is the leaf fresh density
- B_{Aerial} is equal to M_L (kg fw)

Soil attachment is considered by adding the chemical mass in the attached soil on the day of harvest

$$(21) \quad C_L = C_L(t_H) + TS_A C_S$$

where



- $C_L(t_H)$ is the concentration in leaves on the day of harvest (t_H)
- TS_A (g g^{-1} (ww)) is a transfer factor for soil attachment

The parameterisation of the leaf model is given in Table 5.

Table 5. Parameters of the leaf (Legind and Trapp 2009; Trapp and Matthies 1996; Trapp and Legind 2009).

Parameter	Symbol	Value	Unit
Transpiration	Q	1	L d^{-1}
Shoot mass	M_L	1	kg fw
Leaf area	A_L	5	m^2
Soil attachment	TS_A	0.01	g g^{-1} (ww)
Leaf wet density	$\rho_{L,wet}$	1000	kg fw m^{-3}
Leaf dry density	$\rho_{L,dry}$	200	kg dw m^{-3}
Growth rate	k_G	0.035	d^{-1}
Water content	W_L	0.8	L kg fw^{-1}
Air content	G_L	0.1	L kg fw^{-1}
Lipid content	L_L	0.02	kg kg^{-1} (ww)
Correction factor	b	0.95	
Growth period	$t_{lettuce}$	60	d

4.4 Grain

For grains we use a modified leafy vegetables model to calculate uptake into grains. The change of chemical concentration in grains is influx with transpiration water plus gaseous deposition from air plus soil attachment minus diffusion to air, growth and degradation.

$$(22) \quad \frac{dC_G}{dt} = \frac{Q_G}{M_G K_{RW}} C_{R_G} + \frac{A_G g_G}{M_G} C_{A,gas} + \frac{f_{wet} Irr S_{field}}{M_G} C_{River} - \frac{A_G g_G}{K_{GA} M_G} C_G - k C_G$$

where:

- C_G (mg kg fw^{-1}) is the concentration of chemical in grains
- M_G (kg fw) is the mass of grains
- A_G (m^2) is the area of grains
- g_G (m d^{-1}) is the conductance of grains. This is calculated from Equations 12 – 18, but with Q_G and A_G .
- ρ_G (kg fw m^{-3}) is the density of grains



- K_{GA} ($\text{m}^3 \text{ kg fw}^{-1}$) is the partition coefficient between grains and air. This is calculated from Equations 8 and 19, but with parameters for the grain (Table 6) (the carbohydrate fraction (f_{CH}) is found by division of carbohydrate content (CH_G) with density (ρ_{CH})).
- k (d^{-1}) is the sum of k_G (d^{-1}) the growth rate and k_{deg} (d^{-1}) the degradation rate

Soil attachment is considered by adding the chemical mass in the attached soil on the day of harvest (Equation 21).

The parameterisation of the grain model is given in Table 6.

Table 6. Parameters of the grain (Legind and Trapp 2009).

Parameter	Symbol	Value	Unit
Transpiration	Q_G	0.2	L d^{-1}
Grain mass	M_G	1	kg fw
Grain area	A_G	1	m^2
Soil attachment	TS_A	0.001	g g^{-1} (ww)
Grain wet density	$\rho_{G,wet}$	1000	kg fw m^{-3}
Grain dry density	$\rho_{G,dry}$	850	kg dw m^{-3}
Growth rate	k_G	0.035	d^{-1}
Water content	W_G	0.15	L kg fw^{-1}
Air content	G_G	0	L kg fw^{-1}
Lipid content	L_G	0.02	kg kg^{-1} (ww)
Carbohydrate content	CH_G	0.602	kg kg^{-1} (ww)
Carbohydrate density	ρ_{CH}	2	kg L^{-1}
Correction factor	b	0.95	
Growth period	t_{grain}	50	d

4.5 Fruit

The change of chemical concentration in fruits is influx with xylem and phloem plus gaseous and particulate deposition from air minus diffusion to air, growth and degradation.

(23)

$$\frac{dC_F}{dt} = \frac{Q_F}{M_F K_{RW}} C_{R_F} + \frac{A_F g_F}{M_F} C_{A,gas} + \frac{(f_{wet} \Lambda_{part} Rain + f_{dry} v_{dep,dry}) S_{field}}{M_F} TSP_A C_{A,part} - \frac{A_F g_F}{K_{FA} M_F} C_F - k C_F$$

where:

- Q_F (L d^{-1}) is the sum of xylem and phloem flow to fruits
- M_F (kg fw) is the mass of fruits



- A_F (m^2) is the area of fruits
- g_F (m d^{-1}) is the conductance of fruits
- K_{FA} ($\text{m}^3 \text{kg fw}^{-1}$) is the partition coefficient between fruit and air found from Equations 2 and 19 but with parameters for the fruit (Table 7)
- k (d^{-1}) is the sum of k_G (d^{-1}) the growth rate and k_{deg} (d^{-1}) the degradation rate

The xylem flow to fruits is found by averaging with the surface areas of fruits and leaves of the fruit tree (Trapp 2007). The phloem flow into fruits is assumed to be ten times the dry matter content of the fruit with a growing period of 60 days. The concentration of chemical in xylem and phloem are assumed to be the same, so xylem and phloem flow are added to give the total flow to fruits (Table 7).

The area of fruits is found by multiplying the area of one piece of fruit by the number of fruits. The number of fruits is found by dividing the mass of fruits with the mass of one piece of fruit. The area of fruits and leaves of the fruit tree is given in Table 7.

The conductance of fruits is found from Equation 12, but from the permeability of fruits (Equation 24). This is found by adding the permeability of fruit tissue to the calculation of leaf permeability. The permeability of the stomata is found from Equation 18, but from the xylem flow to fruits (Table 7).

$$(24) \quad P_F = \frac{1}{\frac{1}{(P_{c, total} + P_{stomata})} + \frac{1}{P_{tissue}}}$$

where:

- P_{tissue} (m d^{-1}) is the permeability of fruit tissue.

$$(25) \quad P_{tissue} = \frac{D_F}{d_F}$$

where:

- D_F ($\text{m}^2 \text{d}^{-1}$) is the diffusion coefficient in fruit tissue found from Equation 5, but with parameters for the fruit (Table 7)
- d_F (m) is the diffusion path length in the fruit (0.01 m)

The parameterisation of the fruit model is given in Table 7.



Table 7. Parameters of the fruit (Trapp 2007).

Parameter	Symbol	Value	Unit
Fruit mass	M_F	0.4	kg fw
Fruit radius	R_F	0.04	m
Fruit fresh density	$\rho_{F, fresh}$	1000	kg fw m ⁻³
Fruit dry density	$\rho_{F, dry}$	156	kg dw m ⁻³
Growth rate	k_G	0.035	d ⁻¹
Water content	W_F	0.844	L kg fw ⁻¹
Air content	G_F	0.25	L kg fw ⁻¹
Lipid content	L_F	0.006	kg kg ⁻¹ (ww)
Correction factor	b	0.95	
Xylem flow to fruit	Q_{FX}	0.015	L d ⁻¹
Xylem and phloem flow to fruit	Q_F	0.025	L d ⁻¹
Leaf area	$A_{L,F}$	2	m ²
Fruit area	A_F	0.03	m ²
Growth period	t_{fruit}	90	d

The steady state concentrations of chemical in plant tissue, predicted with the leaf, grain and fruit model are compared in Figure 22. It is seen that the concentration of chemical in leaf and grain tissue increases with increasing lipophilicity of the chemical, whereas the concentration of chemical in fruit tissue decreases after a log K_{OW} of 3. This is caused by the transfer from air. The permeability of the cuticle pathway increases with lipophilicity, which is seen for leaf and grain. But for fruit the permeability of fruit tissue decreases, which counteracts this effect and leads to decreasing concentrations in fruit.

It can also be seen that the concentration of chemical in leaf, grain and fruit tissue decreases with increasing volatility from water, most pronounced for leaf and grain, which have larger surface area to volume ratios.

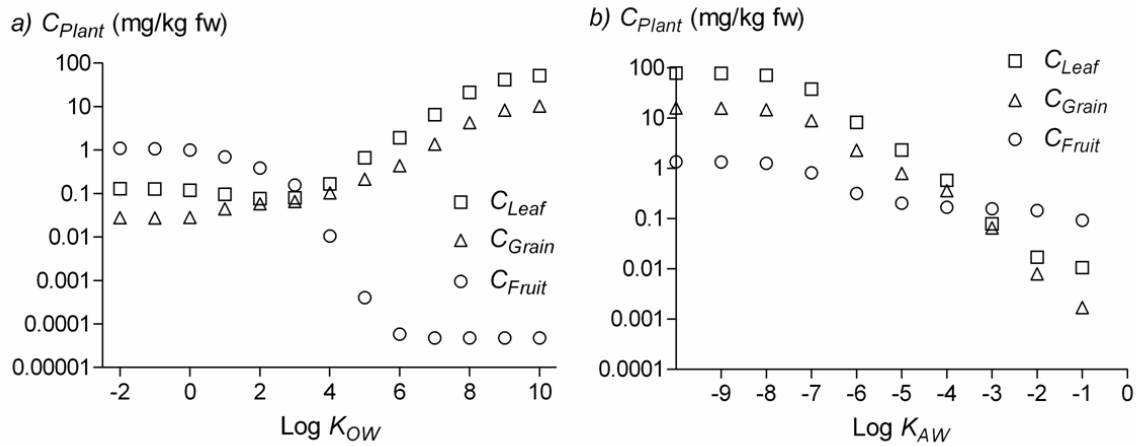


Figure 22. Concentration of chemical in leaf, grain and fruit as a function of lipophilicity and volatility from water, $C_{Soil} = 1 \text{ mg/kg ww}$, $C_{Air} = 0.001 \text{ mg/m}^3$. a) $K_{AW} = 0.001$, b) $K_{OW} = 1000$.

4.6 Animal

The change of chemical mass in animals is from input with diet, drinking water and inhalation minus outflux with lipids, urination and exhalation. For milk cattle there is also outflux by lactation (Trapp et al. 2008). The mass in cattle fat is found by division with the lipid content of the cattle.

$$(26) \quad \frac{dm_C}{dt} = I - k m_C$$

where:

- m_C (mg) is the mass of chemical in cattle
- I (mg d^{-1}) is the sum of daily intake of chemical
- k (d^{-1}) is the loss rate constant

The daily intake of chemical is found from the consumption of grass, drinking water and inhalation.

$$(27) \quad I = F_{Grass} C_{Grass} + F_W C_W + F_A C_A$$

where:

- F_{Grass} (kg ww d^{-1}) is the grass consumption rate of cattle
- C_{Grass} (mg kg ww^{-1}) is the concentration in grass and found from the leaf model without irrigation
- F_W (L d^{-1}) is the drinking and urination rate of cattle
- C_W (mg L^{-1}) is the concentration in drinking water for the cattle
- F_A ($\text{m}^3 \text{d}^{-1}$) is the respiration rate of cattle



The loss rate constant is the sum of losses by outflux, degradation and growth.

$$(28) \quad k = \frac{F}{M_C K_{CF}} + k_{deg} (+k_G)$$

Where:

- F (kg d^{-1}) is the outflux of water, lipids and air from the cattle. For milk cattle lactation is added to the outflux.
- K_{CF} (kg kg^{-1}) is the partition coefficient between cattle body and outflux
- M_C (kg) is the bodyweight of cattle
- k_{deg} (d^{-1}) is the degradation rate in cattle
- k_G (d^{-1}) is the growth rate of cattle (only for beef cattle)

The outflux of water, lipids and air is the sum of drinking rate, lipid excretion rate and respiration rate of the cattle (Eq. 29). For milk cattle, the lactation rate is added to the outflux as a sum of lipids and water in milk (Eq. 30).

$$(29) \quad F = F_W \rho_W + F_L + F_A \rho_A 1000 \text{L m}^3$$

$$(30) \quad F = F_W \rho_W + F_L + F_A \rho_A 1000 \text{L m}^3 + W_M \rho_W F_M + L_M F_M$$

where:

- F_L (kg d^{-1}) is the lipid excretion rate, which is taken as 10% of the lipid content in the grass consumed by the cattle
- ρ_A (kg m^{-3}) is the density of air
- W_M (L kg^{-1}) is the water content of milk
- F_M (kg d^{-1}) is the lactation rate
- L_M (kg d^{-1}) is the lipid content of milk

The partition coefficient between cattle and outflux is determined from the partition coefficients between cattle body and aqueous phase of cattle, K_{CW} , and, outflux and aqueous phase of cattle, K_{FW} .

$$(31) \quad K_{CF} = \frac{K_{CW}}{K_{FW}}$$

where:



- K_{CW} ($L\ kg^{-1}$) is the partition coefficient between cattle body and aqueous phase of cattle
- K_{FW} ($L\ kg^{-1}$) is the partition coefficient between outflux and aqueous phase of cattle

The partition coefficient between cattle body and aqueous phase of cattle is in analogy with Equation 2 determined from the lipid and water content of the cattle body.

$$(32) \quad K_{CW} = W_C + \frac{L_C}{\rho_L} K_{OW}$$

where:

- W_C ($L\ kg^{-1}$) is the water content of the beef cattle body
- L_C ($kg\ kg^{-1}$) is the lipid content of the beef cattle body
- ρ_L ($kg\ L^{-1}$) is the density of cattle lipids

The partition coefficient between outflux and aqueous phase of cattle is calculated from the outflux fractions of water, lipids and air.

$$(33) \quad K_{FW} = f_W + f_L K_{OW} + f_A K_{AW}$$

where:

- f_W ($L\ kg^{-1}$) is the outflux fraction of water
- f_L ($L\ kg^{-1}$) is the outflux fraction of lipid
- f_A ($L\ kg^{-1}$) is the outflux fraction of air

Outflux fractions of water, lipid and air are determined from drinking rate, lipid excretion rate, respiration rate and total outflux (Eq. 34). For milk cattle the lactation rate is also included in the calculation (Eq. 35)

$$(34) \quad f_W = \frac{F_W}{F}, f_L = \frac{F_L/\rho_L}{F}, f_A = \frac{F_A 1000Lm^3}{F}$$

$$(35) \quad f_W = \frac{F_W + W_M F_M}{F}, f_L = \frac{F_L + L_M F_M}{F \rho_L}, f_A = \frac{F_A 1000Lm^3}{F}$$

The parameterisation of the cattle model and milk is given in Table 8.



Table 8. Parameters for cattle and milk (Czub and McLachlan 2004; Danish Cattle Federation 2008; McLachlan 1997; Trapp et al. 2008)

Parameter	Symbol	Value	Unit
Density of cattle lipids	ρ_L	0.8	kg L ⁻¹
Density of air	ρ_A	0.0013	kg L ⁻¹
Drinking rate	F_W	48	L d ⁻¹
Lipid excretion rate	F_L	0.13	kg d ⁻¹
Respiration rate	F_A	150	m ³ d ⁻¹
Grass consumption rate	F_{Grass}	65	kg fw d ⁻¹
Beef			
Bodyweight	M_C	690	kg
Water content	W_C	0.74	L kg ⁻¹
Lipid content	L_C	0.26	kg kg ⁻¹
Growth rate	k_G	0.006	d ⁻¹
Growth period	$t_{slaughter}$	852	d
Milk			
Bodyweight	M_C	460	kg
Water content of cattle	W_C	0.78	L kg ⁻¹
Lipid content of cattle	L_C	0.21	kg kg ⁻¹
Lactation rate	F_M	24.4	kg d ⁻¹
Water content of milk	W_M	0.87	L kg ⁻¹
Lipid content of milk	L_M	0.044	kg kg ⁻¹

[4.7 Milk](#)

The concentration of chemical in milk is found by assuming equilibrium partitioning between milk cattle and milk (Trapp et al. 2008).

$$(36) \quad C_M = K_{MC} C_C$$

where:

- C_M (mg kg⁻¹) is the concentration of chemical in milk
- K_{MC} (kg kg⁻¹) is the partition coefficient between milk and cattle body
- C_C (mg kg⁻¹) is the concentration in milk cattle found from Eq. 26 by division with bodyweight of milk cattle and with parameters for milk cattle

The partition coefficient between milk and cattle body is analogy with Eq. 31 calculated from the partition coefficients between milk and water, and cattle body and water.



$$(37) \quad K_{MC} = \frac{K_{MW}}{K_{CW}}$$

where:

- K_{MW} ($L \text{ kg}^{-1}$) is the partition coefficient between water and milk calculated from Eq. 32, but with parameters for milk instead of cattle
- K_{CW} ($L \text{ kg}^{-1}$) is the partition coefficient between cattle body and water calculated from Eq. 32 with parameters for milk cattle

The parameterisation of the milk compartment is given in Table 8.

The steady state concentrations of chemical in beef cattle and milk, predicted with the animal model are shown in Figure 23. It is seen that the concentration of chemical in beef cattle and milk increases with increasing lipophilicity of the chemical, whereas the concentration of chemical decreases with increasing volatility from water of the chemical. For hydrophilic chemicals the concentration in milk is an order of magnitude higher than the concentration in beef cattle, this is due to a smaller lipid content of milk than of beef cattle.

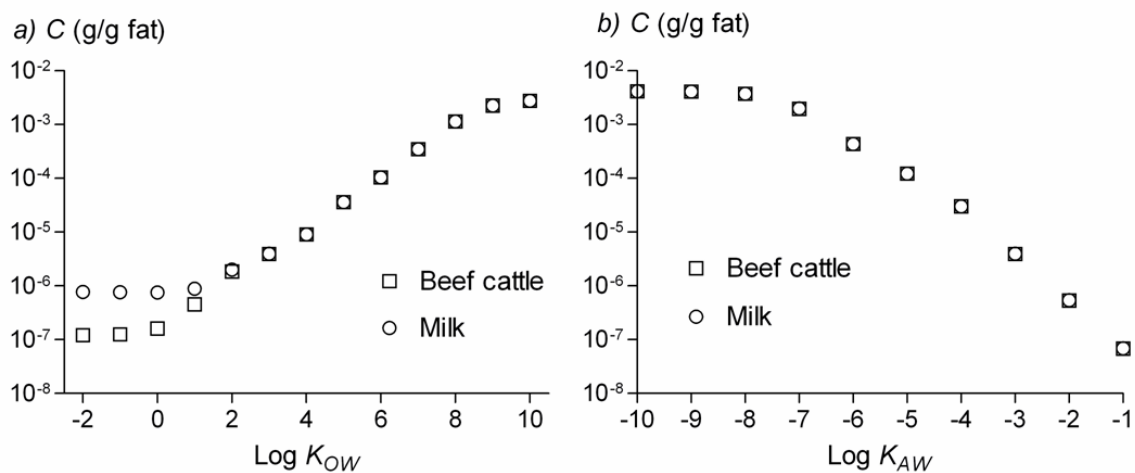


Figure 23. Concentration of chemical in beef cattle and milk as a function of lipophilicity and volatility from water, $C_{Soil} = 1 \text{ mg/kg ww}$, $C_{Air} = 0.001 \text{ mg/m}^3$, $C_{Water} = 1 \text{ mg/L}$. a) $K_{AW} = 0.001$, b) $K_{OW} = 1000$.

5. THE PLANT AND ANIMAL SYSTEM – DEFINITION OF THE MATHEMATICAL MODEL FOR INORGANIC CHEMICALS

This section describes the equations behind the interaction matrix for the 2-FUN plant system for inorganic chemicals (Figure 21). For these, the focus of 2-FUN is on uptake of As, Cd and Pb in plants and animals. Time-dependent concentrations of chemicals in each of the plant, animal and milk compartments are derived from the time-dependent concentrations of chemicals in air and soil.



5.1 Plants

The various crop types and the three selected chemicals require different approaches for the estimation of chemical concentration in plant tissue. One approach is a Freundlich type plant soil relation found from measured values of As, Cd and Pb in soil, carrots, potatoes and lettuce (Swartjes et al. 2007; Versluijs and Otte 2001).

$$(38) C_{Plant} = \frac{10^{(a + b \log (C_{S,t}) + c pH_S + d \log f_{OC} + e \log \%clay)} \rho_{P,dry} STcf_{BCF}}{\rho_{P,fresh}}$$

where:

- C_{Plant} (mg kg fw⁻¹) is the concentration of metal in the plant at harvest
- $C_{S,t}$ (mg kg dw⁻¹) is the (semi) total concentration of metal in soil (determined by acid digestion)
- a , b , c , d and e are empirical parameters given in Table 9 found from the RIVM plant – soil database
- $\rho_{S,wet}$ (kg ww L⁻¹) is the bulk soil density
- $\rho_{S,dry}$ (kg dw L⁻¹) is the dry soil density
- pH_S is the soil pore water pH
- $\%clay$ is the clay content of the soil (g dw g dw⁻¹)
- f_{OC} is the organic carbon content of the soil (g dw g dw⁻¹)
- $\rho_{P,dry}$ (kg dw L⁻¹) is the plant dry density
- $\rho_{P,fresh}$ (kg fw L⁻¹) is the plant fresh density
- $STcf_{BCF}$ is a soil type correction factor related to the average values of organic matter and clay content of the RIVM plant – soil database (Equation 39).

Table 9. Empirical parameters for the uptake of As, Cd and Pb in carrots, potatoes and lettuce (Swartjes et al. 2007; Versluijs and Otte 2001).

Plant	Metal	<i>a</i>	<i>b</i>	<i>c</i>	<i>d</i>	<i>e</i>
Carrot	As	-0.93	0.32	0.01	0.11	-0.11
	Cd	0.74	0.45	-0.16	0.20	0.09
	Pb	-0.64	0.56	-0.04	-0.16	-0.03
Potato	Cd	-0.86	0.36	0.06	-0.13	-0.27
	Pb	-2.0	0.67	0.12	-0.02	-0.50
Lettuce	Cd	1.0	0.28	-0.18	-0.19	0.16
	Pb	-0.60	0.90	-0.07	-0.34	-0.19



$$(39) \quad STcf_{BCF} = \frac{A + B\%clay + C\%OM}{A + B\%clay_{average} + C\%OM_{average}}$$

where:

- A , B and C are empirical parameters given in Table 10
- $\%OM$ is the organic matter content of soil
- $\%clay_{average}$ is the average clay content of the RIVM plant – soil database, 16%
- $\%OM_{average}$ is the average organic matter content of the RIVM plant – soil database, 7%

Table 10. Empirical parameters for the soil type correction (Swartjes et al. 2007).

Parameter	A	B	C
As	15	0.4	0.4
Cd	0.4	0.007	0.021
Pb	50	1	1

A second approach for estimating the concentration of these inorganic chemicals in plant tissue is presented in the CLEA model. This approach assumes that the concentration in the root is directly proportional to the concentration in the soil solution. Roots are in this context not edible roots. The concentration in edible plant parts, C_{Plant} (mg kg fw^{-1}), are found by multiplication with the fraction of metal in the roots that reaches the root store, potato, shoot or fruit by xylem or phloem flow (Jeffries and Martin 2008). (Equation not unit true)

$$(40) \quad C_{Plant} = C_{S,t} \frac{\delta f_{int}}{(\theta + \rho_{S,dry} K_d)}$$

where:

- δ is a correction factor for the soil to plant transport ($\delta = 5$ for Cd, Pb and As)
- f_{int} is the fraction of metal in roots reaching the internal plant system (Cd and As: $f_{int} = 0.5$, for Pb no correction factor for the internal distribution in plants is given. Thorne et al (2005) assumes that 20% of Pb is transported from root to shoots, so this is applied ($f_{int} = 0.2$))
- θ (L L^{-1}) is the water-filled soil porosity
- K_d (L kg dw^{-1}) is the soil water partition coefficient (described in the deliverable related to the soil system)

A third approach is presented in the Xtrafood model for estimation of Cd concentrations in grain. This approach is based on a study of Cd in the UK (Adams et al. 2004).

$$(41) \quad C_G = 10 \left(\frac{(0.12 + 0.43 \log(C_{S,t}) - 0.16 pH_S) \rho_{G,dry}}{\rho_{G,wet}} \right)$$



where:

- $\rho_{G,dry}$ (kg dw m⁻³) is the grain dry density

Table 11. Applicability of the three approaches for estimating As, Cd and Pb concentrations in plants from soil.

Plant	Cd	Pb	As
Root	RIVM	RIVM	(RIVM)
	CLEA	CLEA	CLEA
Potato	RIVM	RIVM	CLEA
	CLEA	CLEA	
Lettuce	RIVM	RIVM	CLEA
	CLEA	CLEA	
Grain	Xtrafood	-	-
Fruit	CLEA	CLEA	CLEA

An overview of the three presented approaches and where they apply are presented in Table 11. It is seen that none of the models have an approach for estimating the concentration of Pb and As in grain. So for 2-FUN we suggest a fourth approach similar to the model OURSON for estimating the concentration of metal in plant tissue. This is based on both transfers from air and soil to plant, whereas the first three approaches estimate transfer from soil only.

$$(42) \quad C_{Plant} = TF_A C_A + \frac{TF_S \rho_{P,dry}}{\rho_{P,fresh}} C_{S,t}$$

where:

- TF_A (m³ kg fw⁻¹) is a transfer factor from air to plant.
- TF_S (kg kg⁻¹ (dw)) is a transfer factor from soil to plant

The transfer factor from soil to plant is either found from databases or literature, or based on any of the three first approaches for estimating transfer of metal from soil to plant (Equations 38, 40 and 41).

For roots, tubers and grain there is only transfer from soil to plant and the steady state concentration in the plant at harvest is given by:

$$(43) \quad C_{Plant} = \frac{TF_S \rho_{P,dry}}{\rho_{P,fresh}} C_{S,t}$$

For the dynamic 2-FUN model version, it can be assumed that the transfer from soil to plant is constant with time and the following expression is valid:



$$(44) \quad \frac{dC_{P,S}}{dt} = \frac{TF_S \rho_{P,dry}}{t_{harvest} \rho_{P,fresh}} C_{S,t} \quad \text{for } t \leq t_{harvest}$$

where:

- $t_{harvest}$ (d) is the growth period of the plant

The parameterisation of the root, tuber and grain model for As, Cd and Pb is given in Tables 3, 4, 6 and 12.

Irrigation can be added to the grain model for metals:

$$(45) \quad \frac{dC_G}{dt} = \frac{TF_S \rho_{G,dry}}{t_{harvest} \rho_{G,fresh}} C_{S,t} + \frac{f_{wet} Irr S_{field}}{M_G} C_{River}$$

This is similar to the approach adopted for organic chemicals. However, the aerial biomass used for calculating the interception fractions (Eq. 20) is assumed to increase linearly with time:

$$(46) \quad \frac{dB_{Aerial}}{dt} = \frac{M_G}{t_{harvest}} \quad \text{for } t \leq t_{harvest}$$

Table 12. Chemical specific transfer factors from soil, TF_S , for the root, tuber (BAPPET 2008) and grain (Brus et al. 2005; Krauss et al. 2002; Lavado et al. 2007; Nan et al. 2002; Pruvot et al. 2006; Williams et al. 2007) model.

Parameter	Symbol	Median		Unit
Root				
Transfer factor (As)	$TF_R(As)$	0.006 (0.001; 0.051)	(5 th ; 95 th)	dw
Transfer factor (Cd)	$TF_R(Cd)$	0.302 (0.048; 2.41)	(5 th ; 95 th)	dw
Transfer factor (Pb)	$TF_R(Pb)$	0.011 (0.001; 0.21)	(5 th ; 95 th)	dw
Tuber				
Transfer factor (As)	$TF_T(As)$	0.002 (0.001; 0.027)	(5 th ; 95 th)	dw
Transfer factor (Cd)	$TF_T(Cd)$	0.085 (0.017; 0.495)	(5 th ; 95 th)	dw
Transfer factor (Pb)	$TF_T(Pb)$	0.002 (0.0005; 0.035)	(5 th ; 95 th)	dw
Grain				
Transfer factor (As)	$TF_G(As)$	0.003 (0; 0.024)	(min; max)	dw
Transfer factor (Cd)	$TF_G(Cd)$	0.151 (0.054; 0.594)	(5 th ; 95 th)	dw
Transfer factor (Pb)	$TF_G(Pb)$	0.0032 (0.0019; 0.0074)	(5 th ; 95 th)	dw



For leaf and fruit there is transfer from air to plant as well as from soil to plant and the steady state concentration in the plant at harvest can as a first estimate be found from:

$$(47) \quad C_P = \frac{TF_S C_{S,t} \rho_{P,dry}}{\rho_{P,fresh}} + \frac{A_P v_{dep}}{2 M_P (k_G + k_W)} C_A$$

where:

- k_W (d^{-1}) is the weathering rate ($0.05 d^{-1}$)

The transfer factor, TF_S , for leaf and fruit is calculated by subtracting an estimated average contribution from air (second part in Eq. 47) from the total concentration in the plant before division by the concentration in soil.

For the dynamic 2-FUN model version for leaves, contribution from air is split into irrigation, wet and dry particulate deposition like for the organic chemicals:

$$(48) \quad \frac{dC_L}{dt} = \frac{TF_S \rho_{L,dry}}{t_{harvest} \rho_{L,fresh}} C_{S,t} + \frac{(f_{wet} \Lambda_{part} Rain + f_{dry} v_{dep,dry}) S_{field}}{M_L} TSP_A C_{A,part} + \frac{f_{wet} Irr S_{field}}{M_L} C_{River} - k_W C_L$$

For the dynamic 2-FUN fruit model, the contribution from air is split into wet and dry particulate deposition:

$$(49) \quad \frac{dC_F}{dt} = \frac{TF_S \rho_{F,dry}}{t_{harvest} \rho_{F,fresh}} C_{S,t} + \frac{(f_{wet} \Lambda_{part} Rain + f_{dry} v_{dep,dry}) S_{field}}{M_F} TSP_A C_{A,part} - k_W C_L$$

The aerial biomass used for calculating the interception fractions (Eq. 20) is assumed to increase linearly with time for the metals (Eq. 46)

The parameterisation of the leaf and fruit model for As, Cd and Pb is given in Tables 5, 7 and 13.



Table 13. Metal specific transfer factors from soil, TF_s , for the leaf and fruit model (BAPPET 2008; U.S.EPA 1996).

Parameter	Symbol	Median		Unit
Leaf				
Transfer factor (As)	$TF_L(As)$	0.01 (0.002; 0.13)	(5 th ; 95 th)	dw
Transfer factor (Cd)	$TF_L(Cd)$	0.99 (0.001; 6.63)	(5 th ; 95 th)	dw
Transfer factor (Pb)	$TF_L(Pb)$	0.018 (0.001; 0.25)	(5 th ; 95 th)	dw
Fruit				
Transfer factor (As)	$TF_T(As)$	0.002 (0.002; 0.006)	(min; max)	dw
Transfer factor (Cd)	$TF_T(Cd)$	0.141 (0.019; 1.2)	(5 th ; 95 th)	dw
Transfer factor (Pb)	$TF_T(Pb)$	0.005 (0.001; 0.023)	(5 th ; 95 th)	dw

The steady state concentrations of As, Cd and Pb in crops (Eqs. 43 and 47) were estimated for Denmark. Input concentration were: $C_{S,t}$ (As): 2 mg kg dw⁻¹, $C_{S,t}$ (Cd): 0.33 mg kg dw⁻¹, $C_{S,t}$ (Pb): 20 mg kg dw⁻¹ (Samsøe-Petersen et al. 2002) and C_A (As): 0.4 ng m⁻³, C_A (Cd): 2.3 ng m⁻³, C_A (Pb): 4.3 ng m⁻³ (Kemp et al. 2008). These modelled levels were compared to measured values (Figure 24). The values were in close agreement, except for As in fruit and grain, where the model underestimated the transfer.

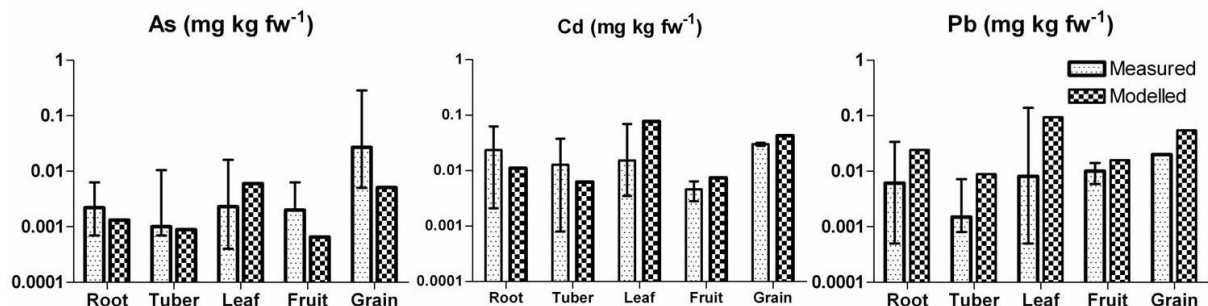


Figure 24. Modelled versus measured values for Denmark (Fromberg et al. 2005; Samsøe-Petersen et al. 2002; Wiersma et al. 1986). Measured values for grain are wheat (As) and wheat flour (Cd and Pb), for fruit (As) apple juice was measured.

5.2 Animals

For the animal part of the 2-FUN system we suggest to use a transfer factor relating the dose of chemical that the animal receives from grass, water and air to the concentration of chemical in meat (muscle) and milk:

$$(50) \quad C_M = TF_M (F_{Grass} C_{Grass} + F_W C_W + F_A C_A)$$

where:

- TF_M (d kg fw⁻¹) is the dose-related transfer factor to meat or milk



The parameterisation of the meat and milk metal model is given in Tables 8 and 14.

Table 14. Chemical specific transfer factors, TF_M , for the meat and milk model (Crout et al. 2004; Howard et al. 2009; Stevens 1991; Stevens 1992).

Parameter	Symbol	Average x 10^{-3}		Unit
Meat				
Transfer factor (As)	$TF_M(As)$	1.2 (0.3; 2.4)	(min; max)	d kg fw ⁻¹
Transfer factor (Cd)	$TF_M(Cd)$	2.0 (0; 60)	(min; max)	d kg fw ⁻¹
Transfer factor (Pb)	$TF_M(Pb)$	0.38 (0.02; 1.6)	(min; max)	d kg fw ⁻¹
Milk				
Transfer factor (As)	$TF_M(As)$	0.075 (0; 0.15)	(min; max)	d kg fw ⁻¹
Transfer factor (Cd)	$TF_M(Cd)$	0.064 (0; 8.4)	(min; max)	d kg fw ⁻¹
Transfer factor (Pb)	$TF_M(Pb)$	0.12 (0.007; 1.2)	(min; max)	d kg fw ⁻¹

The steady state concentrations of As, Cd and Pb in meat and milk (Eq. 47) were estimated for Denmark. The modelled concentrations of metals in leaves were used as an estimate for the concentration of chemicals in grass for cow consumption. The model results were compared to measured values (Figure 25). The values were in close agreement, except for As in meat and milk, where the model underestimated the transfer.

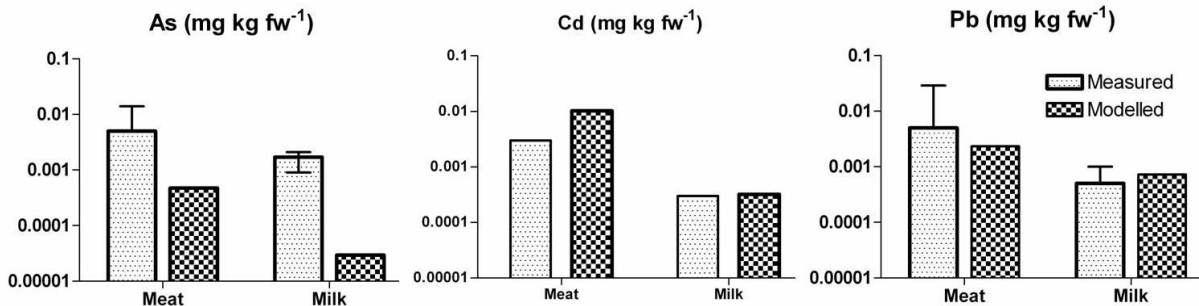


Figure 25. Modelled versus measured values for Denmark (Fromberg et al. 2005).



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